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EFFECT OF THE SPECIMEN SIZE ON NECKING DEVELOPMENT IN METALS AND ALLOYS DURING SUPERPLASTIC DEFORMATION

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Abstract. A model is proposed that describes the development of individual and multiple necks in superplastically deformed materials. Within the model, the examined samples have the form of round bars and are subjected to tensile superplastic deformation without strain hardening. It is demonstrated that neck development and necking-induced failure occur faster with a decrease in strain rate sensitivity and/or an increase in the fraction of the sample length occupied by necks. This means that high values of strain to failure observed in small specimens of superplastically deformed ultrafine-grained metals and alloys, where diffuse necking happens in the whole specimen, can be significantly reduced in larger specimens where the necking regions occupy only a small part of the sample.

Keywords: superplastic deformation, necking, ductility, failure, ultrafine-grained materials

1. Introduction

It is known that the ductility of metals and alloys under superplastic deformation is often limited by cavitation or diffuse necking (e.g., [1]). In particular, diffuse necking is often observed in ultrafine-grained (ufg) alloys demonstrating superplastic deformation or superplastic behavior (e.g., [2,3]). Due to the difficulty in making nanostructured materials large enough for standard mechanical testing, to measure the mechanical properties of such materials, many researchers have been using small samples [4]. In such samples the neck, if it appears, propagates over the entire sample length and represents a gradual decrease in the sample thickness from the sample edges to its center. This is in contrast to the case of large samples, where a neck during superplastic deformation can occupy only a part of the sample length, although multiple necking can occur [5-7].

At the same time, recent investigations [4,8,9] demonstrated that the sample length can have a significant effect on the ductility of metals. In particular, it was experimentally demonstrated that the gauge length can affect the onset of necking and postnecking behaviour of ufg and coarse-grained Cu [8,9]. The gauge length effect on the ductility of Cu has been attributed [4,9] to the difference in the fractions of the specimen length occupied by the neck in small and large samples. However, no relation has been established that would allow one to estimate the speed of the neck development and strain to failure in large samples based on the corresponding parameters in small samples and the strain rate sensitivity of specimens. To fill this gap, here we suggest a model that describes the development of individual and multiple necks in superplastically deformed materials and calculate the effect of the specimen length on the ductility of such materials.



Fig. 1. Deformed bar with multiple necks

2. Model

Consider a plastically deformed round bar under a uniaxial tension (Fig. 1). Assume that plastic deformation of the bar is accompanied by the formation of identical multiple necks that develop during plastic deformation. We denote the fraction of the specimen length occupied by necks as f_{neck} . In considering plastic deformation of the bar, we will use the long wavelength approximation [10-13]. This approximation assumes that the stress state and strain rate are the same at every cross section of the bar, and the stress state represents uniaxial tension σ . This approximation neglects the Bridgman effect [14] associated with the formation of hydrostatic tension, in addition to uniaxial tension, in the neck regions. However, the comparison of the long wavelength approximation with more refined models [10] demonstrated that in the case of high strain rate sensitivity (which is realized in the examined situation of superplastic deformation), the relatively simple long-wavelength approximation becomes very accurate. Therefore, we will use this approximation in further analysis.

3. Calculation of necking development during superplastic deformation

Within this approximation, we will expand the approach adopted by [10] for the analysis of a bar with a single neck to the examined case of multiple necks. To do so, we consider two cross sections, A and B, of the bar. The true stresses, σ_A and σ_B , in these cross sectional

areas, S_A and S_B , are related as

$$\sigma_A S_A = \sigma_B S_B = F \,, \tag{1}$$

where *F* is the magnitude of the tensile force acting on the bar (Fig. 1). We then consider one of the neck regions in the bar and suppose that there is an initial nonuniformity. Let us introduce the coordinate system (x, y) with the origin in the center of the neck region (Fig. 1) and denote the length of the neck as 2L (so that the neck occupies the region $-L \le x \le L$). Then the variation of the initial cross sectional area $S^i(x)$ in the neck region is assumed to be [10]

$$S^{i}(x) = S^{i}_{B}f(\tilde{x}), \qquad (2)$$

where S_B^i is the area of the cross section in the regions without necking, and $\tilde{x} = x/L$. Following [10], we take the initial imperfection of the cross sectional area in the form

$$f(\tilde{x}) = 1 - \eta \frac{1 + \cos(\pi \tilde{x})}{2},$$
(3)

where $\eta > 0$ is the imperfection amplitude. For simplicity, in considering superplastic deformation or superplastic behavior, we focus on the common situation where strain hardening is absent. In this case, the true strain σ does not depend on true strain ε but depends on strain rate $\dot{\varepsilon}$. We also employ the model strain-rate-dependent constitutive law (e.g., [10])

$$\sigma = \sigma_R (\dot{\varepsilon} / \dot{\varepsilon}_R)^m, \tag{4}$$

where σ_R and $\dot{\varepsilon}_R$ are the reference stress and strain rate, respectively. The true strain ε is related to the engineering strain ε_e as $\varepsilon_e = e^{\varepsilon} - 1$, which yields: $\dot{\varepsilon}_e = e^{\varepsilon} \dot{\varepsilon}$. From the condition of the volume conservation during plastic deformation, we have: $S(1 + \varepsilon_e) = S^i$, which can be rewritten as $S = S^i e^{-\varepsilon}$. Substitution of the latter relation to formulae (1)–(4) gives: $e^{-\varepsilon/m} \dot{\varepsilon} = f(\tilde{x})^{-1/m} e^{-\varepsilon_B/m} \dot{\varepsilon}_{-}$ (5)

$$\mathcal{E} = f(x) \quad e^{-x} \quad \mathcal{E}_B.$$
 (5)
From (5), we have:

$$\int_{0}^{\varepsilon} e^{-\varepsilon'/m} d\varepsilon' = f(\tilde{x})^{-1/m} \int_{0}^{\varepsilon_{B}} e^{-\varepsilon'_{B}/m} d\varepsilon'_{B}, \qquad (6)$$

which yields:

$$\varepsilon = -m\log[1 - f(\tilde{x})^{-1/m}(1 - e^{-\varepsilon_B/m})].$$
⁽⁷⁾

From (7) the stretch λ (defined as $\lambda = \varepsilon_e + 1 = e^{\varepsilon}$) can be related to the stretch λ_B at cross section B as

$$\lambda = [1 - f(\tilde{x})^{-1/m} (1 - \lambda_B^{-1/m})]^{-m}.$$
(8)

The average stretch of the bar λ_{av} (defined as the ratio of the lengths of the strained and unstrained bar) can be obtained from (8) as

$$\lambda_{av} = \lambda_B (1 - f_{neck}) + f_{neck} \int_0^1 [1 - f(\tilde{x})^{-1/m} (1 - \lambda_B^{-1/m})]^{-m} d\tilde{x}.$$
(9)

To analyze the development of necking with plastic deformation, we calculate the ratio Δ of the cross sectional area, S_A , at the center of the neck to the cross sectional area, S_B , of the regions without necking. The ratio Δ follows as

$$\Delta = \frac{S_A}{S_B} = \frac{\sigma_B}{\sigma_A} = \frac{\dot{\varepsilon}_B^m}{\dot{\varepsilon}_A^m}.$$
(10)

To relate the strain rates appearing on the right hand side of formula (10) to the stretch λ_{B} , using (7), we express the strain rate $\dot{\varepsilon}$ as

$$\dot{\varepsilon} = \frac{f(\tilde{x})^{-1/m} e^{-\varepsilon_B/m}}{1 - f(\tilde{x})^{-1/m} (1 - e^{-\varepsilon_B/m})} \dot{\varepsilon}_B \,. \tag{11}$$

Substituting (11) to (10) and using the relations $\lambda_B = e^{\varepsilon_B}$ and $\varepsilon_A = \varepsilon(\tilde{x} = 0)$, one obtains:

$$\Delta = [1 - (1 - \eta)^{-1/m} (1 - \lambda_B^{-1/m})]^m (1 - \eta) \lambda_B.$$
(12)

4. Results and discussion

Using formulae (9) and (12), we plot the dependencies of Δ on the average engineering strain $\varepsilon_e^{av} = \lambda_{av} - 1$. These dependencies are shown in Fig. 2, for $\eta = 0.01$ and various values of the parameters *m* and f_{neck} . Figure 2 demonstrates the known and intuitively evident fact that the development of necking (characterized by a decrease of Δ from 1 (when necking is absent) down to zero (when necking leads to failure) occurs faster for the materials with smaller values of strain rate sensitivity *m*.



Fig. 2. Dependencies of the ratio Δ of the cross sectional area at the neck center to that in the regions without necks on the engineering strain ε_e^{av} for a plastically deformed round bar, at various values of strain rate sensitivity m and two different values of the fraction f_{neck} of neck regions. The solid lines correspond to the case $f_{neck} = 0.2$ while the dashed lines depict the situation where $f_{neck} = 1$

Also, in the initial stage of necking development (characterized by $\Delta > 0.9$), for a specified engineering strain ε_e^{av} , the parameter Δ is nearly independent of f_{neck} . At the same time, when necking becomes pronounced (that is, Δ becomes sufficiently small), the development of necking occurs at smaller strains for a smaller value of the fraction f_{neck} of necking regions. This effect becomes especially pronounced for high values of strain rate sensitivity m. If we assume that in small specimens there is only one neck, which occupies the whole length of the bar (that is, $f_{neck} = 1$), while in larger ones necks occupy only a small part of the bar, we can conclude from the above than in large specimens necking develops faster (that is, at smaller average strain) than in small ones.



Fig. 3. Dependencies of the engineering strain to failure ε_c for a plastically deformed round bar on the fraction of neck regions f_{neck} , for various values of strain rate sensitivity m

Now calculate the engineering strain to failure for the plastically deformed bar that fails by necking. The critical value λ_c of the average stretch λ_{av} at which necking leads to failure is obtained from the relation $\Delta = 0$ and formula (12) as [10] $\lambda_c = [1 - (1 - \eta)^{1/m}]^{-m}$, (13)

and the corresponding critical value ε_c of the average engineering strain ε_e^{av} (that is, strain to failure) is given by $\varepsilon_c = \lambda_c - 1$. The dependencies of the engineering strain to failure ε_c on the fraction of neck regions f_{neck} are plotted in Fig. 3, for $\eta = 0.01$ and various values of

strain rate sensitivity *m*. Figure 3 clearly demonstrates that the strain to failure ε_c strongly increases with an increase in the fraction f_{neck} of necking regions, and this effect becomes especially strong for large values of strain rate sensitivity typical of superplastic deformation. This implies that very high strain to failure observed (e.g., [2,3,15-17]) in short ufg specimens with high strain rate sensitivity (characterized by $f_{neck} = 1$) may not be observed in similar long specimens where the value of f_{neck} can be small.

5. Conclusions

Thus, in this paper, we have suggested a model describing the development of individual and multiple necks in superplastically deformed materials. In the framework of the model, we have considered a round bar under tension, which is superplastically deformed without strain hardening. Within the long wavelength approximation, we have calculated the normalized cross sectional area in the center of neck regions and strain to failure as functions of strain rate sensitivity and volume fraction occupied by necks. We have demonstrated that neck development and necking-induced failure speed up with a decrease in strain rate sensitivity and/or an increase in the volume fraction occupied by necks. The latter effect (faster neck development and a decrease in the strain to failure with an increase of the fraction of sample length occupied by necks) is especially pronounced in the case of a high strain rate sensitivity. This implies that record values of strain to failure observed (e.g., [2,3,15-17]) in ufg metals and alloys in the form of bars with a small length (where the neck occupies the entire specimen) can be significantly reduced in large enough specimens where the necking regions occupy only a small part of the sample.

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THERMOMECHANICAL INTERACTIONS DUE TO TIME HARMONIC SOURCES IN A TRANSVERSELY ISOTROPIC MAGNETO THERMOELASTIC ROTATING SOLIDS IN LORD-SHULMAN MODEL

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Abstract. The present research deals with the mathematical modelling of two dimensional transversely isotropic magneto thermoelastic initially stressed solid due to time-harmonic source with generalized Lord-Shulman (LS) theory of thermoelasticity. The Fourier transform has been used to find the solution to the problem. The expressions for the displacement components, stress components, and temperature distribution are obtained in the transformed domain. The effect of time-harmonic source is depicted graphically on the resulting quantities.

Keywords: transversely isotropic Magneto thermoelastic, mechanical and thermal stresses, time-harmonic source

Nomenclature

- δ_{ii} Kronecker delta,
- D_{ijkl} Elastic parameters,
- β_{ij} Thermal elastic coupling tensor,
- *T* Absolute temperature,
- T_0 Reference temperature,
- φ conductive temperature,
- t_{ii} Stress tensors,
- e_{ii} Strain tensors,
- P_{mi} Pre stress tensor,
- u_i Components of displacement,
- ρ Medium density,
- C_E Specific heat,
- α_{ij} Linear thermal expansion coefficient,

- K_{ij} Thermal conductivity,
- ω Frequency,
- τ_0 Relaxation Time,
- $\boldsymbol{\Omega}$ Angular Velocity of the Solid,
- F_i Components of Lorentz force,
- *H*₀ Magnetic field intensity vector,
- J Current Density Vector,
- **u** Displacement Vector,
- μ_0 Magnetic permeability,
- ε_0 Electric permeability,
- $\delta(t)$ Dirac's delta function,
- **h** induced magnetic field vector,
- *E* induced electric field vector,

1. Introduction

A lot of research and attention has been given to deformation and heat flow in a continuum using thermoelasticity theories during the past few years. When sudden heat/external force is applied in a solid body, it transmits time-harmonic wave by thermal expansion. The change at some point in the medium is beneficial to detect the deformed field near mining shocks, seismic and volcanic sources, thermal power plants, high-energy particle accelerators, and many emerging technologies. The study of the time-harmonic source is one of the broad and dynamic areas of continuum dynamics. Therefore, an unbounded rotating elastic medium with angular velocity, with rotation and relaxation time, and without energy dissipation in generalized thermoelasticity has been studied in this research.

Marin [1] had proved the Cesaro means of strain and kinetic energies of dipolar bodies with finite energy. Marin [2] investigated and solved the initial-boundary value problem without recourse either to an energy conservation law or to any boundedness assumptions on the thermoelastic coefficients in thermoelastic bodies with voids. Ailawalia et al. [3] had studied a rotating generalized thermoelastic medium in the presence of two temperatures beneath hydrostatic stress and gravity with different kinds of sources using integral Yadav solved transversely isotropic rotating transforms. Singh and [4] the magnetothermoelastic medium equations by cubic velocity equation of three plane waves without anisotropy, rotation, and thermal and magnetic effects. Banik and Kanoria (2012) studied the thermoelastic interaction in an isotropic infinite elastic body with a spherical cavity for the TPL(Three-Phase-Lag) heat equation with two-temperature generalized thermoelasticity theory and has shown variations between two models: the two-temperature GN theory in presence of energy dissipation and two-temperature TPL model and has shown the effects of ramping parameters and two-temperature.

Mahmoud [5] had considered the impact of rotation, relaxation times, magnetic field, gravity field, and initial stress on Rayleigh waves and attenuation coefficient in an elastic half-space of granular medium and obtained the analytical solution of Rayleigh waves velocity by using Lame's potential techniques. Abd-alla and Alshaikh [6] had discussed the influence of magnetic field and rotation on plane waves in transversely isotropic thermoelastic medium under the GL theory in presence of two relaxation times to show the presence of three quasi plane waves in the medium. Marin et al. [7] has modelled a micro stretch thermoelastic body with two temperatures and eliminated divergences among the classical elasticity and research.

Sharma et al. [8] investigated the 2-D deception in transversely isotropic homogeneous thermoelastic solids in presence of two temperatures in GN-II theory with an inclined load (linear combination of normal load and tangential load). Kumar et al. [9] investigated the impact of Hall current in a transversely isotropic magnetothermoelastic in the presence and absence of energy dissipation due to the normal force. Kumar et al. [10] studied the conflicts caused by thermomechanical sources in a transversely isotropic rotating homogeneous thermoelastic medium with a magnetic effect as well as two temperatures and applied to the thermoelasticity Green–Naghdi theories with and without energy dissipation using thermomechanical sources. Lata et al. [11] studied two temperature and rotation aspect for GN-II and GN-III theory of thermoelasticity in a homogeneous transversely isotropic magnetothermoelastic medium for the case of the plane wave propagation and reflection. Ezzat et al. [12] proposed a mathematical model of electro-thermoelasticity for heat conduction with memory-dependent derivative. Kumar et al. [13] analyzed the Rayleigh waves in a transversely isotropic homogeneous magnetothermoelastic medium in presence of two temperatures, with Hall current and rotation.

Marin et.al. [14] studied the GN-thermoelastic theory for a dipolar body using mixed initial BVP and proved a result of Hölder's-type stability. Lata [15] studied the impact of

energy dissipation on plane waves in sandwiched layered thermoelastic medium of uniform thickness, with two temperatures, rotation, and Hall current in the context of GN Type-II and Type-III theory of thermoelasticity. Ezzat and El-Bary [16] had applied the magnetothermoelasticity model to a one-dimensional thermal shock problem of functionally graded half-space based on memory-dependent derivative. Kumar et al. [17] investigated the deformations in a homogeneous transversely isotropic magneto-Visco thermoelastic medium under GN type I and II theories in presence of rotation and two temperatures with thermomechanical sources. Despite this several researchers working on a different theory of thermoelasticity as Marin [18], Marin [19], Atwa [20], Marin [21], Marin and Baleanu [22], Bijarnia and Singh [23], Ezzat et al. [24], Ezzat et al. [25], Ezzat et al. [26], Ezzat and El-Bary [27], Ezzat and El-Bary [28], Ezzat et al. [29], Chauthale et al. [30] and Shahani and Torki [31].

In spite of these, not much work has been carried out in thermomechanical interactions in transversely isotropic magneto thermoelastic solid with rotation and relaxation time and without energy dissipation due to time-harmonic source in generalized LS theories of thermoelasticity. Keeping these considerations in mind, analytic expressions for the displacement components, stress components, and temperature distribution in twodimensional homogeneous, transversely isotropic magneto-thermoelastic solids without energy dissipation, with rotation and various frequencies of the time-harmonic source.

2. Basic equations

Following Zakaria [32], the simplified Maxwell's linear equation of electrodynamics for a slowly moving and conducting elastic solid are

$$curl \, \boldsymbol{h} = \boldsymbol{J} + \varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t},\tag{1}$$

$$curl \mathbf{E} = -\mu_0 \frac{\partial \mathbf{h}}{\partial t},\tag{2}$$

$$E = -\mu_0 \left(\frac{\partial u}{\partial t} + H_0 \right), \tag{3}$$

div $h = 0.$

Maxwell stress components are given by

$$T_{ij} = \mu_0 (H_i h_j + H_j h_i - H_k h_k \delta_{ij}).$$
(5)
For an anisotropic prostressed thermoelestic medium the constitutive equation is

For an anisotropic pre-stressed thermoelastic medium, the constitutive equation is given by

$$t_{ij} = D_{ijkl}e_{kl} + e_{jm}P_{mi} - \beta_{ij}T,$$
(6)

and the equation of motion for a uniformly rotating pre-stressed medium in the rotating frame of reference with angular velocity $\mathbf{\Omega}$ in the presence of external force is given by

$$t_{ij,j} + F_i = \rho\{ \ddot{\boldsymbol{u}}_i + (\boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \mathbf{u}))_i + (2\boldsymbol{\Omega} \times \dot{\boldsymbol{u}})_i \},$$
(7)

where $\Omega = \Omega n$, *n* is a unit vector representing the direction of the axis of rotation. The term $\Omega \times (\Omega \times \mathbf{u})$ is the additional centripetal acceleration due to the time-varying motion only, and the term $2\Omega \times \dot{u}$ is the Coriolis acceleration which occurs for a moving frame of reference only. The total stress in the half-space is composed of Hooke's mechanical stress and Maxwell's stress. The Lorentz force F_i is (8)

$$F_i = \mu_0 (\boldsymbol{J} \times \boldsymbol{H}_0) \ .$$

The Lord-Shulman model of heat conduction equation in the presence of an external source of heat Q is given by

$$K_{ij}T_{,ij} + \rho(Q + \tau_0 \dot{Q}) = \beta_{ij}T_0(\dot{e}_{ij} + \tau_0 \ddot{e}_{ij}) + \rho C_E(\dot{T} + \tau_0 \ddot{T}),$$
(9)
where

$$\beta_{ij} = \mathcal{C}_{ijkl} \alpha_{ij},\tag{10}$$

$$e_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \quad i, j = 1, 2, 3,$$
(11)

 $\beta_{ij} = \beta_i \delta_{ij}, K_{ij} = K_i \delta_{ij}, C_{ijkl} = D_{ijkl} + \delta_{jl} P_{ki}, i \text{ is not summed.}$ Here $D_{ijkl}(D_{ijkl} = D_{klij} = D_{jikl} = D_{ijlk})$ are elastic parameters.

3. Formulation and solution of the problem

We consider a pre-stressed 2-D homogeneous transversely isotropic magneto thermoelastic medium, permeated by an initial magnetic field $H_0 = (0, H_0, 0)$ acting along y-axis. This initial magnetic field produces an induced magnetic field h = (0, h, 0) and induced electric field $E = (E_1, 0, E_3)$. The rectangular Cartesian co-ordinate system (x, y, z) having origin on the surface (z = 0) with z-axis pointing vertically into the medium is introduced. The surface of the half-space is subjected to a thermomechanical force acting at z = 0. In addition, we consider that

$$\mathbf{\Omega} = (0, \Omega, 0). \tag{12}$$

Following Lata et al. [10] from the generalized Ohm's law we have $J_2 = 0$. (13)

And the density components J_1 and J_3 are given as

$$J_{1} = -\varepsilon_{0}\mu_{0}H_{0}\frac{\partial^{2}w}{\partial t^{2}},$$

$$J_{3} = \varepsilon_{0}\mu_{0}H_{0}\frac{\partial^{2}u}{\partial t^{2}}.$$
(14)
(15)

In addition, the equations of displacement vector $\mathbf{u} = (u, v, w)$ and temperature change T for 2-dimensional motion of transversely isotropic thermoelastic solid are: u = u(x z t) v = 0 w = w(x z t) and T = T(x z t)(16)

$$C_{11}\frac{\partial^2 u}{\partial x^2} + C_{13}\frac{\partial^2 w}{\partial x \partial z} + C_{44}\left(\frac{\partial^2 u}{\partial z^2} + \frac{\partial^2 w}{\partial x \partial z}\right) - \beta_1 \frac{\partial T}{\partial x} - \mu_0 J_3 H_0 = \rho \left(\frac{\partial^2 u}{\partial t^2} - \Omega^2 u + 2\Omega \frac{\partial w}{\partial t}\right), \quad (17)$$

$$(C_{13} + C_{44})\frac{\partial^2 u}{\partial x \partial z} + C_{44}\frac{\partial^2 w}{\partial x^2} + C_{33}\frac{\partial^2 w}{\partial z^2} - \beta_3\frac{\partial T}{\partial z} - \mu_0 J_1 H_0 = \rho \left(\frac{\partial^2 w}{\partial t^2} - \Omega^2 w - 2\Omega\frac{\partial u}{\partial t}\right), \quad (18)$$

$$K_{1}\frac{\partial^{2}T}{\partial x^{2}} + K_{3}\frac{\partial^{2}T}{\partial z^{2}} + \rho(Q + \tau_{0}\dot{Q}) = \rho C_{E}(\dot{T} + \tau_{0}\ddot{T}) + T_{0}\frac{\partial}{\partial t}\left\{\beta_{1}\left(1 + \tau_{0}\frac{\partial}{\partial t}\right)\frac{\partial u}{\partial x} + \beta_{3}\left(1 + \tau_{0}\frac{\partial}{\partial t}\right)\frac{\partial w}{\partial z}\right\},$$
(19)
and

$$t_{11} = C_{11}e_{11} + C_{13}e_{13} - \beta_1 T,$$
(20)

$$t_{20} = C_{10}\rho_{11} + C_{13}\rho_{13} - \beta_{2}T$$
(21)

$$\begin{aligned} & (21) \\ & (1) \\ &$$

where
$$C_{11} = D_{11} + P_{11}$$
, $C_{13} = D_{13}$, $C_{33} = D_{33} + P_{33}$, $C_{44} = D_{44} + P_{11}$.
 $\beta_1 = (C_{11} + C_{12})\alpha_1 + C_{13}\alpha_3$,
 $\beta_3 = 2C_{13}\alpha_1 + C_{33}\alpha_3$,
where $\alpha_1 = \alpha_2$ is the set there a base of C_{12} is the set of C_{13} is the set

where α_1 , α_3 are linear thermal expansion coefficients.

We consider that the medium is initially at rest. Therefore, the preliminary and symmetry conditions are given by

 $u(x, z, 0) = 0 = \dot{u}(x, z, 0),$

 $w(x, z, 0) = 0 = \dot{w}(x, z, 0),$

 $T(x, z, 0) = 0 = \dot{T}(x, z, 0)$ for $z \ge 0, -\infty < x < \infty$,

u(x, z, t) = w(x, z, t) = T(x, z, t) = 0 for t > 0 when $z \to \infty$.

Assuming the time-harmonic behaviour as

$$(u, w, T, Q)(x, z, t) = (u, w, T, Q)(x, z)e^{i\omega t},$$
where ω is the angular frequency.
(23)

To simplify the solution, mention below dimensionless quantities are used:

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$$x' = \frac{x}{L}, \quad u' = \frac{\rho c_1^2}{L\beta_1 T_0} u, \quad t' = \frac{c_1}{L} t, \quad w' = \frac{\rho c_1^2}{L\beta_1 T_0} w, \quad T' = \frac{T}{T_0}, \quad t'_{11} = \frac{t_{11}}{\beta_1 T_0}, \quad t'_{33} = \frac{t_{33}}{\beta_1 T_2}, \quad t'_{31} = \frac{t_{31}}{\beta_1 T_2}, \quad z' = \frac{z}{L}, \quad h' = \frac{h}{H_2}, \quad \Omega' = \frac{L}{C} \Omega.$$
(24)

 $\beta_1 T_0, \beta_1 T_0, L, H_0, C_1$ Making use of (23) and then using dimensionless variables of eq. (24) in Eqs. (17)-(19), after suppressing the primes, yield

$$\frac{\partial^2 u}{\partial x^2} + \delta_4 \frac{\partial^2 w}{\partial x \partial z} + \delta_2 \left(\frac{\partial^2 u}{\partial z^2} + \frac{\partial^2 w}{\partial x \partial z} \right) - \frac{\partial T}{\partial x} = \left(\frac{\varepsilon_0 \mu_0^2 H_0^2}{\rho} + 1 \right) (-\omega^2 u) - \Omega^2 u + 2\Omega i \omega w, \tag{25}$$

$$\delta_1 \frac{\partial^2 u}{\partial x \partial z} + \delta_2 \frac{\partial^2 w}{\partial x^2} + \delta_3 \frac{\partial^2 w}{\partial z^2} - \frac{\beta_3}{\beta_1} \frac{\partial T}{\partial z} = \left(\frac{\varepsilon_0 \mu_0^2 H_0^2}{\rho} + 1\right) (-\omega^2 w) - \Omega^2 w + 2\Omega i \omega u, \tag{26}$$

$$\frac{\partial^2 T}{\partial x^2} + \frac{K_3}{K_1} \frac{\partial^2 T}{\partial z^2} + \rho \left(1 + \tau_0 \frac{c_1}{L} i\omega \right) Q = \delta_5 \frac{\partial}{\partial t} \left(1 + \tau_0 \frac{c_1}{L} i\omega \right) T + \\ + \delta_6 i\omega \left(1 + \tau_0 \frac{c_1}{L} i\omega \right) \left[\beta_1 \frac{\partial u}{\partial x} + \beta_3 \frac{\partial w}{\partial z} \right],$$
(27)

where $\delta_1 = \frac{c_{13} + c_{44}}{c_{11}}$, $\delta_2 = \frac{c_{44}}{c_{11}}$, $\delta_3 = \frac{c_{33}}{c_{11}}$, $\delta_4 = \frac{c_{13}}{c_{11}}$, $\delta_5 = \frac{\rho c_E c_1 L}{K_1}$, $\delta_6 = -\frac{T_0 \beta_1 L}{\rho c_1 K_1}$. Apply Fourier transforms defined by

$$\hat{f}(\xi, z, \omega) = \int_{-\infty}^{\infty} f(x, z, \omega) e^{i\xi x} dx.$$
(28)

On Eqs. (25)–(27), we obtain a system of equations

$$\begin{bmatrix} -\xi^2 + \delta_2 D^2 + \delta_7 \omega^2 + \Omega^2] \hat{u}(\xi, z, \omega) + [\delta_4 Di\xi + \delta_2 Di\xi - 2\Omega i \omega] \hat{w}(\xi, z, \omega) + \\ + (-i\xi) \hat{T}(\xi, z, \omega) = 0, \qquad (29)$$

$$\begin{bmatrix} \delta_1 Di\xi + 2\Omega i\omega]\hat{u}(\xi, z, \omega) + [-\delta_2 \xi^2 + \delta_3 D^2 + \delta_7 \omega^2 + \Omega^2] \hat{w}(\xi, z, \omega) - \\ -\frac{\beta_3}{\beta_1} D\hat{T}(\xi, z, \omega) = 0,$$
(30)

$$\begin{bmatrix} -\delta_6 \omega \delta_8 \beta_1 \xi] \hat{u}(\xi, z, \omega) + [\delta_6 i \omega \delta_8 \beta_3 D] \hat{w}(\xi, z, \omega) + \\ + \left[\xi^2 - \frac{\kappa_3}{\kappa_1} D^2 + \delta_5 \delta_8 i \omega \right] \hat{T}(\xi, z, \omega) = \rho \delta_8 \hat{Q}(\xi, z, \omega),$$
(31)

where $\delta_7 = \frac{\varepsilon_0 \mu_0^2 H_0^2}{\rho} + 1$, $\delta_8 = 1 + \tau_0 \frac{C_1}{L} i\omega$.

Here we are considering that there is no external supply of heat source i.e. by taking $\hat{Q}(\xi, z, s) = 0$, the non-trivial solution exists if the determinant of the coefficient matrix of $[\hat{u}, \hat{w}, \hat{T}]$ of (29)-(31) vanishes and the characteristic equation is $(AD^{6} + BD^{4} + CD^{2} + E)(\hat{u}, \hat{w}, \hat{T}) = 0,$ (32) where

$$\begin{split} \mathbf{A} &= \delta_2 \delta_3 \vartheta_7 - \vartheta_5 \delta_2 \frac{\beta_3}{\beta_1}, \\ \mathbf{B} &= \delta_3 \vartheta_1 \vartheta_7 + \delta_2 \delta_3 \vartheta_6 + \delta_2 \vartheta_7 \vartheta_3 - \vartheta_5 \vartheta_9 \delta_2 - \vartheta_8 \delta_1 i \xi \vartheta_7, \\ \mathbf{C} &= \delta_3 \vartheta_1 \vartheta_6 + \vartheta_1 \vartheta_3 \vartheta_7 - \vartheta_1 \vartheta_5 \vartheta_9 + \delta_2 \vartheta_6 \vartheta_3 + \vartheta_4 \vartheta_8 \vartheta_9 - \vartheta_8 \delta_1 i \xi \vartheta_6 - 4\Omega^2 \omega^2 \vartheta_7 + \vartheta_2 \delta_1 i \xi \vartheta_5 - \vartheta_2 \vartheta_4 \delta_3, \\ \mathbf{E} &= \vartheta_3 \vartheta_1 \vartheta_6 - 4\Omega^2 \omega^2 \vartheta_6 - \vartheta_2 \vartheta_4 \vartheta_3, \\ \vartheta_1 &= -\xi^2 + \delta_7 \omega^2 + \Omega^2, \\ \vartheta_2 &= -i\xi, \\ \vartheta_3 &= -\delta_2 \xi^2 + \delta_7 \omega^2 + \Omega^2, \\ \vartheta_4 &= -\delta_6 \delta_8 \omega \beta_1 \xi, \end{split}$$

$$\vartheta_{5} = \delta_{6} \delta_{8} i \omega \beta_{3},$$

$$\vartheta_{6} = \xi^{2} + \delta_{5} \delta_{8} i \omega,$$

$$\vartheta_{7} = -\frac{\kappa_{3}}{\kappa_{1}},$$

$$\vartheta_{8} = \delta_{1} i \xi,$$

$$\vartheta_{9} = -\frac{\beta_{3}}{\beta_{1}}.$$

The roots of the Eq. (32) are $\pm \lambda_{i}$, $(i = 1, 2, 3)$, are obtained by using the radiation

condition $\tilde{u}, \tilde{w}, \tilde{T} \to 0$ as $z \to \infty$ and can be written as

$$\hat{u}(\xi, z, \omega) = \sum_{j=1}^{3} A_j e^{-\lambda_j z},\tag{33}$$

$$\widehat{w}(\xi, z, \omega) = \sum_{j=1}^{3} d_j A_j e^{-\lambda_j z},$$

$$\widehat{T}(\xi, z, \omega) = \sum_{j=1}^{3} l_j A_j e^{-\lambda_j z},$$
(34)
(35)

where $A_i(\xi, \omega), j = 1, 2, 3$ being undetermined constants and d_j and l_j are given by

$$d_{j} = \frac{\delta_{2}\zeta_{7}\lambda_{j}^{4} + (\vartheta_{7}\vartheta_{1} + \delta_{2}\vartheta_{6})\lambda_{j}^{2} + \vartheta_{1}\vartheta_{6} - \vartheta_{4}\vartheta_{2}}{(\delta_{3}\vartheta_{7})\lambda_{j}^{4} + (\delta_{3}\vartheta_{6} + \vartheta_{3}\vartheta_{7} - \vartheta_{5}\vartheta_{9})\lambda_{j}^{2} + \vartheta_{3}\vartheta_{6}},$$

$$l_{j} = \frac{\delta_{2}\delta_{3}\lambda_{j}^{4} + (\delta_{2}\zeta_{3} + \vartheta_{1}\delta_{3} - \delta_{1}\vartheta_{8}i\xi)\lambda_{j}^{2} - 4\Omega^{2}\omega^{2} + \vartheta_{3}\vartheta_{1}}{(\delta_{3}\vartheta_{7})\lambda_{j}^{4} + (\delta_{3}\vartheta_{6} + \vartheta_{3}\vartheta_{7} - \vartheta_{5}\vartheta_{9})\lambda_{j}^{2} + \vartheta_{3}\vartheta_{6}}.$$

4. Boundary conditions

Impulsive line tractions on the surface (z = 0). We consider that the mechanical force is applied on the surface (z = 0) i.e.

$$t_{33} = -F_1 \psi_1(x) e^{i\omega t},$$

$$t_{31} = -F_2 \psi_2(x) e^{i\omega t},$$

$$\frac{\partial T}{\partial z} + hT = 0,$$
(36)
(37)
(38)

where F_1 , F_2 is the magnitude of the force applied on the boundary, $\psi_1(x)$ and $\psi_2(x)$ specify the vertical and horizontal traction distribution functions respectively along the x-axis, h is heat transfer coefficient and $h \rightarrow 0$ equation (38) corresponds to the insulated boundary and $h \rightarrow \infty$, equation (38) corresponds to the isothermal boundary.

Applying the Fourier transform defined by (28) on the boundary conditions (36)-(38), and using the value of t_{33} and t_{31} from equations (21)-(22) and using values of \hat{u} , \hat{w} and \hat{T} from equations (33)-(35) in the transformed equations (36)-(38), we find the solution of the problem by using Cramer's rule to obtain the values of A_j and again using these values of $A_{j,j}$ =1,2,3 in equations (33)-(35) and equations (21)-(22) we obtain the components of displacement, temperature, and stress, in the transformed domain as

$$\hat{u} = \frac{F_1 \hat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 \Gamma_{1j} e^{-\lambda_j z} \right] e^{i\omega t} + \frac{F_2 \hat{\psi}_2(\xi)}{\Gamma} \left[\sum_{j=1}^3 \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t}, \tag{39}$$

$$\widehat{w} = \frac{F_1 \widehat{\psi}_1(\xi)}{\Gamma} \left| \sum_{j=1}^3 d_j \Gamma_{1j} e^{-\lambda_j z} \right| e^{i\omega t} + \frac{F_2 \widehat{\psi}_2(\xi)}{\Gamma} \left| \sum_{j=1}^3 d_j \Gamma_{2j} e^{-\lambda_j z} \right| e^{i\omega t}, \tag{40}$$

$$\hat{T} = \frac{F_1 \hat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 l_j \Gamma_{1j} e^{-\lambda_j z} \right] e^{i\omega t} + \frac{F_2 \hat{\psi}_2(\xi)}{\Gamma} \left[\sum_{j=1}^3 l_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t},$$
(41)

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$$\widehat{t_{11}} = \frac{F_1 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 S_j \Gamma_{1j} e^{-\lambda_j z} \right] e^{i\omega t} + \frac{F_2 \widehat{\psi}_2(\xi)}{\Gamma} \left[\sum_{j=1}^3 S_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t}, \tag{42}$$

$$\widehat{t_{13}} = \frac{F_1 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 N_j \Gamma_{1j} e^{-\lambda_j z} \right] e^{i\omega t} + \frac{F_2 \widehat{\psi}_2(\xi)}{\Gamma} \left[\sum_{j=1}^3 N_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t}, \tag{43}$$

$$\widehat{t_{33}} = \frac{F_1 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 M_j \Gamma_{1j} e^{-\lambda_j z} \right] e^{i\omega t} + \frac{F_2 \widehat{\psi}_2(\xi)}{\Gamma} \left[\sum_{j=1}^3 M_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t}, \tag{44}$$

where

$$\begin{split} &\Gamma_{11} = -N_2 R_3 + R_2 N_3, \\ &\Gamma_{12} = N_1 R_3 - R_1 N_3, \\ &\Gamma_{13} = -N_1 R_2 + R_1 N_2, \\ &\Gamma_{21} = M_2 R_3 - R_2 M_3, \\ &\Gamma_{22} = -M_1 R_3 + R_1 M_3, \\ &\Gamma_{23} = M_1 R_2 - R_1 M_2, \\ &\Gamma = -M_1 \Gamma_{11} - M_2 \Gamma_{12} - M_3 \Gamma_{13}, \\ &N_j = -\delta_2 \lambda_j + i\xi d_j, \\ &M_j = i\xi - \delta_3 d_j \lambda_j - \frac{\beta_3}{\beta_1} l_j, \\ &R_j = (-\lambda_j + h) l_j, \\ &S_j = -i\xi - \delta_4 d_j \lambda_j - l_j. \end{split}$$

Concentrated normal force. We obtain the solution with concentrated normal force on the surface (z = 0) by taking $\psi_{1}(x) = \delta(x) \psi_{2}(x) = \delta(x)$ (45)

$$\psi_1(x) = \delta(x), \quad \psi_2(x) = \delta(x). \quad (45)$$
Applying Fourier transform defined by Eq. (28) on Eq. (45), we obtain
$$\hat{\psi}_1(\xi) = 1, \quad \hat{\psi}_2(\xi) = 1. \quad (46)$$

Using eq. (46) in (39)-(44), the components of displacement, stress, and temperature change are obtained.

Uniformly distributed force. We obtain the solution with uniformly distributed force applied on the surface (z = 0) for the case of a uniform strip load of non-dimensional width 2m applied at the origin of coordinate system x = z = 0 by taking

$$\psi_1(x), \psi_2(x) = \begin{cases} 1 \text{ if } |x| \le m\\ 0 \text{ if } |x| > m \end{cases}$$
(47)

The Fourier transforms of $\psi_1(x)$ and $\psi_2(x)$ with respect to the pair (x, ξ) in the dimensionless form after suppressing the primes becomes

$$\hat{\psi}_1(\xi) = \hat{\psi}_2(\xi) = \left\{ \frac{2\sin(\xi m)}{\xi} \right\}, \ \xi \neq 0.$$
(48)

Using (48) in (39)-(44), the components of displacement, stress, and temperature can be obtained.

Linearly distributed force. We obtain the solution with linearly distributed force applied on the surface (z = 0) having 2 m as the width of the strip load by taking

$$\{\psi_1(x), \psi_2(x)\} = \begin{cases} 1 - \frac{|x|}{m} \text{ if } |x| \le m \\ 0 \text{ if } |x| > m \end{cases}$$
(49)

by using () and applying the transform defined by (20) on (41), we get $\hat{\psi}_1(\xi) = \hat{\psi}_2(\xi) = \left\{\frac{2\{1-\cos(\xi m)\}}{\xi^2 m}\right\}, \ \xi \neq 0$

by using () and applying the transform defined by (20) on (41), we get

13

(50)

$$\hat{\psi}_1(\xi) = \hat{\psi}_2(\xi) = \left\{ \frac{2\{1 - \cos(\xi m)\}}{\xi^2 m} \right\}, \ \xi \neq 0.$$
(50)

Using (50) in (39)-(44), the components of displacement, stress, and temperature are obtained.

Thermoelastic interactions due to the thermal source. Thermal source is applied at surface (z = 0), so the boundary conditions become

$$t_{33} = 0,$$
 (51)
 $t_{31} = 0,$ (52)

$$\frac{\partial T}{\partial z} + hT = F_3 \psi_1(x) e^{i\omega t},\tag{53}$$

where, $\psi_1(x)$ specifies the source distribution function along z-axis, F_3 is the constant temperature applied on the boundary surface. If h = 0, Eq. (53) corresponds to temperature gradient boundary whereas $h \to \infty$, Eq. (53) corresponds to the temperature input boundary. Applying the Fourier transform defined by (28) on the boundary conditions (51)-(53), and using the value of t_{33} and t_{31} from Eqs. (21)-(22) and using values of \hat{u} , \hat{w} and \hat{T} from Eqs. (33)-(35) in the transformed Eqs. (51)-(53), we find the solution of the problem by using Cramer's rule to obtain the values of A_j and again using these values of A_j , j=1,2,3 in Eqs. (33)-(35) and Eqs. (21)-(22) we obtain the components of displacement, temperature, and stress, in the transformed domain as

$$\hat{u} = \frac{\widehat{F_{3}\psi_{1}(\xi)}}{\Gamma} \left[\sum_{j=1}^{3} \Gamma_{2j} e^{-\lambda_{j} z} \right] e^{i\omega t},$$
(54)

$$\widehat{w} = \frac{F_3 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 d_i \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t},\tag{55}$$

$$\hat{T} = \frac{F_3 \hat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 l_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t},\tag{56}$$

$$\widehat{t_{11}} = \frac{F_3 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 S_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t},$$
(57)

$$\widehat{t_{13}} = \frac{F_3 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 N_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t},$$
(58)

$$\widehat{t_{33}} = \frac{F_3 \widehat{\psi}_1(\xi)}{\Gamma} \left[\sum_{j=1}^3 M_j \Gamma_{2j} e^{-\lambda_j z} \right] e^{i\omega t},$$
(59)

where

$$\begin{split} &\Gamma_{11} = -N_2 R_3 + R_2 N_3, \\ &\Gamma_{12} = N_1 R_3 - R_1 N_3, \\ &\Gamma_{13} = -N_1 R_2 + R_1 N_2, \\ &\Gamma_{21} = M_2 R_3 - R_2 M_3, \\ &\Gamma_{22} = -M_1 R_3 + R_1 M_3, \\ &\Gamma_{23} = M_1 R_2 - R_1 M_2, \\ &\Gamma = -M_1 \Gamma_{11} - M_2 \Gamma_{12} - M_3 \Gamma_{13}, \\ &N_j = -\delta_2 \lambda_j + i\xi d_j; j = 1, 2, 3, \\ &M_j = i\xi - \delta_3 d_j \lambda_j - \frac{\beta_3}{\beta_1} l_j; j = 1, 2, 3, \\ &R_j = (-\lambda_j + h) l_j; j = 1, 2, 3, \end{split}$$

 $S_j = -i\xi - \delta_4 d_j \lambda_j - l_j.$

Concentrated thermal source. We obtained the solution with concentrated normal thermal source on the surface (z = 0) by taking $\psi_1(x) = \delta(x)$. (60)

$$\psi_1(x) = o(x)$$
.
Applying Fourier transform defined by Eq. (2)

Applying Fourier transform defined by Eq. (28) on Eq. (60), we obtain
$$\hat{\psi}_1(\xi) = 1.$$

Using (53) in (54)-(59), the components of displacement, stress, and temperature are obtained.

Uniformly distributed thermal source. We obtained the solution with uniformly distributed thermal source applied to the surface (z = 0) for the case of a uniform strip load of non-dimensional width 2m applied at the origin of coordinate system x = z = 0 by taking

$$\psi_1(x) = \begin{cases} 1 \text{ if } |x| \le m\\ 0 \text{ if } |x| > m \end{cases}$$
(62)

The Fourier transforms of $\psi_1(x)$ with respect to the pair (x, ξ) in the dimensionless form after suppressing the primes becomes

$$\hat{\psi}_1(\xi) = \left\{ \frac{2\sin(\xi m)}{\xi} \right\}, \ \xi \neq 0.$$
(63)

Using (55) in (54)-(59), the components of displacement, stress, and temperature are obtained.

Linearly distributed thermal source. We obtained the solution with linearly distributed force applied on the surface (z = 0) having 2 m as the width of the strip load by taking

$$\{\psi_1(x),\} = \begin{cases} 1 - \frac{|x|}{m} \text{ if } |x| \le m \\ 0 \text{ if } |x| > m \end{cases}$$
(64)

by using (24) and applying the transform defined by (28) on (56), we get

$$\hat{\psi}_1(\xi) == \left\{ \frac{2\{1 - \cos(\xi m)\}}{\xi^2 m} \right\}, \ \xi \neq 0.$$
(65)

Using (64) in (54)-(59), the components of displacement, stress, and temperature are obtained.

5. Inversion of the transformation

For obtaining the expressions of displacement component u, normal displacement component w, temperature change T, stress components t_{11} , t_{13} and t_{33} given by Eqs. (39)-(44) and (54)-(59) in the physical domain, we invert the expressions using the formula

$$\tilde{f}(x,z,\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\xi x} \hat{f}(\xi,z,\omega) d\xi = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\cos(\xi x)f_e - i\sin(\xi x)f_o| d\xi,$$
(66)

where f_o is odd and f_e is the even parts of $f(\xi, z, s)$ respectively, which is solved numerically by using the software MATLAB

6. Results and discussion

To demonstrate the theoretical results and effect of angular frequency, and relaxation time, the physical data for cobalt material, which is transversely isotropic, is taken from Dhaliwal & Singh [34] is given as $D_{11} = 3.07 \times 10^{11} Nm^{-2}$, $D_{33} = 3.581 \times 10^{11} Nm^{-2}$, $D_{13} = 1.027 \times 10^{10} Nm^{-2}$, $D_{44} = 1.510 \times 10^{11} Nm^{-2}$, $\beta_1 = 7.04 \times 10^6 Nm^{-2} deg^{-1}$, $\beta_3 = 6.90 \times 10^6 Nm^{-2} deg^{-1}$, $\rho = 8.836 \times 10^3 Kgm^{-3}$, $C_E = 4.27 \times 10^2 jKg^{-1} deg^{-1}$, $K_1 = 0.690 \times 10^2 Wm^{-1} K deg^{-1}$, $K_3 = 0.690 \times 10^2 Wm^{-1} K^{-1}$, $T_0 = 298 \text{ K}$, $H_0 = 1 \text{ Jm}^{-1} \text{ nb}^{-1}$, $\varepsilon_0 = 8.838 \times 10^{-12} \text{ Fm}^{-1}$, L = 1, $\Omega = 0.5$, $F_1 = 1$, $F_2 = 1$, $F_3 = 1$, $P = P_{11} = P_{33} = 0.1$.

Using the above values, the displacement component u, normal displacement component w, temperature change T, stress components t_{11} , t_{13} and t_{33} in Eqs. (39)-(44) and (54)-(59) are further obtained in the physical domain by using the software MATLAB and

(61)

have been plotted graphically for transversely isotropic magneto-thermoelastic medium to study the effect of frequency of time-harmonic sources.

Case 1: Mechanical force and concentrated load with time-harmonic source frequency and rotation

Figure 1 to Figure 6 show the variations of the displacement components (u and w), temperature T and stress components (t_{11} , t_{13} and t_{33}) for a transversely isotropic magneto-thermoelastic medium with mechanical force and concentrated load and with combined effects of relaxation time, rotation, time-harmonic source frequency in generalized thermoelasticity without energy dissipation respectively. The displacement component u illustrates the same pattern for $\omega = 0.25$, 0.5 and 0.75 but having different magnitudes and shows the opposite pattern for = 1.0. The displacement component w illustrates the same pattern with different magnitude temperature T sharply decreases for the initial range of x for all the values of for ω . Stress components (t_{11} , t_{13} and t_{33}) in Fig. 4 to Fig. 6 vary (increase or decrease) during the initial range of distance near the loading surface of the time-harmonic source and follow a small oscillatory pattern for the rest of the range of distance.



Fig. 1. Variations of displacement component **Fig. 2.** Variations of displacement component u with distance x w with distance x



Fig. 3. Variations of temperature T with distance x



Fig. 4. Variations of stress component t₁₁ with distance x

Thermomechanical interactions due to time harmonic sources in a transversely isotropic magneto thermoelastic...



 t_{13} with distance x

Fig. 6. Variations of the stress component t_{33} with distance x

Case II: Mechanical force and linearly distributed load with time-harmonic source frequency, rotation

Figure 7 to Figure 12 show the variations of the displacement components (u and w), temperature T and stress components (t_{11} , t_{13} and t_{33}) for a transversely isotropic magneto-thermoelastic medium with mechanical force and linearly distributed load and with combined effects of relaxation time, rotation, time-harmonic source frequency in generalized thermoelasticity without energy dissipation respectively. The displacement components (u and w) and temperature T illustrate the variation in the initial range of distance and then shows the small oscillatory pattern. Stress components (t_{11} , t_{13} and t_{33}) in Fig. 10 to Fig. 12 vary (increase or decrease) during the initial range of distance near the loading surface of the time-harmonic source and follow a small oscillatory pattern for the rest of the range of distance.



Fig. 7. Variations of displacement component u with distance x



Fig. 8. Variations of displacement component w with distance x



Fig. 9. Variations of temperature T with distance x



Fig. 11. Variations of the stress component t_{13} with distance x

Fig. 10. Variations of stress component t₁₁ with distance x



Fig. 12. Variations of the stress component t_{33} with distance x

Case III: Mechanical force and uniformly distributed load with time-harmonic source frequency and rotation

Figure 13 to Figure 18 show the variations of the displacement components (u and w), temperature T and stress components (t_{11} , t_{13} and t_{33}) for a transversely isotropic magnetothermoelastic medium with mechanical force and uniformly distributed load and with combined effects of relaxation time, rotation, time-harmonic source in generalized thermoelasticity without energy dissipation respectively. The displacement components (uand w), temperature T and Stress components t_{13} illustrate the same pattern but having different magnitudes with frequency. Stress components (t_{11} and t_{33}) in Fig. 16 to Fig. 18 vary (increase or decrease) during the initial range of distance near the loading surface of the time-harmonic source and follow the small oscillatory pattern for the rest of the range of distance. Higher the value of ω higher the stress near the loading surface.



Fig. 17. Variations of the stress component t_{13} with distance x

Fig. 18. Variations of the stress component t_{33} with distance x

Case IV: Thermal source and concentrated load with time-harmonic source frequency and rotation

Figure 19 to Figure 24 show the variations of the displacement components (u and w), temperature T and stress components (t_{11} , t_{13} and t_{33}) for a transversely isotropic magneto-thermoelastic medium with thermal source and concentrated load and with combined effects of relaxation time, rotation, a time-harmonic source in generalized thermoelasticity without energy dissipation respectively. The displacement components (u and w) and Stress component t_{13} illustrate the same pattern but having different magnitudes of frequency. Temperature T and Stress components (t_{11} , t_{33}) show the same behaviour for different values of ω .



Fig. 19. Variations of displacement component u with distance x



Fig. 21. Variations of temperature T with distance x

Fig. 20. Variations of displacement component w with distance x



Fig. 22. Variations of stress component t₁₁ with distance x



Fig. 23. Variations of the stress component t_{13} with distance x



Case V: Thermal Source and linearly distributed load with time-harmonic source frequency and rotation

Figure 25 to Figure 30 show the variations of the displacement components (u and w), temperature T and stress components (t_{11} , t_{13} and t_{33}) for a transversely isotropic magneto-thermoelastic medium with thermal source and linearly distributed load and with combined effects of relaxation time, rotation, time-harmonic source in generalized thermoelasticity without energy dissipation respectively. The displacement components (u and w) illustrate the same pattern but having different magnitudes with frequency. Temperature T decreases during the initial range of distance near the loading surface of the time-harmonic source. Stress components (t_{11} , t_{13} and t_{33}) in Fig. 28 to Fig. 30 show the different behaviour with different frequencies.



Fig. 25. Variations of displacement component u with distance x



Fig. 26. Variations of displacement component w with distance x



Fig. 27. Variations of temperature T with distance x



Fig. 29. Variations of the stress component t_{13} with distance x



Fig. 28. Variations of stress component t₁₁ with distance x



Fig. 30. Variations of the stress component t_{33} with distance x

Case VI: Thermal source and uniformly distributed load with time-harmonic source frequency and rotation

Figure 31 to Figure 36 show the variations of the displacement components (*u* and *w*), temperature T and stress components (t_{11} , t_{13} and t_{33}) for a transversely isotropic magneto-thermoelastic medium with thermal source and uniformly distributed load and with combined effects of relaxation time, rotation, time-harmonic source in generalized thermoelasticity without energy dissipation respectively. The displacement components (*u* and *w*) and temperature T illustrate the different patterns with all values of frequencies. Stress components (t_{11} , t_{13} and t_{33}) in Fig. 34 to Fig. 36 show the different patterns with different frequencies. Stress component shows the same oscillatory pattern for $\omega = 0.5, 0.75$ and 1.0 and the opposite pattern for $\omega = 0.25$.





Fig. 31. Variations of displacement component u with distance x

Distance x Fig. 32. Variations of displacement component w with distance x







4

ω = .50, τ₀=0.5

ω = .75, τ₀=0.5

ω = 1.0, τ₀=0.5

6

Distance x

8

10

7. Conclusions

0.2

0.0

-0.2

-0.4

From the above investigation, it is observed that frequency of time-harmonic source with LS-theory plays a key role in the oscillatory behaviour of the physical quantities both near as

-3

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well as just as far from the source. The physical quantities differ with the change in angular frequency. The result gives the inspiration to study magneto-thermoelastic materials as an innovative domain of applicable thermoelastic solids. The shape of curves shows the impact of different angular frequencies and fixed relaxation time and rotation on the body and fulfills the purpose of the study. The outcomes of this research are extremely helpful in the dynamic response of time-harmonic sources in transversely isotropic magneto-thermoelastic medium with rotation which is beneficial to detect the deformation field such as geothermal engineering; advanced aircraft structure design, thermal power plants, composite engineering, geology, high-energy particle accelerators and in real life as in geophysics, auditory range, geomagnetism, etc. The proposed model in this research is relevant to different problems in thermoelasticity and thermodynamics.

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ON THE DEFORMATION OF A COMPOSITE ROD IN THE FRAMEWORK OF GRADIENT THERMOELASTICITY

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Abstract. The gradient thermoelasticity problem for a composite rod based on the applied one-parameter model is investigated. To find the Cauchy stresses, the Vishik-Lyusternik asymptotic approach is used, taking into account the presence of boundary-layer solutions in the vicinity of the rods' boundaries and interface. A new dimensionless parameter equal to the ratio of the second rod length and the gradient parameter are introduced. Simplified formulas are constructed in order to find the distribution of the Cauchy stresses depending on the new parameter. After finding the Cauchy stresses distribution, moment stresses, total stresses, displacements, and deformations are further calculated. The dependence of the Cauchy stress jump on the ratio of the rods' physical characteristics and the scale parameter is investigated. The analysis of the results provided is performed.

Keywords: composite rod, gradient model, thermoelasticity, Cauchy stresses, moment stresses, asymptotic approach, boundary layer

1. Introduction

An interest in studying the stress-strain state (SSS) of composite structures of small sizes is associated with the prospects for the development of microelectronics, nanostructures, aerospace systems, and highly sensitive equipment. In such structures, especially in coatings, the sizes of the studied elements may become comparable with the characteristic sizes of the material's microstructure. In addition, large stress concentrations can occur at the interface between dissimilar materials, which greatly affects the product strength. In classical mechanics, the constitutive equations do not include any scale parameters; therefore, they cannot be used in modeling scale effects. At present, gradient elasticity theories are commonly used to model the effects observed in ultrathin structures, as well as in nanostructured materials, geomaterials, and biomaterials which include length dimension parameters in the constitutive relations.

The gradient elasticity theory is a generalization of the classical theory of elasticity. It was formulated in the 60s of the last century in the works of Toupin [1] and Mindlin [2,3]. Subsequently, a large number of researchers dealt with the development of the gradient elasticity theory [4-27]. The scientific schools of Aifantis [4-9] and Lurie [13-20] made a particularly large contribution to the development of gradient mechanics. In the gradient elasticity theory, the strain energy density depends not only on the strain but also on the first strain gradient. The mathematical formulation of the gradient theory of elasticity in the general case is completely determined by the variational Lagrange principle. The equilibrium equations of the gradient theory with respect to displacements or stresses have a higher order of differential equations compared to the classical theory, and in order to construct a solution, it is required to satisfy additional boundary conditions. Note that the practical use of the

model [3] raises the question of identifying five additional gradient modules. To overcome this difficulty, the applied gradient deformation models were proposed: the three-parameter model by D.C.C. Lam [23], the one-parameter models by E.C. Aifantis [7] and S.A. Lurie [13].

On the basis of the one-parameter model of the gradient elasticity theory, many problems have been recently solved, both one-dimensional and two-dimensional. In [10], the solutions of the gradient elasticity theory for a rod were obtained, both for static and dynamic statements. In [9], the problems of the gradient theory of elasticity for composite bodies are considered. The conditions of conjugation at the interface of materials modified in comparison with the classical theory are obtained. For the one-dimensional problem, the exact analytical solutions are obtained. In [16,17], a refined gradient theory on the bending of scaledependent hyperfine rods was constructed. In [13], the equilibrium problem of a two-layer coating under the influence of localized normal load in the framework of the plane problem is numerically studied. The problem statement is given on the basis of the interfacial layer model, which is a one-parameter version of the gradient theory of elasticity. Based on the variational formulation, the authors obtained the equilibrium equations, boundary conditions, and conjugation conditions. The solution was carried out using the integral Fourier transform and its numerical inversion. The dependence of the stress distribution on the layer thickness and the gradient parameter of the model are investigated. In [26], based on a three-parameter gradient model, the static deformation of a two-layer microplate was studied. It was found that the Cauchy stresses break at the boundary of the layers. In [27], the problem of bending a microbeam with a partial coating was solved. To study the scale effects, an additional scale parameter was introduced - the ratio of the coating thickness to the gradient parameter. The effect of a decrease in the scale parameter on changes in the distribution of displacements, stresses, and the neutral line was studied. It is found out that gradient effects play an important role when the scale parameter is less than unity.

Starting from the 70s of the last century, gradient theories have begun to be applied to problems in the mechanics of coupled fields [12,14,15,18,19,21]. In [12], the formulation of the dynamic coupled problem of gradient thermoelasticity was obtained. Further, gradient models began to be employed to more accurately estimate the SSS of inhomogeneous thermoelastic bodies, including the layered ones made of functionally graded materials (FGM). FGM is a composite material manufactured by mixing different material components (e.g., ceramic and metal ones) and is characterized by a smooth change of properties along with the coordinate [28]. So, in [21], the SSS of a long thick-walled FGM cylinder under the influence of thermal and mechanical load is numerically studied. The material characteristics of the cylinder vary exponentially in the radial direction. The influence of the inhomogeneity parameter and the gradient parameter on the distribution of stresses and displacements is studied. In [14], the formulation of the unbound gradient thermoelasticity problem based on the model of the interfacial layer for the coating-substrate system is presented under the assumption of the one-dimensionality of the original problem. As a result of the numerical solution, graphs of the distribution of stresses and strains are built, taking into account the influence of both thermomechanical characteristics, and the gradient parameter.

In this work, we study the SSS of a composite rod under thermomechanical loading based on the applied one-parameter model [7]. We have chosen a one-dimensional problem to study due to the fact that for such a problem one can obtain simplified analytical solutions that can be further used to analyze the stress state of thin coatings. The study begins with finding the temperature distribution. Then, on the basis of the Vishik-Lyusternik asymptotic approach, simplified analytical expressions for the Cauchy stresses in a dimensionless form are obtained. After finding the Cauchy stresses distribution, we calculate moment stresses,
total stresses, strains and displacements. A comparative analysis of the results obtained is performed.

2. Constitutive relations of gradient mechanics

In 1968, R.D. Mindlin and N.N. Eshel, put forward a position that the strain energy density is a function of not only the strain tensor but also the first strain gradient [3]. For a linear isotropic material, the expression for the strain energy density has the form:

$$w = \frac{1}{2}\lambda\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}\varepsilon_{ij} + c_1\varepsilon_{ij,j}\varepsilon_{ik,k} + c_2\varepsilon_{ii,k}\varepsilon_{kj,j} + c_3\varepsilon_{ii,k}\varepsilon_{jj,k} + c_4\varepsilon_{ij,k}\varepsilon_{ij,k} + c_5\varepsilon_{ij,k}\varepsilon_{kj,i}.$$
 (1)

Here λ and μ are the Lame parameters, c_1 , c_2 ,..., c_5 are the additional gradient

parameters, $\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i})$ is the tensor of small deformations of an elastic body. Note that

the practical use of this model raises the question of identifying additional modules.

To overcome this difficulty, B.S. Altan and E.C. Aifantis [7] proposed an applied oneparameter gradient deformation model based on a simplified form of the strain energy density.

Putting in (1)
$$c_1 = c_2 = c_5 = 0$$
, $c_3 = \frac{1}{2}\lambda l^2$, $c_4 = \mu l^2$, we get:

$$w = \frac{1}{2}\lambda\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}\varepsilon_{ij} + l^2(\frac{1}{2}\lambda\varepsilon_{ii,k}\varepsilon_{jj,k} + \mu\varepsilon_{ij,k}\varepsilon_{ij,k}).$$
(2)

Here l is a gradient parameter with a length dimension and associated with sizes of microstructural inhomogeneities.

The constitutive relations for the components of the Cauchy stress tensor τ_{ij} , moment stress tensor m_{ijk} , and total stress tensor σ_{ij} have the form [7]:

$$\tau_{ij} = \frac{\partial w}{\partial \varepsilon_{ij}},\tag{3}$$

$$m_{ijk} = \frac{\partial w}{\partial \varepsilon_{ij,k}} = l^2 \tau_{ijk,k} , \qquad (4)$$

$$\sigma_{ij} = \tau_{ij} - m_{ijk,k} = (1 - l^2 \nabla^2) \tau_{ij} \,.$$
(5)

The mathematical formulation of the gradient theory of elasticity in the general case is completely determined by the variational Lagrange principle. By varying the functional compiled in [7], we obtain the equilibrium equation:

$$\sigma_{ij,j} = 0, \tag{6}$$

and the natural static boundary conditions on the surface S bounding the region V are as follows:

$$m_{ijk,k}n_{j}n_{k} = q_{i}, \ \tau_{ij}n_{j} - m_{ijk,k}n_{j} - (m_{ijk,k}n_{k})_{,j} + (m_{ijk,k}n_{j}n_{k})_{,s}n_{s} = t_{i}.$$
(7)

Here t_i , q_i are the vectors of the given forces in the body volume and on its surface, n_i are the components of the unit normal vector to the body surface at the considered point. The formulation of the problem is supplemented by the kinematic boundary conditions: $u_i = \overline{u_i}$,

$$u_{i,l}n_l = \frac{\partial \overline{u}_i}{\partial n}$$

In the case of the problem of unbound thermoelasticity, according to [21], we will replace ε_{ij} with $\varepsilon_{ij} - \gamma T \delta_{ij}$ in the equation (2), where γ is the temperature stress coefficient, δ_{ij} is the Kronecker symbol. In addition, the equilibrium equation (6) and the mechanical

boundary conditions (7) must be supplemented by the equation of classical thermal conductivity:

$$\left(k_{ij}T_{,i}\right)_{,i} = 0 \tag{8}$$

and thermal boundary conditions

 $T|_{S_1} = 0, \ T|_{S_2} = T_0.$ (9)

Here $S = S_1 + S_2$ is the body surface.

As an example, we consider the equation of equilibrium, thermal conductivity, and the constitutive relations of gradient thermoelasticity for an inhomogeneous rod:

$$\begin{aligned}
 \sigma' &= 0, & (10) \\
 (k(x)T')' &= 0, & (11) \\
 \sigma &= \tau - l^2 \tau'', & (12) \\
 \tau &= E(x)u' - \gamma(x)T(x), & (13) \\
 m &= l^2 \tau' & (14)
 \end{aligned}$$

In the formulas (10) - (14), the prime sign denotes the derivative with respect to x.

3. Statement of the gradient thermoelasticity problem for a composite rod

Consider the equilibrium of a composite thermoelastic rod with a length H at the junction at the point $x = H_0$, under the influence of a combined thermo-mechanical load. One end of the rod x = 0 is rigidly fixed and maintained at zero temperature; at the other end x = H the force p_0 acts, and the temperature T_0 is maintained. The Young modulus E, the thermal conductivity k and the thermal stress coefficient γ are piecewise continuous functions of the coordinate x. Because the equilibrium equations in gradient theory have an increased order of differential equations compared to the classical theory, then the additional boundary conditions are also required. As additional boundary conditions, we take u'(0) = 0, m(H) = 0. In addition, according to [14,15], the interface conditions for temperature, heat flux, displacements, strains, total stresses, and moment stresses must be satisfied at the junction. Further in the formulas, we denote the functions and parameters corresponding to the first and second rod by the indices "1" and "2", respectively. To simplify the calculations, we assume that the gradient parameter is the same for each rod, i.e. $l_1 = l_2 = l$.

The original aim of the study was to find the distribution of the Cauchy stresses $\tau(x)$ along the length of the composite rod. For this, we express the total stresses $\sigma(x)$, moment stresses m(x), and displacement gradients u'(x) through the Cauchy stresses. Then the formulation of the thermoelasticity problem in terms of the Cauchy stresses will take the form:

$$\tau_1' - l^2 \tau_1''' = 0, \ \tau_2' - l^2 \tau_2''' = 0, \tag{15}$$

$$(k_1(x)T_1')' = 0, \qquad (k_2(x)T_2')' = 0,$$
(16)

$$T_1(0) = 0, \ T_2(H) = T_0, \tag{17}$$

$$\tau_1(0) = 0, \ \tau_2'(H) = 0, \ \tau_2(H) - l^2 \tau_2''(H) = p_0, \tag{18}$$

$$T_1(H_0) = T_2(H_0), \ k_1(H_0)T_1'(H_0) = k_2(H_0)T_2'(H_0),$$
(19)

$$\frac{\tau_1(H_0) + \gamma_1(H_0)T_1(H_0)}{E_1(H_0)} = \frac{\tau_2(H_0) + \gamma_2(H_0)T_2(H_0)}{E_2(H_0)},$$
(20)

$$\tau_1'(H_0) = \tau_2'(H_0), \ \tau_1(H_0) - l^2 \tau_1''(H_0) = \tau_2(H_0) - l^2 \tau_2''(H_0).$$
(21)

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On the deformation of a composite rod in the framework of gradient thermoelasticity

Let us write out the dimensionless problem (15)-(21) by introducing the following dimensionless parameters and functions:

$$\xi = \frac{x}{H}, \ h_0 = \frac{H_0}{H}, \ \alpha = \frac{1}{H}, \ \beta_0 = \frac{\gamma_0 T_0}{E_0}, \ P_0 = \frac{p_0}{E_0}, \ W_i = \frac{\gamma_0 T_i}{E_0}, \ \Omega_i = \frac{\tau_i}{E_0}, \ M_i = \frac{m_i}{E_0 H}, \ S_i = \frac{\sigma_i}{E_0}, \ \overline{s_i} = \frac{E_i}{E_0}, \ \overline{k_i} = \frac{k_i}{k_0}, \ \overline{\gamma_i} = \frac{\gamma_i}{\gamma_0}, \ i = 1, 2, \ k_0 = \max_{x \in [0,H]} k(x), \ \gamma_0 = \max_{x \in [0,H]} \gamma(x), \ E_0 = \max_{x \in [0,H]} E(x).$$

The dimensionless boundary value problem of thermoelasticity (15) - (21) takes the form:

$$\Omega_1' - \alpha^2 \Omega_1'' = 0, \ \Omega_2' - \alpha^2 \Omega_2'' = 0,$$
(22)

$$\left(\overline{k_1}(\xi)W_1'\right)' = 0, \left(\overline{k_2}(\xi)W_2'\right)' = 0,$$
(23)

$$W_1(0) = 0, W_2(1) = \beta_0,$$
 (24)

$$\Omega_1(0) = 0, \ \Omega_2'(1) = 0, \ \Omega_2(1) - \alpha^2 \Omega_2''(1) = P_0,$$
(25)

$$W_1(h_0) = W_2(h_0), \ k_1(h_0)W_1'(h_0) = k_2(h_0)W_2'(h_0),$$
(26)

$$\frac{\Omega_1(h_0) + \overline{\gamma}_1(h_0)W_1(h_0)}{\overline{s}_1(h_0)} = \frac{\Omega_2(h_0) + \overline{\gamma}_2(h_0)W_2(h_0)}{\overline{s}_2(h_0)},$$
(27)

$$\Omega_1'(h_0) = \Omega_2'(h_0), \quad \Omega_1(h_0) - \alpha^2 \Omega_1''(h_0) = \Omega_2(h_0) - \alpha^2 \Omega_2''(h_0).$$
(28)

4. Solving the thermoelasticity problem for a rod

The solution of the thermoelasticity problem (22) - (28) begins with finding the temperature distribution along the length of the composite rod based on the solution of the classical heat conduction problem (23), (24), (26).

In case when both rods are made of inhomogeneous materials, the solution to the problem of thermal conductivity (23), (24), (26) has the form:

$$W_{1}(\xi) = \beta_{0} \frac{f_{1}(\xi)}{f_{1}(h_{0}) + f_{2}(1)}, \quad W_{2}(\xi) = \beta_{0} \frac{f_{1}(h_{0}) + f_{2}(\xi)}{f_{1}(h_{0}) + f_{2}(1)}, \quad f_{1}(\xi) = \int_{0}^{\xi} \frac{d\eta}{\overline{k_{1}}(\eta)}, \quad f_{2}(\xi) = \int_{h_{0}}^{\xi} \frac{d\eta}{\overline{k_{2}}(\eta)}.$$
(29)

In case both rods are made of homogeneous materials, by setting in (29) $\overline{k_1} = const$ and $\overline{k_2} = const$, we obtain:

$$W_{1}(\xi) = \beta_{0} \frac{\overline{k_{2}}\xi}{\overline{k_{1}} + h_{0}(\overline{k_{2}} - \overline{k_{1}})}, \quad W_{2}(\xi) = \beta_{0} \frac{\overline{k_{1}}\xi + h_{0}(\overline{k_{2}} - \overline{k_{1}})}{\overline{k_{1}} + h_{0}(\overline{k_{2}} - \overline{k_{1}})}.$$
(30)

After finding the temperature distribution, further, in order to find the Cauchy stresses, it is necessary to solve the boundary-value problem (22), (25), (27), (28). The accurate analytical solutions were obtained in the work when both rods were made of homogeneous materials. These solutions are cumbersome and therefore are not presented here: they are used to evaluate the accuracy of the approximate analytical solution.

The problem (22), (25), (27), (28) contains the differential equations (22) with a small parameter in the highest derivative and is singularly perturbed. We obtain the approximate analytical solution to the boundary value problem (22), (25), (27), (28) based on the Vishik-Lyusternik method [29,30].

According to the scheme of the Vishik-Lyusternik method, we construct the first iterative process. To do this, we present solutions for each of the equations (22) in the form of an expansion for the small parameter α in the form:

$$\Omega_1(\xi,\alpha) \cong G_1(\xi,\alpha) = g_1^{(0)}(\xi) + \alpha g_1^{(1)}(\xi) + \alpha^2 g_1^{(2)}(\xi) + \dots,$$
(31)

$$\Omega_2(\xi,\alpha) \cong G_2(\xi,\alpha) = g_2^{(0)}(\xi) + \alpha g_2^{(1)}(\xi) + \alpha^2 g_2^{(2)}(\xi) + \dots$$
(32)

Substituting the expansions (31), (32) into (22) and performing the splitting by α powers, we obtain the sequence of boundary value problems:

Obviously, by solving each of the problems (33), it is impossible to satisfy all the boundary and conjugation conditions. It is necessary to build on additional boundary layer solutions that should quickly fade away with distance from the border.

According to the scheme of the Vishik-Lyusternik method, we construct the second iterative process. For the first rod, the boundary layers are localized in the vicinity of the attachment point $\xi = 0$ and the interface point $\xi = h_0$ with the second rod. For the second rod, the boundary layers are in the vicinity of $\xi = h_0$ and $\xi = 1$. We introduce the tensile coordinates in the vicinity of the boundaries $\eta_1 = \frac{\xi}{\alpha}$, $\eta_2 = \frac{\xi - h_0}{\alpha}$, $\eta_3 = \frac{h_0 - \xi}{\alpha}$, $\eta_4 = \frac{\xi - 1}{\alpha}$. Thus, the expressions for the Cauchy stresses of each rod can be represented as:

$$\Omega_{1}(\xi,\alpha) \cong G_{1}(\xi,\alpha) + Z_{1}\left(\frac{\xi}{\alpha},\alpha\right) + Z_{2}\left(\frac{\xi-h_{0}}{\alpha},\alpha\right),$$
(34)

$$\Omega_{2}(\xi,\alpha) \cong G_{2}(\xi,\alpha) + Z_{3}\left(\frac{h_{0}-\xi}{\alpha},\alpha\right) + Z_{4}\left(\frac{\xi-1}{\alpha},\alpha\right),$$
(35)

where
$$Z_{1}\left(\frac{\xi}{\alpha}, \alpha\right) = z_{1}^{(0)}\left(\frac{\xi}{\alpha}\right) + \alpha z_{1}^{(1)}\left(\frac{\xi}{\alpha}\right) + \alpha^{2} z_{1}^{(2)}\left(\frac{\xi}{\alpha}\right) + ...,$$

 $Z_{2}\left(\frac{\xi - h_{0}}{\alpha}, \alpha\right) = z_{2}^{(0)}\left(\frac{\xi - h_{0}}{\alpha}\right) + \alpha z_{2}^{(1)}\left(\frac{\xi - h_{0}}{\alpha}\right) + \alpha^{2} z_{2}^{(2)}\left(\frac{\xi - h_{0}}{\alpha}\right) + ...,$
 $Z_{3}\left(\frac{h_{0} - \xi}{\alpha}, \alpha\right) = z_{3}^{(0)}\left(\frac{h_{0} - \xi}{\alpha}\right) + \alpha z_{3}^{(1)}\left(\frac{h_{0} - \xi}{\alpha}\right) + \alpha^{2} z_{3}^{(2)}\left(\frac{h_{0} - \xi}{\alpha}\right) + ...,$
 $Z_{4}\left(\frac{\xi - 1}{\alpha}, \alpha\right) = z_{4}^{(0)}\left(\frac{\xi - 1}{\alpha}\right) + \alpha z_{4}^{(1)}\left(\frac{\xi - 1}{\alpha}\right) + \alpha^{2} z_{4}^{(2)}\left(\frac{\xi - 1}{\alpha}\right) +$

In the expansions (34), (35) we restrict ourselves to only zero approximations. Then approximate solutions can be represented as:

$$\Omega_{1}(\xi,\alpha) \cong g_{1}^{(0)}(\xi) + z_{1}^{(0)}\left(\frac{\xi}{\alpha}\right) + z_{2}^{(0)}\left(\frac{\xi - h_{0}}{\alpha}\right),$$
(36)

$$\Omega_{2}(\xi,\alpha) \cong g_{2}^{(0)}(\xi) + z_{3}^{(0)}\left(\frac{h_{0}-\xi}{\alpha}\right) + z_{4}^{(0)}\left(\frac{\xi-1}{\alpha}\right).$$
(37)

The functions $g_1^{(0)}(\xi)$, $g_2^{(0)}(\xi)$ coincide with the solution of the problem for a composite rod obtained on the basis of the classical model of thermoelasticity and have the form:

$$g_1^{(0)}(\xi) = g_2^{(0)}(\xi) = P_0.$$
(38)

To find the first boundary-layer solution $z_1^{(0)}(\eta_1)$, given that $\frac{d^2}{d\xi^2} = \frac{1}{\alpha^2} \frac{d^2}{d\eta_1^2}$, $\frac{d^4}{d\xi^4} = \frac{1}{\alpha^4} \frac{d^4}{d\eta_1^4}$, we obtain the equation $z_1^{(0)'} - z_1^{(0)'''} = 0$, (39) with the solution $z_1^{(0)} = 0$, $z_1 = 0$, (39)

$$z_1^{(0)} = C_1 + C_2 e^{\eta_1} + C_3 e^{-\eta_1}.$$
(40)
Since the boundary-layer solution $z_1^{(0)}(\eta_1)$ must asymptotically tend to zero for

 $\eta_1 \rightarrow \infty$, we assume $C_1 = C_2 = 0$ in (40). Therefore, $z_1^{(0)} = C_3 e^{-\frac{\varsigma}{\alpha}}$.

To find the second boundary-layer solution $z_2^{(0)}(\eta_2)$, we have the equation:

$$z_2^{(0)'} - z_2^{(0)'''} = 0$$
, (41)
which solution has the form:

$$z_2^{(0)} = C_4 + C_5 e^{\eta_2} + C_6 e^{-\eta_2} \,. \tag{42}$$

As far as the boundary-layer solution $z_2^{(0)}(\eta_2)$ also has to tend asymptotically to zero for $\eta_2 \rightarrow -\infty$, we assume in (42) $C_4 = C_6 = 0$. So, $z_2^{(0)} = C_5 e^{\frac{\xi - h_0}{\alpha}}$. The expressions for the Cauchy stress in the first rod will take the form:

$$\Omega_1(\xi,\alpha) = P_0\left(1 - e^{-\frac{\xi}{\alpha}}\right) + C_5 e^{\frac{\xi - h_0}{\alpha}}.$$
(43)

To find C_3 , we proceed to satisfy the boundary condition on the left end of the rod $\xi = 0$: $\Omega_1(0) = g_1^{(0)}(0) + z_1^{(0)}(0) = P_0 + C_3 = 0$. From this, we have $C_3 = -P_0$. Here we take into account that when $\xi = 0$, only the first boundary-layer solution manifests itself $z_1^{(0)}$ since the value h_0 is such that the influence of the second boundary layer solution $z_2^{(0)}$ can be omitted due to the small size of $e^{-\frac{h_0}{\alpha}}$.

Then the Cauchy stress in the first rod will take the form:

$$\Omega_1(\xi,\alpha) \cong P_0\left(1 - e^{-\frac{\xi}{\alpha}}\right) + C_5 e^{\frac{\xi - h_0}{\alpha}}.$$
(44)

Given the physical meaning, we similarly determine the third and fourth boundary-layer solutions in the form $z_3^{(0)} = C_7 e^{\frac{h_0 - \xi}{\alpha}}$, $z_4^{(0)} = C_8 e^{\frac{\xi - 1}{\alpha}}$. From the condition $\Omega'_2(1) = 0$ follows the relationship between the constants C_7 and C_8 in the form $C_8 = C_7 e^{\frac{h_0 - 1}{\alpha}}$. The expressions for the stress in the second rod will take the form:

$$\Omega_2(\xi,\alpha) \cong P_0 + C_7 \left(e^{\frac{h_0 - \xi}{\alpha}} + e^{\frac{h_0 - 1}{\alpha}} e^{\frac{\xi - 1}{\alpha}} \right).$$
(45)

The Unknowns C_5 and C_7 are determined from the boundary conditions (27), (28), assuming $1 - e^{\frac{h_0}{\alpha}} \cong 1$ in the calculations.

Then the expressions for the dimensionless Cauchy stresses, denoting by $\delta_0 = \frac{1-h_0}{\alpha}$ the ratio of the length of the second rod and the gradient parameter α , can be represented as:

$$\Omega_{1}(\xi,\alpha) \cong P_{0}\left(1-e^{-\frac{\xi}{\alpha}}\right) + K\left(1-e^{-2\delta_{0}}\right)e^{\frac{\xi-h_{0}}{\alpha}},$$
(46)

$$\Omega_{2}(\xi,\alpha) \cong P_{0} - \mathbf{K}\left(e^{\frac{h_{0}-\xi}{\alpha}} + e^{-\delta_{0}}e^{\frac{\xi-1}{\alpha}}\right),\tag{47}$$

where

$$K = \frac{P_0(\overline{s_1}(h_0) - \overline{s_2}(h_0)) + W_1(h_0)(\overline{s_1}(h_0)\overline{\gamma_2}(h_0) - \overline{s_2}(h_0)\overline{\gamma_1}(h_0))}{\overline{s_1}(h_0) + \overline{s_2}(h_0) + (\overline{s_1}(h_0) - \overline{s_2}(h_0))e^{-2\delta_0}}.$$
(48)

If we put in (46), (47) $\alpha = 0$, then we obtain the expressions for stresses corresponding to the classical thermoelasticity: $\Omega_1 = \Omega_2 = P_0$.

From the formulas (46), (47) it follows that at the point $\xi = h_0$ there is a stress jump. Neglecting the magnitude $P_0 e^{-\frac{h_0}{\alpha}}$ compared with 2*K*, we get the expression for the stress jump:

$$\Delta\Omega = \Omega_1 - \Omega_2 \cong 2K \,. \tag{49}$$

The value of the stress jump, according to (48), (49), is determined by the mechanical stress P_0 , the temperature $W_1(h_0)$, and the relation between thermoelastic characteristics and the parameter δ_0 . From the formula (48) it follows that if a continuous change in the thermomechanical characteristics through the junction of the rods is ensured, then there will be no Cauchy stress jump.

If $\delta_0 \leq 1$ (the relative length of the second rod is comparable to or less than the value of the gradient parameter α), then scale effects will appear, consisting in the dependence of the Cauchy stress jump on the value of the parameter δ_0 . When $\delta_0 = 0$ the Cauchy stress jump is minimal; with the increase δ_0 from 0 to $\delta_0 \sim 1$ comes the exponential increase of $\Delta\Omega$. At $\delta_0 = 0$, the value $\Delta\Omega$ for a rod made of homogeneous parts, in the case of mechanical loading, is determined by the formula

$$\Delta \Omega \cong P_0 \left(1 - \frac{\overline{s}_2}{\overline{s}_1} \right). \tag{50}$$

If the elastic modulus of the first rod is greater than that of the second one, we have the following in the dimensionless form: $\overline{s_1} = 1$, $\overline{s_2} \in [0,1)$. The maximum stress jump, equal to $\Delta \Omega \cong P_0$, will be at $\overline{s_2} = 0$. If the elastic modulus of the first rod is less than the second one, we have: $\overline{s_2} = 1$, $\overline{s_1} \in [0,1)$. The absolute value of the maximum stress jump $|\Delta \Omega| \rightarrow +\infty$ will be at $\overline{s_1} \rightarrow 0$.

At $\delta_0 \gg 1$ (the relative length of the second rod is much larger than the gradient parameter α), the exponents $e^{-\delta_0}$ are very small quantities. Then in the expressions (46)-(48) one can put $1 - e^{-2\delta_0} \cong 1$, $e^{-\delta_0} e^{\frac{\xi-1}{\alpha}} \cong 0$, $\overline{s_1}(h_0) + \overline{s_2}(h_0) + (\overline{s_1}(h_0) - \overline{s_2}(h_0))e^{-2\delta_0} \cong \overline{s_1}(h_0) + \overline{s_2}(h_0)$.

In this case, the value of the stress jump $\Delta\Omega$ is independent of the specific parameter value δ_0 , and it is determined by the ratio of thermomechanical characteristics. The value $\Delta\Omega$

for a rod made of homogeneous parts, in the case of mechanical loading, at $\delta_0 \gg 1$, is determined by the formula

$$\Delta \Omega \cong 2P_0 \frac{\overline{s_1} - \overline{s_2}}{\overline{s_1} + \overline{s_2}}.$$
(51)

The absolute value of the maximum stress jump in this case is $|\Delta\Omega| \cong 2P_0$ and will be reached for $\overline{s_1} = 1$, $\overline{s_2} = 0$ or $\overline{s_2} = 1$, $\overline{s_1} = 0$.

After finding the laws of distribution of the dimensionless Cauchy stresses along the coordinate ξ , we further calculate the dimensionless moment stresses $M_i = \alpha^2 \Omega'_i$, and the dimensionless strains $E_i = \frac{1}{\overline{s_i}} (\Omega_i + \overline{\gamma_i} W_i)$, i = 1, 2. The total stresses $S_i = \Omega_i - M'_i$, based on boundary conditions (25), (28), are the same and equal $S_1(\xi) = S_1(\xi) = P_0$ regardless of the material and gradient characteristics of the rods. The displacements distributions U_i , i = 1, 2 by the coordinate ξ are found by integrating the expressions for strains E_i , given the boundary condition $U_1(0) = 0$ and the conjugation condition $U_1(h_0) = U_2(h_0)$.

5. Computation results

This section presents the results of calculations on finding the distribution of dimensionless Cauchy stresses, moment stresses, total stresses, strains, and coordinate displacements for both mechanical and thermal loading.

Example 1. Consider the case of mechanical loading of a composite rod ($\beta = 0$, $P_0 = 0.1$), the parts of which are made of homogeneous materials with the following characteristics: $\delta_0 = 5$, $\overline{s_1} = 0.5$, $\overline{s_2} = 1$. The influence of the gradient parameter α magnitude on the accuracy of the calculation of the dimensionless Cauchy stresses by the asymptotic formulas (46), (47) is studied. During the calculations, it was found that the error in the approximate calculation of the dimensionless Cauchy stresses does not exceed 1% at $\alpha \leq 0.02$.



Fig. 1. Distribution graphs along the coordinate ξ: a) dimensionless Cauchy stresses;b) dimensionless moment stresses under mechanical loading



Fig. 2. Distribution graphs along the coordinate ξ : a) dimensionless strains; b) dimensionless displacements during mechanical loading

Figures 1 and 2 show images of the distribution of the dimensionless Cauchy stresses (Fig. 1a), the moment stresses (Fig. 1b), the strains (Fig. 2a), and the displacements (Fig. 2b) at $\alpha = 0.01$. The value h_0 is determined from the expression $h_0 = 1 - \delta_0 \alpha$.

From Figure 1a it follows that the Cauchy stresses: 1) near the end face $\xi = 0$ decay exponentially to zero in accordance with the boundary condition $\Omega_1(0) = 0$; 2) experience a jump at the point $\xi = h_0$, which values, according to (51), is determined by the ratio of the elastic modulus of the rods. From Figure 1b it follows that the moment stresses equal to zero, except for the vicinity of the fixing and conjugation points, and reach a peak at the point of contact of the rods.

Figure 2a depicts the strains and displacements.

In the case of mechanical loading, we study the dependence of the jump of the Cauchy stresses $\Delta\Omega$ at the point $\xi = h_0$, calculated by the formula (49), on the value of the parameter δ_0 at $P_0 = 0.1$, $\alpha = 0.01$ and various ratios of the elastic modulus. Figure 3 presents the results of calculations of the dependence of the stress jump on the parameter δ_0 for: 1) $\overline{s_1} = 1$, $\overline{s_2} = 0.5$ (Fig. 3a); 2) $\overline{s_1} = 0.5$, $\overline{s_2} = 1$ (Fig. 3b). In this case, the solid line shows the dependence $\Delta\Omega(\delta_0)$, obtained in the course of the exact analytical solution, and the dots – on the basis of the formula (49).



Fig. 3. Graph of the dependence of the jump in the dimensionless Cauchy stresses on the parameter δ_0 under mechanical loading

From Figure 3 it follows that the minimum Cauchy stress jump occurs when $\delta_0 \ll 1$, i.e. when the length of the second rod is much less than the gradient parameter α . As you increase δ_0 , the stress jump increases exponentially. Starting from $\delta_0 > 3$, i.e. when the length of the second rod becomes 3 times greater than the gradient parameter α , $\Delta\Omega$ almost reaches a stationary value.

Example 2. Consider the case of thermal loading of a composite rod ($\beta_0 = 0.1, P_0 = 0$), the parts of which are made of homogeneous materials with the following characteristics: $\alpha = 0.01, \ \delta_0 = 8, \ \overline{s_1} = 1, \ \overline{s_2} = 1, \ \overline{k_1} = 1, \ \overline{k_2} = 0.25, \ \overline{\gamma_1} = 0.5, \ \overline{\gamma_2} = 1.$ To find the temperature at the point h_0 , we use the first formula (30).



Fig. 4. Distribution graphs along the coordinate ξ: a) dimensionless Cauchy stresses;b) dimensionless moment stresses under thermal loading



Fig. 5. Distribution graphs along the coordinate ξ : a) dimensionless strains; b) dimensionless displacements during mechanical loading

Figures 4-5 show images of the distribution of the dimensionless functions: the Cauchy stresses (Fig. 4a), the moment stresses (Fig. 4b), the strains(Fig. 5a), and the displacements (Fig. 5b). The error in calculating the distribution of the dimensionless functions was less than 1%.

From Figure 4a, it follows that the Cauchy stresses are equal to zero, with the exception of the vicinity of the junction of the rods, where a stress jump occurs, due to the difference in the coefficients of the thermal stresses of the rods. From Figure 4b it follows that the moment stresses are equal to zero, with the exception of the vicinity of the junction of the rods and reach a peak at the junction point of the rods.

The magnitude of the Cauchy stress jump during the thermal way of loading the rod made of homogeneous parts is:

$$\Delta \Omega \cong 2 \frac{W_1(h_0) \left(\overline{s_1} \overline{\gamma}_2 - \overline{s_2} \overline{\gamma}_1\right)}{\overline{s_1} + \overline{s_2} + (\overline{s_1} - \overline{s_2}) e^{-2\delta_0}}.$$
(52)

For the case of thermal loading, we study the dependence of the Cauchy stress jump $\Delta\Omega$ at a point $\xi = h_0$ on the parameter δ_0 at $\beta_0 = 0.1$, $\overline{k_1} = 1$, $\overline{k_2} = 0.25$, $\overline{s_1} = 0.5$, $\overline{s_2} = 1$, $\overline{\gamma_1} = 1$, $\overline{\gamma_2} = 0.8$, $\alpha = 0.01$. The value h_0 , necessary to find the temperature, is determined from the expression $h_0 = 1 - \delta_0 \alpha$. In Figure 6, the solid line shows the dependence obtained in the course of the exact analytical solution, and the dots – on the basis of approximate formulas.

On the deformation of a composite rod in the framework of gradient thermoelasticity



Fig. 6. Graph of the dependence of the jump in the dimensionless Cauchy stresses on the parameter δ_0 under thermal loading

From Figure 6 it follows that in the case of thermal loading, the maximum rate of change of the function $\Delta\Omega(\delta_0)$ is observed at $\delta_0 < 1$, i.e. when the length of the second rod is less than the gradient parameter α . For $\delta_0 > 1$, with an increase of δ_0 , a smooth change in function $\Delta\Omega(\delta_0)$ is observed.

6. Conclusion

A statement of the gradient thermoelasticity problem for a composite rod based on the oneparameter Aifantis model is given. After finding the temperature distribution from the solution of the classical heat conduction problem, simplified analytical expressions for finding the Cauchy stresses are obtained on the basis of the asymptotic Vishik-Lyusternik approach. The cases of thermal and mechanical loading of the rod are considered. A new scale parameter is introduced, equal to the ratio of the length of the second rod and the gradient parameter. After finding the distribution of the Cauchy stresses, moment stresses, total stresses, displacements, and deformations are calculated. It was revealed that, within the framework of the gradient theory, the deformations are continuous at the point of contact of the rods. This fact explains the jump in the Cauchy stresses in the vicinity of the point of the rod conjugation. The magnitude of the Cauchy stress jump depends on both the ratio of thermomechanical characteristics and the value of the scale parameter. The dependence of the Cauchy stress jump on the scale parameter is investigated. It was found out that the stress jump function changes most rapidly at values of the scale parameter less than the length of the second rod. The moment stresses are continuous, equal to zero, except for the vicinity of the fixing and conjugation points, and reach a peak at the rods' conjugation point. The total stresses, which are a combination of the Cauchy stresses and the first gradient of the moment stresses, are continuous in each rod and equal to the value of the mechanical load at the rod's end.

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BURST-LIKE SHAPE MEMORY RECOVERY AND CALORIMETRIC EFFECT IN Cu-Al-Ni ALLOY SINGLE CRYSTALS AT CYCLIC TEST

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Abstract. Here we report on compressive stress-strain behavior, ordinary and burst-like shape memory (SM) strain recovery, and associated caloric effects in Cu - 14.02% wt. Al - 4.0% wt. Ni single crystals which have multiphase martensitic structure at room temperature. The effect of repetitive thermo-mechanical cycling on the recovery of the shape memory deformation is investigated. The stress-strain curves of the specimens are smooth in all tests. Immediately after quenching, crystals exhibited burst-like strain recovery accompanied by the jumping of the whole specimen in each deformation-recovery. After several days from quenching, crystals showed weaker jumping which was also reducing with each thermomechanical cycle. The average values of the integral thermal effect remained the same from cycle to cycle. Although the starting temperature of burst-like reverse martensitic transformation stochastically varied from cycle to cycle, it showed a general tendency to decrease with an increasing number of cycles until the burst-like effect disappears completely. The heating rate does not significantly affect the position of the DSC peak. Low temperature aging of the specimens resulted in the gradual weakening and disappearance of the burst-like strain recovery. Thus, thermal treatment and loading regimes should be optimized for highcycle applications of Cu-Al-Ni alloys.

Keywords: shape memory alloys (SMA); strain recovery; martensitic phase transformation; differential scanning calorimetry (DSC)

1. Introduction

High-quality single crystalline shape memory alloys (SMA) outperform conventional polycrystalline materials in actuator applications in terms of precise control of deformation and long fatigue life [1,2].

Thermomechanical and shape memory properties of single crystalline SMAs are strongly anisotropic. For instance, the recoverable shape memory strain differs considerably for different crystallographic directions. Some SMA single crystals, like Ni-Fe-Ga-Co, Cu-Al-Fe-Mn, and Cu-Al-Ni, also exhibit strong anisotropy of shape memory kinetics [3,4]. For certain orientations, these crystals manifest an extraordinarily fast rate of strain recovery. This effect is also referred to as "burst-like strain recovery" [3-7]. In contrast to the shape recovery in conventional SMAs which occurs slowly over a wide temperature range of about 10 K showing relatively low temperature sensitivity, the burst-like strain recovery occurs in a very narrow temperature interval less than a few tenths of a degree [5,6]. The burst-like recovery of shape memory (SM) strain completes almost instantly and is often accompanied by the jumping of the sample. The initial velocity of the sample exceeds up to 30 m/s [3,6].

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Actually, the phenomenon of burst-like martensitic transitions has been known for many years. Machlin and Cohen [8] were possibly the first to report burst martensitic transformations in Fe-Ni and Fe-Ni-C alloys. Later, burst-like martensitic transformations were observed in Au-Cd, Ni-Ti, Fe-Ni-C, Pu-Ga alloys [9]. Such transformations occur apparently instantaneously in the time interval of an audible click [9]. The duration of the burst was estimated by Entwistle [10] to be about 10^{-4} to 10^{-3} s. However, direct experimental evidence for that is lacking. Most of the authors report that the burst usually stops before the transformation is complete. In contrast to that, we observed complete burst-like strain recovery in Ni-Fe-Ga-Co [3,6] and Cu-Al-Ni single crystals [11]. The origin of this effect can be ascribed to interphase stresses. A more in-depth analysis of the influence of elastic interphase stresses on the parameters of martensite–austenite transitions in SMA crystals can be found in [11-13].

In recent decades, Cu-based SMAs have emerged as potential material for a variety of applications, such as high damping materials, sensors, and actuators [1]. Although Cu-Al-Ni crystals are well-known SMA materials [12,14], some of their properties like burst-like shape memory strain recovery require more in-depth investigation. Our present knowledge on the effect of burst-like strain recovery is limited only to sporadic observations of the effect in Cu-Al-Ni alloy crystals and estimations of the transformation energy [11].

Up to now, burst-like shape recovery has been observed in Ni-Fe-Ga-Co, Cu-Al-Ni, and Cu-Al-Fe-Mn shape memory alloy crystals [3-6,11], which can restore the original shape almost instantaneously in a very narrow temperature range. The burst-like recovery of SM strain is often accompanied by the jumping of the sample. It is of interest whether this effect is reproducible at multiple cyclic repetitions. We observed a good reproducibility in Ni₄₉Fe₁₈Ga₂₇Co₆ crystals, however, multiple cyclic operations were limited by the natural fragility of the crystals. In this study, we focus on burst-like SM recovery at cyclic operation in Cu-Al-Ni crystals and calorimetric effects associated with strain recovery.

Picornell et al. [15,16] were probably among the first researchers who reported anomalous DSC peaks during the burst-like shape recovery. They observed a sharp calorimetric peak during the heating of compressively pre-deformed Cu-Al-Ni single crystals. The peak was ascribed to the γ' - β type transformation of the mechanically formed γ' martensite to the high temperature β phase. The γ' martensitic phase disappeared after the first heating run, therefore, in the second cycle, the DSC peak reverted back to its typical form corresponding to a β - β' transformation.

The objective of this article is to investigate new shape memory materials based on Cu-Al-Ni single crystals and their treatment for future applications of burst-like strain recovery.

2. Materials and Methods

Cu – 14.02% wt. Al – 4.0% wt. Ni single crystal were pulled from own melt on a seed orientated along [001] direction by Stepanov growth technique. This growth technology provides high quality and nearly net shape crystals with smooth side surfaces. Cylindrical $(\emptyset 5 \times 10 \text{ mm}^3, \text{ mainly for the mechanical test})$ and prismatic $(1.5 \times 2.5 \times 4.5 \text{ mm}^3 \text{ for mechanical and calorimetrical experiments})$ specimens were cut from 5 mm-diameter crystal rods by spark erosion. The specimens were annealed at 1233 K for 15 min and quenched in water at room temperature. Some experiments were performed on the specimens after additional aging at 455K during 4h. The samples were polished and etched in an aqueous solution of HNO₃ to remove erosion slag and mechanically deformed layers. All specimens were compressed to a full shape memory strain which was over 8% along [001] in each experiment. The compression was performed at a near room temperature (~290-295 K) using an Instron 1342 testing machine at a strain rate of $5 \times 10^{-4} \text{ s}^{-1}$. Transformation temperatures and latent heats of

transformations in the undeformed samples after thermal treatment were measured using a Mettler Toledo 822e differential scanning calorimeter with 10 K/min rate of cooling/heating. A heat flux type differential scanning calorimeter (DSC6300, Seiko Instr.) was used for calorimetric measurements of heat flows during the strain recovery in deformed specimens. Details of the calorimetric method can be found in [17].

The rate of shape recovery was measured by a homemade laser interferometer setup with a measurement range of $10^{-7} - 10^{-2}$ m/s [18]. When heated to the transformation temperature, the deformed specimens underwent SM strain recovery which in some cases was accompanied with a shockwave travelling in [001] direction leading to jumping of the whole crystal. The jump was registered by a video camera for estimation of initial speed of the specimens. More than 60 experiments on compression and SM strain recovery were conducted with one specimen in several experimental series.

3. Results and discussion

According to differential scanning calorimetry (DSC) curves shown in Fig. 1, samples quenched at room temperature had both martensitic and austenitic phases. DSC heating and cooling diagrams reveal two main peaks with complex features implying the superposition of several processes. They can be ascribed to multiphase transformations with characteristic (start and finish) temperatures of 245K, 262K, and 281K, 301K at heating and 253K, 248K, and 243K, 233K at cooling, respectively. So martensitic and austenitic phases are present in the initial specimens at room temperature before their deformation by compression. A small difference between the latent heats of the direct and reverse transformations indicates good reversibility of the martensitic transformations. The broad asymmetric shape of the DSC peaks are probably because of multistage martensitic phase transformations.



Fig. 1. DSC curves of Cu-Al-Ni single crystal after quenching near transformation temperatures at the first cooling and heating

Figure 2 shows compression $(\sigma-\varepsilon)$ curves for the crystal after quenching in water (a) and quenching followed by aging. Both stress-strain curves look relatively smooth and have no sharp stress drops similar to those observed in Cu–13.5 (13.6) wt.%Al–4.0wt%Ni [11,16] and other crystals with burst-like recovery [3,6,15,19]. The curves show good reproducibility after loading-recovery cycling (over 60 cycles). After unloading, the SM strain is about 8%.

Figure 3 shows interferometer data of the shape recovery rate near the temperature of phase transformation for the sample heated at a constant rate of 2 K/min. It should be noted that the magnitude of the shape recovery rate goes above the upper limit of the instrument range and therefore cannot be measured by the laser interferometer.



Fig. 2. Stress–strain curves of Cu-Al-Ni single crystalline sample under uniaxial compression along [100] at temperature of 293K; for the sample after quenched (1) and for quenched and aged (2)



Fig. 3. Rate of strain recovery in deformed Cu-Al-Ni crystal versus time at heating near the temperature of reverse martensitic transformation measured by laser interferometer (heating rate is 2 K/min)

On top of that, burst-like shape recovery is accompanied by jumping of the sample (Fig. 4), which complicates the measurements of strain in the specimens. For that reason, we employed an alternative approach and estimated the burst like shape recovery rate from the initial velocity of the jumping samples. Experimental measurements using a kinetic method [5,6] showed that the start velocity can exceed 20-30 m/s, which can serve as a rough

indication of shape recovery rate. Indeed, the real strain recovery rate can be much faster than that value and possibly can approach the speed of a shock wave in solid.



Fig. 4. Video snapshot showing a jump of a 30 g load as a result of burst-like shape memory strain recovery in 1.6g grams Cu-Al-Ni crystal. The initial speed of the crystal is 12 m/s. The launcher consists of a guide tube, an SMA crystal (inside the tube), and a heater

Table 1. Jump express test. Jump strength score: 3 is strong, 2 is medium, 1 is weak jump (or its absent). Heating rate is about ~45 K/min

Number of test	1	2	3	4	5	6	7	8	9	10	11	12	13
Days after quenching	0	0	1	1	1	1	1	1	1	1	5	5	9
Temperature of furnace (T, K)	343	339	337	342	337	340	337	339	341	347	335	342	331
Jump strength (arb. units)	3	3	3	3	3	3	3	3	3	3	2	3	1

The results of the jump test are shown in Table 1 where jump energy was evaluated using a semi-quantitate score from 1 to 3 (1 – the lowest, 3 – the highest). As can be seen from the table, there is a general trend that the jump energy and transformation temperature decrease with time after quenching. The jumps were not observed at temperatures below 330K at the heating rate of 45K/min. Instead only slight trembling or sideways falls of the specimen without jumping were observed.

Figure 5a shows a typical DSC peak for the crystal deformed along [001] during the shape recovery acquired at 0.1 K/min. The peak appears to be very asymmetrical so the maximum of the heat flow practically coincides with the onset of the transformation. It is noteworthy that the curve of DSC heat flow versus temperature (Fig. 5b) forms a loop instead of a peak. This effect can be explained by rapid heat consumption during the burst-like recovery of shape memory deformation which cannot be compensated by the heater. This results in the self-cooling of the sample so that the temperature deviates from the linear progression and drops down by 0.5°C. The reversal of the temperature trend produces a loop on the DSC curve.



Fig. 5. DSC measurement of heat flow in quenched Cu-Al-Ni crystal versus time (a) and temperature (b) during shape recovery along [001]



Fig. 6. DSC curves for undeformed Cu-Al-Ni specimens: 1, 2 – cooling and heating of quenched crystal; 3, 4-cooling and heating of quenched and aged crystal. DSC peak of deformed crystals after quenching and aging is shown in the inset (5)

Figure 6 shows DSC curves for the Cu-Al-Ni crystal deformed along [001] direction after quenching (curve a) and after quenching followed by aging (curve b). Aging is known to increase the degree of an order [21]. Also aging increases transformation temperatures by about 30-40 K for pristine crystals and ~25-30 K for deformed specimens. It means that at room temperature martensitic transformation is almost completed, and the crystal is in the austenitic phase. Besides, samples after the thermal treatment were less prone to fast recovery of SM strain. These samples exhibited only weak jumps.

Figure 7a shows DSC curves for the sample compressed along [001] after a different number of deformation-recovery cycles. The maximum of the DSC curve shifts to lower temperatures with an increasing number of cycles. Thus, aging and thermo-mechanical cycling have the opposite effects on the transformation temperature.



Fig. 7. DSC curves for Cu-Al-Ni crystal deformed along [001]. The shift of transformation temperature at increasing of cycle number (a); DSC peaks at a heating rate 1K/min and 17 K/min

It is interesting to note that the reverse transformation temperature for the deformed specimen at 1 K/min in cycle 1 and 17 K/min in cycle 2 are the same (Fig. 7b). The effect is similar to that we have recently observed in Ni-Fe-Ga-Co single crystals [22] albeit it is weaker.

4. Summary

We investigated shape memory and associated caloric effects in Cu-Al-Ni crystals. The shape recovery process shows extremely high sensitivity to temperature and completes almost instantly when a critical temperature is reached. DSC study revealed anomalous heat intake during the burst-like shape recovery. The DSC peak position does not show any strong dependence on the heating rate. In contrast, the DSC peak position exhibits a clear shift to lower temperatures with an increasing number of deformation-recovery cycles and time after quenching.

We suggest that the burst-like effect is related to interphase boundary stresses which are typical for multiphase crystals. For that reason, the effect is stronger in quenched crystals and weaker in aged crystals. Relaxation of interphase boundary stresses results in a weaker burstlike effect. The mechanism of relaxation requires further investigation.

Our findings suggest that Cu-Al-Ni crystals and other SMA materials with burst-like shape recovery have the potential as new functional materials and can be used in various technical applications. However, further research and development aimed at the stabilization of the burst-like effect are needed.

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ALGORITHM FOR POSITIONING OF ROTARY ACTUATORS BASED ON SHAPE MEMORY Cu-Al-Ni TENSILE FORCE ELEMENTS

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Abstract. This paper considers positioning algorithms for rotary actuators based on shape memory Cu-Al-Ni crystals. The actuator function scheme is provided. An algorithm for positioning of the actuator based on an actual rotary angle has been developed. Experimental results on the control algorithm and the actuator are presented. The functional characteristics of the actuator (rotation speed and positioning accuracy) are considered.

Keywords: shape memory effect, Cu–Al–Ni single crystals, cyclic rotary actuator, positioning algorithms

1. Introduction

Actuators based on shape memory alloys (SMA) are characterized by a high power-to-weight ratio and silent operation [1]. These properties make them ideal candidates for applications in robotics [2-3]. Typically a Cu-Al-Ni wire, usually shaped into a helical spring, is used as a force element in rotary and linear SMA actuators [4-5]. Due to a small diameter and high electrical resistance, the SMA wire can be directly heated by passing an electrical current through it. Unfortunately, force elements of this type typically have a low power output. An alternative approach is to use SMA cylindrical rods as force elements. In this case, the SMA force element has to be heated externally by a dedicated heater, but the developed force is substantially higher compared to that of a helical shaped force element. For example, a 3-mm-diameter SMA rod can develop a force up to 1500 N. In this paper we consider SMA actuators with rod-shaped force elements.

In our previous publications [6-12] we investigated the design of cyclic rotary and linear actuators based on the shape memory effect in relation to the properties of Cu-Al-Ni single crystals. This publication follows up on our earlier study of the design and control system for a cyclic rotary actuator [13] and describes the positioning system of such an actuator with rod-shaped force elements.

2. Actuator design

A detailed description and design of the cyclic rotary actuator used in this study can be found in Ref. [13]. Figure 1 shows the actuator scheme. The actuator consists of two Cu–Al–Ni force elements each having an individual electric heater (not shown in Fig. 1). The shaft is supported by two rolling bearings mounted in a supporting body. The rotation angle of the shaft is measured by a rotary transducer which is attached to one end of the shaft by a coupling bushing. One end of each force element is hinged to the actuator body by means of a sleeve and a pin. Another end is connected by the sleeve to a lever, which is rigidly attached to the output shaft.



Fig. 1. Actuator scheme

Force elements are 148 mm in length and have a cylindrical section with a diameter of 3 mm. Both ends of the force element have an M6 male screw thread. Each force element has a dedicated heater consisting of a Ni-Cr alloy wire insulated with silica fiber and wound in coils around the force element. Temperatures of the force elements are measured by thermocouples placed between the coils of the heating wire. The end of the thermocouple is coated by thermal conductive grease in order to get good thermal contact with the force element.

The main parameters of the actuator are shown in Table 1.

	Designation	Value	Units
Diameter of force element	d	3	mm
Length of undeformed force element	L	148	mm
Reversible deformations	\mathcal{E}_{SM}	0.08	
Heating element power	Р	135	W
Operating temperature	Т	60 - 200	°C
Type of thermocouple		Chromel-Alumel	

 Table 1. Actuator parameters

In this paper, we focus on an in-depth analysis of actuator performance characteristics in the positioning mode.

3. Logic scheme of an actuator control system

The actuator control system consists of the following elements: a personal computer, an Arduino microcontroller, a software for actuator control, a 270W power supply, a 5V DC–DC

stabilizer, two k-type thermocouples, two thermocouples signals amplifiers, and two high current transistors.

A functional diagram of the actuator control system is shown in Fig. 2. The controller collects the data from the sensors, i.e. the temperature of each force element and the angular position of the shaft and sends them to the PC. The control software on the PC analyzes the sensor data and input parameters set by a user ("input parameters" on Fig. 2) and adjusts heating/cooling accordingly. The output power of the heaters is controlled by pulse-width modulation (PWM) of the transistors in the power supply circuit. Also, the software displays reading from the sensors and plots the results in real-time ("output parameters" in Fig. 2).



Fig. 2. Functional diagram of the actuator control system

4. A control algorithm

Realization of the control algorithm. The control algorithm was implemented using the MatLab software package. The Arduino Uno microcontroller was communicated via a Serial-USB port using the MatLab Support Package for Arduino Hardware.

In our prior work [13] we described the control algorithm for an actuator working in a cyclic mode. There MatLab script was used to calculate the desired temperature of each force element. The power supplied to each of the heaters was adjusted using a proportional-integral (PI) controller to achieve that temperature set point.

In this paper, we present an updated version of that algorithm. The key difference is the addition of the position feedback provided by the angular transducer. A proportional (P) controller is used to position the actuator shaft at the desired angle. The control diagram is shown in Fig. 3.



Fig. 3. Angle control diagram

The actuator positioning without a load. We conducted a series of experiments to test the actuator control algorithm and analyze the specifics of using shape memory elements in actuators.

The first experiment demonstrates the actuator performance when the shaft rotates from 0° to 60° and then back to 0° . Figure 4a shows the dependence of the angular position and temperature versus time. Figure 4b shows strain-temperature hysteresis loops for both force elements. As one can see the dependence of the angle versus time is nonlinear; the fastest motion is achieved in the range from 15° to 60° where the rotation speed is approximately constant and can be controlled. It is noteworthy that the heating of the first force element mirrors the cooling of the second force element and vice versa (Fig. 4a). This effect originates from the very logic of the temperature control algorithm. The hysteresis loops of thermomechanical behavior of elements almost coincide with each other. The regions of the curve in the vicinity of the start and end temperatures of the phase transformations are special in the sense that the temperature variation does not produce any significant displacement. These regions can be defined as 80° C-120°C and 150°C -160°C for the heating branch, and 150°C-120°C and 100°C-80°C for the cooling branch. Thus, we can conclude that the optimal stroke is about 50° (i.e. from 10° to 60°), which is 77% of maximum stroke.



Fig. 4. Cyclic rotation: a) the actuator parameters diagram; b) hysteresis diagrams

The next experiment demonstrates the actuator performance going through the following consecutive motions: from 0° to 50° , then a rotation from this position to 30° , then from 30° to 27° , and finally from 27° to 26° (Fig. 5 and Fig 6). It can be seen that the P controller can achieve the desired angle position for small and large angular displacements. The investigation and analysis of the positioning limit will be given in the next works.



Fig. 5. Rotation from some angle totarget angle: a) from 0° to 50° b) from 50° to 30°





In the next experiments we investigated how the actuator control algorithm copes with large and small changes of the angular position (Fig. 7). It can be seen that the difference between the starting position and the setpoint does have a significant impact on the rotation time. Typically the actuator can reach the target position in one or two oscillations.



Fig. 7. Rotation from 0° to 10° , 30° , 50°

The conducted experiments yielded the following important conclusions:

- shape memory elements can be successfully employed in rotary cyclic actuators;
- precise control of actuator position can be achieved by the use of a P controller;
- the rotation angle difference does significantly impact the rotation time;
- the actuator can equally well cope with large and small angular displacements.

5. Conclusion

The actuator design and functional diagram are provided. An algorithm for positioning the actuator based on an actual angular position is designed. Experimental results on the performance of the control algorithm and the actuator are presented. The stabilization time is the same for large and small angular displacements. The positioning accuracy is better than 1°. It is sufficient to use P controller for angular position and PI controller for temperature. Further research should be aimed at the investigation of the actuator performance under load.

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THE DYNAMIC MECHANISM OF LOW-TEMPERATURE INSTABILITY OF PLASTIC DEFORMATION IN METALS

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Abstract. Under the assumption of structural softening of plastic deformation in metals, a solution of the system of equations for the ensemble of dislocations is obtained describing a running front for the dislocation density (soliton). Such dislocation charge is able to destroy deformation barriers and cause an athermal mechanism of the instability of the low-temperature plastic deformation.

Keywords: low-temperature deformation, kinetic instability, dynamic pile-up of dislocations

1. Introduction

Nowadays, the unstable character of plastic deformation is considered as a universal property of solid bodies, which is able to manifest itself in a wide range of temperatures [1]. In crystalline materials, it is caused by self-consistent collective movement of dislocations under the action of external and internal stresses [2,3]. At helium temperatures, the instability of plastic deformation (the serrated deformation) has been found in a large number of materials and it is typical at very low temperatures[4, 5]. Its character is determined by numerous parameters related to both the deformation conditions (deformation rate, temperature) and the properties of the material itself (lattice type, grain size, etc.).

Several hypotheses [6,7] have been proposed to explain the physical nature of the serrated deformation. Physically, this phenomenon has much to do with the softening of the material. A typical cause of the strength loss is the anomalous damping of dislocations (negative friction) as it was first established by Cottrell [8]. This effect is most pronounced in alloys, where the dependence of the damping force F(v) acting on dislocations on their velocities v is depicted by an *N*-shaped curve at elevated temperatures. At low temperatures, this instability [F(v) < 0] can have a dynamical nature and be due, for example, to the dispersion of the elastic moduli at high dislocation velocities [9] or to the thermoplastic instability [10,11].

In addition to this mechanism of the plastic deformation instability at low temperatures, there can be instability associated with a "dry"-friction type of the strength loss of material (structural softening). In the last case, the moving dislocations destroy obstacles that impede them (e.g., precipitates [7]) and the barrier damping of dislocations is decreased. In the framework of this model, in the present paper a theoretical study of wave modes of plastic deformation due to softening of metals at low temperatures.

2. Dynamical equations of dislocation ensemble

Mathematically, the problem of unstable modes of plastic deformation can be formulated using a set of nonlinear equations describing the time evolution of the density of continuously distributed dislocations. These evolution equations follow from the conservation law of the Burgers vector of a system of dislocations. This vector is conserved during various reactions and multiplication of dislocations [9]. The Burgers vector conservation law can be written in the form of a differential consistency equation

$$\partial \alpha_{ik} / \partial t + e_{ilm} \partial j_{mk} / \partial x_l = 0,$$

which relates the tensors of the density α_{ik} and the flux j_{ik} of dislocations [9], These tensors are expressed in terms of the scalar dislocation density $\rho_a(\mathbf{r}, t)$ as

$$\alpha_{ik} = \sum_{a} l_i b_k^a \rho_a, \quad j_{ik} = e_{ijm} \sum_{a} l_j b_k^a \rho_a v_m^a,$$

where $\mathbf{v}_{a}(\mathbf{r},t)$ is the average velocity of dislocation glide and the index *a* enumerates the possible directions of the Burgers vector **b** of a dislocation relative to the unit vector **l** tangential to the dislocation line. The set of evolution equations for the dislocation density $\rho_{a}(\mathbf{r},t)$ follows from the consistency equation and has the form

$$\frac{\partial \rho_a}{\partial t} + \operatorname{div} \rho_a \mathbf{v}_a = G_a(\rho_a),\tag{1}$$

which reduces to the continuity equation, if the local interaction of dislocations is neglected $(G_a = 0)$. This can be done if the plastic deformation is localized in a narrow slip band and is dynamical in character. In this case (further considered here) the equation of motion for dislocations, from which the velocity $\mathbf{v}_a(\mathbf{r}, t)$ can be found, has the form [9]

$$m^* \frac{dv_k^a}{dt} = e_{ijm} l_j b_k^a \left\{ \sigma_{mk}^{\text{ext}} - \sigma_{mk}^{\text{f}} \left(C_j, \psi_j \right) \right\} - F_i \left(\mathbf{v}^a \right).$$
⁽²⁾

In the right-hand side of equation (2), the first term is the Peach-Kohler force per unit of the dislocation length, with σ_{mk}^{ext} being the component of the external stress tensor in the slip plane of dislocations; $\sigma_{mk}^{\text{f}}(C_j, \psi_j)$ is the "dry"-friction stress caused by various local obstacles, which are distributed in space with density C_j and have stopping-force characteristics ψ_j ; m^* is the effective dislocation mass; and $F_i(\mathbf{v}^a)$ is the dissipative friction force.

Equations (1) and (2) are derived under the assumption that the radius of curvature R_c of the dislocation lines is much larger than the average spacing \bar{r} between dislocations. In this approximation, dislocations as a whole can be treated as straight lines, and, when studying the evolution of the entire ensemble of dislocations, one can divide this ensemble into smaller ensembles, each of which is a system of parallel dislocation lines. In this paper, we will investigate the dynamics of one of these ensembles.

Let us consider an ensemble of dislocations in a slip band of a width L > r. The x axis is taken to be along the slip direction of the given slip system of dislocations. Let the plastic flow involve a subsystem of positive edge dislocations ($\mathbf{b} \perp \mathbf{l}$) characterized by a density $\rho_+(\mathbf{r},t) = \rho(\mathbf{r},t)$ with its equilibrium value being equal to $\rho_+^0(\mathbf{r},t) = \rho_0$. Then the plastic flow in the chosen slip band is described by the set of equations

$$m^* \left(\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} \right) = b \left\{ \sigma_{\text{ext}} - \sigma_{\text{f}} \left(C_j, \psi_j \right) \right\} - F(v),$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0.$$
(4)

Dry-friction stress σ_f is usually considered as a fitting parameter. However, in the case of structural crystal softening, the quantities C_i and ψ_i can be a function of dislocation

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density ρ ; therefore, one should generally assume that $\sigma_f = \sigma_f(\rho)$.

The set of equations (3) and (4) has a time-independent uniform solution:

 $\rho = \rho_0, \quad v = v_0, \tag{5}$

where v_0 is determined from the requirement of the right-hand side of equation (3) being equal to zero,

$$F(v_0) = b\sigma_{\text{ext}} - b\sigma_{\text{f}}(\rho_0) = b\sigma_{\text{t}},$$
(6)

while the density ρ_0 is determined from the boundary conditions.

Let us analyze the stability of the time-independent uniform solution (5) of the set of Eqns. (3) and (4) taking into account the above assumptions about $\sigma_{int}(\rho)$ and $\sigma_{f}(\rho)$. Linearizing the original equations and introducing dimensionless quantities

$$n(x,t) = \frac{\rho(x,t)}{\rho_0} - 1, \quad u(x,t) = \frac{\nu(x,t)}{\nu_0} - 1, \tag{7}$$

we arrive at the equations

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = +an - \gamma u, \tag{8}$$

$$\frac{\partial n}{\partial t} + \frac{\partial n}{\partial x'} + \frac{\partial u}{\partial x'} = 0.$$
(9)

Here, we have also introduced the dimensionless variables $x' = x/\tau v_0$ and $t' = t/\tau$ and the parameters $\tau = m^* v_0 / b\sigma_t$, $a = -\sigma'_f (\rho_0) \rho_0 / \sigma_t$, and $\gamma = F'(v_0) v_0 / b\sigma_t$. For wavelike solutions $n, u \sim \exp(\lambda t' - ikx')$, we obtain the dispersion relation

$$\lambda^{2} + \lambda(\gamma - 2ik) - ik(\gamma + a) - k^{2} = 0,$$

from which it follows that the unstable-mode branch is characterized by $\lambda_{+} = \mu + i\omega$ given by

$$\mu = -\frac{\gamma}{2} + \frac{1}{2\sqrt{2}} \left[\gamma^2 + \sqrt{\gamma^4 + 16k^2 a^2} \right]^{/2},\tag{10}$$

$$\omega = k + \frac{ak}{\gamma + 2\mu}.$$
(11)

Therefore, the solution becomes unstable $(\text{Re}\lambda_+ = \mu > 0)$ in two cases,

 $\gamma < 0$

and

 $a > 0, \quad \gamma > 0. \tag{13}$

In the case of inequality (12), we have an instability that is associated with negative friction [F'(v) < 0] in the dislocation dynamics (we will refer to this instability as that of the first type), while in the case of inequality (13), an instability (of the second type) occurs because the barrier damping of the dislocations in the slip band becomes weaker as the dislocation density increases.

As follows from formula (10), the instabilities corresponding to inequalities (12) and (13) occur in the wavenumber range $0 < k^2 < \infty$. The fact that the spectrum of unstable modes contains zero-wavelength harmonics signifies that the set of equations (3) and (4) has no stationary nonhomogeneous solutions in the class of continuous functions. This will not be the case if the viscosity of the dislocation "gas" is taken into account. Physically, viscosity arises because moving dislocations pass into adjacent slip planes, thereby transferring their momentum into those planes. In gases, this is known to be the reason for internal friction between layers [12].

It can easily be shown that if the right-hand side of equation (3) contains the term ηv_{xx}

(12)

responsible for viscosity (η is the coefficient of dynamic viscosity), the spectrum of the unstable modes will be limited and, therefore, the problem will become regular. In this case, expressions (10) and (11) for the branch of unstable modes are redefined by the change in a parameter γ ($\gamma \rightarrow \gamma + \nu k^2$, where $\nu = \eta/m^* v_0^2 \tau$ is the dimensionless coefficient of kinematic viscosity).

3. Stationary structural softening waves

Let us consider a model that exhibits instability associated with structural softening (a > 0). For the sake of definiteness, we assume that the dissipative damping of the dislocations is purely viscous; i.e., F(v) = Bv, where *B* is the viscous damping constant. In this case, the parameter γ involved in the condition for the instability of plastic deformation is equal to unity. We also assume that the dependence of the dry-friction stress on the dislocation density has the form $\sigma_f \sim (K + \rho)^{-1}$, where *K* is a constant (the Michaelis-Menten law [13]). In our problem, this law can be shown to be valid by using the following line of reasoning.

Let dislocations cut obstacles (e.g., precipitates) when moving through them so that these obstacles exhibit less resistance to each subsequent dislocation moving in the same slip plane and their stopping-force characteristics ψ_j decrease. On the other hand, the deformation (cutting) of an obstacle by dislocations leads to an increase in the obstacle's surface energy; therefore, the obstacles tend to relax to their initial state with initial stoppingforce characteristic ψ_{0j} . Taking these processes into account, one can write the kinetic equation for the variable ψ_i

$$\frac{\partial \Psi_j}{\partial t} = \frac{\Psi_{0j} - \Psi_j}{\tau_{\psi}} - \kappa \Psi_j \rho, \tag{14}$$

which, combined with equations (3) and (4), forms a complete set. Here, τ_{ψ} is the relaxation time to equilibrium value ψ_{0j} and $\kappa(C_{0j})$ is a constant characterizing the interaction between the dislocations and stoppers. We assume that the recovery of the configuration of the obstacles occurs rather quickly ($\tau_{\psi} \ll \tau$). Therefore, ψ_j varies adiabatically and one can put $\partial \psi_j / \partial t = 0$ in equation (14); from which it follows that $\psi_j(\rho) = \psi_{0j} / (1 + \kappa \tau_{\psi} \rho)$. Further, putting $\sigma_f \sim \psi_j$, we finally obtain $\sigma_f(\rho) = \sigma_{0f} / (1 + \kappa \tau_{\psi} \rho)$, where σ_{0f} is the friction stress in the absence of softening. It should be noted that the work-softening mechanism considered above is not the only possible one for which the density of structural defects C_j is constant.

With the assumptions formulated above, the original equations take the form

$$m^* \left(\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x}\right) = \eta \frac{\partial^2 v}{\partial x^2} + b\sigma_{\text{ext}} \left(-\frac{b\sigma_{0\text{f}}}{1 + \kappa \tau_{\psi} \rho}\right) - Bv, \qquad (15)$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0.$$
(16)

From equation (15), the steady-state velocity can easily be determined to be $v_0 = b[\sigma_{ext} - \sigma_{0f}/(1 + \kappa \tau_{\psi} \rho)]/B$. This value can differ significantly from the velocity $v = b(\sigma_{ext} - \sigma_{0f})/B$ in the absence of the softening effect. For example, if the crystal softening is limited by friction stress, we have $\sigma_{eff} = \sigma_{ext} - \sigma_{0f} << \sigma_{ext}$. In this case, $v << v_0 \approx b\sigma_{ext}/B(1 + p)$, where the parameter $p = (\kappa \tau_{\psi} \rho_0)^{-1}$ is less than or of order unity.

We will seek inhomogeneous wavelike solutions of equations (15) and (16) in the class

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of self-similar solutions by putting $v = v(\xi)$ and $\rho = \rho(\xi)$, where $\xi = x - ct$. Substituting these into the original equations, we obtain

$$\eta \frac{\partial^2 v}{\partial \xi^2} + R(v) \frac{dv}{d\xi} = -Q(v) = -\frac{\partial U}{\partial v},$$
(17)

$$\rho = \rho_0 \frac{c - v_0}{c - v}, \quad (v < c), \tag{18}$$

where

$$R(v) = -m^*(v-c), \quad Q(v) = B(v-v_0) \left[\frac{a(1+p)v_0}{p(c-v)+c-v_0} - 1 \right].$$

Equation (17) describes a nonlinear oscillator with a damping force $R(v)v'_{\xi}$. Therefore, the problem is reduced to investigating the motion of a particle in an effective potential well U(v), which has the form of an integral of Q(v). The function Q(v) vanishes at singular points $v = v_0$ and $v = v_0[1+(c/v_0-1-a(1+p))/p] = v_c$, at which the potential U(v) has extremal values. The maximum of U is reached at $v = \min\{v_0, v_c\}$, while the minimum is at $v = \max\{v_0, v_c\}$. The equilibrium state at $v = v_c$, which arises in the system because of the change of variables, is always absolutely unstable, in contrast to the physically reasonable state at $v = v_0$. This means that the solutions of equation (17) that describe finite motion can exist only in the vicinity of the minimum of the potential $U - U(v_0)$ for $c < v_0(1+a)$. (It is easy to verify that $v_c < v_0$ if $c < v_0(1+a)$). Possible solutions that describe infinite motion must satisfy the condition $v(\pm \infty) = v_0$, which can be the case only if c > v(1+a), i.e., when the motion is represented in the (v_v, v'_{ξ}) phase plane by a separatrix going out and then entering the saddle point $(v_0, 0)$.

First, we consider possible solutions of equation (17) that describe finite motion, which is a self-oscillation of the variable v. This oscillation will be undamped if the work of the damping force is equal to zero in the average, which will be the case if $c \le c_0 = v_0$.

The maximum wave velocity $(c = c_0)$ corresponds to small-amplitude oscillations, $|v - v_0| < v_0$. Stationary waves of a relatively large amplitude propagate with a velocity c, which is only slightly less than c_0 . In this case, the stationary wavelike solutions of equations (15) and (16) correspond to the limit cycle of equation (17) in the (v, v'_{ξ}) phase plane. The wave velocity c is uniquely determined by the wave amplitude, which, in turn, depends on the given initial conditions.

Now, we consider solitary waves in the system described by equations (17) and (18). As indicated above, equation (17) describes the motion of a particle of mass η in potential U(v) in the presence of damping force $R(v)v'_{\xi}$, which depends on the velocity of propagation of the solitary wave c. The possible values of c lie in the interval $c_{\min} < c < c_{\max}$. The lower limit $c_{\min} = v_0(1+a)$ is determined by the boundary conditions $v(\pm \infty) = v_0$, while the upper limit $c_{\max} = v_0[1+a(1+p)]$ follows from the condition $v_c < c$, i.e., from the condition for the positivity of density ρ .



Fig. 1. The shape of solitary waves in the form of solitons for density $\rho(x,t)$ and velocity v(x,t) of dislocations, normalized to ρ_0 and v_0 , respectively

For a given potential U(v), there is only one value of the velocity c at which the energy loss due to damping in an infinite motion of the particle (corresponding to the motion along the separatrix in the phase plane) is strictly equal to zero. A numerical solution of equation (17) reveals that, in this case, the motion along a closed trajectory in the phase plane corresponds to a soliton-like solution (Fig. 1).

4. Summary

Thus, the model considered in the article describes the formation of a slip band, in the front of which there is a dislocation charge moving at a velocity close to the velocity of dislocations. Such dislocation charge is able to destroy dislocation barriers (precipitates, grain boundaries, etc.) and cause an athermal mechanism of the instability of low-temperature plastic deformation

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AUTOWAVE MECHANISM OF LOCALIZATION OF LOW-TEMPERATURE PLASTIC DEFORMATION

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Abstract. The mechanism of localization of low-temperature plastic deformation is investigated within the framework of the thermal activation model. The localization mechanism is considered as a result of the autowave character of the stationary solution of a system of equations that describes both the processes of thermal conductivity and plastic deformation. It is established that the stationary solution of the initial problem is given by the wave fronts of switching waves of temperature and plastic deformation. It is shown that the considered autowave mechanism determines the process of localization of high-temperature areas of plastic deformation in the cross-section of the sample in the form of either a neck or separate deformation bands.

Keywords: Deformation localization, thermally activated plastic deformation, low temperatures, autowaves

1. Introduction

An important problem of modern materials science is the instability and localization of plastic deformation of mono- and polycrystals in the low temperature region [1]. This phenomenon consists of the serrated deformation and deformation stratification of crystals into local zones of intense shear formation at temperatures of the order of 0.5-50 K, i.e. bands of deformation inside an almost undeformed crystal. Localization of deformation was found in many metals. However, the nature of this phenomenon remains largely unclear [2,3].

Since the localization of deformation is associated with an increase in the plastic flow velocity in a certain slip band, this increase is usually explained by a sharp increase either in the dislocation density in the localized zone, or in the velocity of dislocations (depending on temperature). Physically, this process is related to the excitation of the corresponding wave fronts, similar to the appearance of the Luders bands at elevated temperatures [4]. On the other hand, there is a point of view that the appearance of the deformation bands at very low temperatures is due solely to thermal effects. In this regard, this paper proposes a model for the formation of a localized slip band in the framework of the thermoactivation model of plastic deformation.

2. Autowave model

We investigate a model, which is often used to establish a criterion of plastic deformation instability at thermal activation sliding of dislocations, for the occurrence of autowave solutions [5,6]. Then for thin enough metal samples ($R \ll L$, where R is the radius of the cylindrical sample, L is the length of the sample) the processes of deformation and thermal conductivity (non-uniform along the cylinder axis) can be described by the following system
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of equations[7,8]

$$C\frac{\partial T}{\partial t} - \kappa \frac{\partial^2 T}{\partial x^2} = -\frac{2h}{R}(T - T_0) + \sigma \dot{\epsilon}.$$
(1)

$$\frac{\partial \epsilon(t)}{\partial t} = \dot{\epsilon}, \qquad \dot{\epsilon} = v \exp[-W/k_B T],$$
(2)

Here the equation (1) is the thermal conductivity equation, where T is the temperature of the metal sample, κ is the thermal conductivity coefficient, T_0 is the ambient temperature, h is the heat transfer coefficient, σ is deforming stress, C is the heat capacity of the sample, which is taken to be a constant value for simplicity as in [5].

The thermal activation mode of plastic deformation is characterized by the Eq. (2), where $\dot{\epsilon}$ is the local rate of plastic deformation in the deformation zones, ϵ is the value of plastic deformation, *W* is the activation energy, ν is a pre-exponential multiplier, k_B is the Boltzmann constant.

The system (1), (2) belongs to the class of autowave systems if the right side of the Eq. (1)

$$F(T) = \sigma v \exp[-W/k_B T] - \frac{2h}{R}(T - T_0)$$
(3)

has a descending section in a certain temperature interval and the deforming stress σ must intersect the abscissa axis at least in three points [9]. From the condition F(T) = 0 we get the dependence $\sigma = \sigma(T)$, which is characteristic for the stationary case:

$$\sigma = \frac{2h}{Ru} (T - T_0) \exp(W/k_B T).$$
⁽⁴⁾

This dependency is N-like shape (see Fig. 1) under condition $\alpha = W/k_BT > 4$ [10] and this implies that the autowave mode of plastic deformation (for typical values of the parameters [5]) is possible only at a sample temperature below $T < W / 4k_B \approx 15K$.



Fig. 1. Dependency $\sigma = \sigma(T)$ when the parameter $\alpha = W / k_B T > 4$

The line $\sigma = \sigma_e$ can intersect the $\sigma(T)$ dependency in different ways. Let us consider the case when the intersection occurs at three points (Fig. 1).

For further analysis, we write the system (1), (2) as a single equation entering a dimensionless temperature $\theta = T/T_0$

$$\frac{d\theta}{dt} = \eta \frac{\partial^2 \theta}{\partial x^2} + f(\theta),$$
(5)
where

$$f(\theta) = \mu \sigma \exp\left[-\frac{\alpha}{\theta}\right] - \beta(\theta - 1),$$

$$\mu = \nu/CT_{\theta}, \ \beta = 2h/CR, \ \eta = \kappa/C.$$
(6)

The graph of the dependency $f(\theta)$ at a given external stress level $\sigma = \sigma_e$ is shown in Fig. 2. In this case, the system (5), (6) has three equilibrium states: two stable states corresponding to temperatures $\theta = \theta_1$ and $\theta = \theta_3$ and unstable one corresponding to $\theta = \theta_2$.



Fig. 2. Dependence of the right side of the heat equation (5) on the normalized temperature $\theta = T / T_0$

To find stationary running solutions of the system (5) let us go to the self-similar variable $\xi = x - ct$ assuming $\theta = \theta(\xi)$. Substituting a solution of the assumed type in the original system, we obtain

$$-c\frac{d\theta}{d\xi} = +\eta \frac{d^2\theta}{d\xi^2} + f(\theta).$$
(7)

We choose the following boundary conditions for the variable $\theta(x,t)$: $\theta(-\infty,0) = \theta_3$, $\theta(\infty,0) = \theta_1$.

We will study the system (7) on the phase plane (θ, W), assuming $W = d\theta/d\xi$. We have $\eta \frac{dW}{d\xi} = -cW - f(\theta),$ (8)

$$\frac{d\theta}{d\xi} = W.$$
(9)

This system has three fixed points on the plane (θ, W) $(\theta_1, 0), (\theta_2, 0)$ and $(\theta_3, 0)$.

The point $(\theta_2, 0)$ is the focus, and the singular points $(\theta_1, 0)$ and $(\theta_3, 0)$ are saddle points, through which two trajectories pass (Fig. 3). The only stable stationary solution is described by a separatrix going from saddle to saddle, which corresponds to a certain value of the switching wave speed *c*.

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Fig. 3. Phase plane of the variables $\theta - W$

The system (8), (9) can be reduced to the boundary problem $\eta W \frac{dW}{d\theta} - cW - f(\theta) = 0,$

with the boundary conditions $W(\theta_1) = W(\theta_3) = 0$.

To get analytical results we approximate $f(\theta)$ by cubic trinomial $f(\theta) = -\gamma(\theta - \theta_1)(\theta - \theta_2)(\theta - \theta_3)$ and, assuming $W = \delta(\theta - \theta_1)(\theta - \theta_3)$, obtain

$$c = \sqrt{\frac{\eta\gamma}{2}}(\theta_1 + \theta_3 - 2\theta_2). \tag{11}$$

By integrating the function $W = d\theta/d\xi = \delta(\theta - \theta_1)(\theta - \theta_3)$ we find the profile of the wave solution

$$\theta(x,t) = \theta_1 + (\theta_3 - \theta_1) \left[1 + C_0 \exp\left(\frac{x - ct}{\Lambda}\right) \right]^{-1},$$
(12)

where $\Lambda = \sqrt{8\eta/\gamma} (\theta_3 - \theta_1)^{-1}$ is characteristic width of the wave front, C_0 is an integration constant.

The obtained solution is a temperature wave of heating $\theta = \theta(x - ct)$ from the state θ_1 to the state θ_3 running to the right for c > 0 to which the wave of plastic deformation softening $\dot{\varepsilon}(x-ct)$ corresponds. The wave speed sign is determined by the condition (11), i.e. c > 0 is implemented at $\theta_1 + \theta_3 > 2\theta_2$ under appropriate level of deforming stresses σ_e . At some critical stress $\sigma_e = \sigma_c$, when the condition $\theta_1 + \theta_3 = 2\theta_2$ holds, the solution is a standing wave.

It should be noted that the original system is invariant with respect to a change of sign x. Therefore, the solution of the equation (5) could be looking for the self-similar variable $\xi = x + ct$ with boundary conditions of the form: $\theta(\infty, 0) = \theta_3$, $\theta(-\infty, 0) = \theta_1$. In this case, the general solution of the system takes the form similar to (13), but the corresponding switching wave propagates in the opposite direction at the same speed c > 0:

$$\theta(x,t) = \theta_1 + (\theta_3 - \theta_1) \left[1 + C_0 \exp\left(\frac{x+ct}{\Lambda}\right) \right]^{-1}.$$
(13)

In physically realistic conditions for the appearance of wave solutions, for example, when a slip band with corresponding heating to the temperature θ_3 is formed in cross section of a sample, the actual form of the running wave fronts is shown in Fig. 4 and it corresponds

(10)

to the temperature zone of localization in a certain section of the crystal, which expands with the speed 2c.



Fig. 4. Localized heating zone of a sample formed in its cross-section

3. Conclusion

The original system of equations (1), (2) was considered above under the constant load condition ($\sigma = \sigma_e = const$). In reality, this condition is got on a special machine that maintains the tensile speed of a metal sample constant and is described by the equation

$$\frac{\partial \sigma}{\partial t} = G^* [\dot{\varepsilon}_0 - \frac{1}{L} \int_0^L \dot{\varepsilon}(x, t) dx], \tag{14}$$

where $G^* = Kh_0/S$ is the effective modulus of elasticity, K is machine-sample system stiffness, h_0 and S are height and cross-section of the sample, $\dot{\varepsilon}_0$ is the specified rate of plastic deformation.

Solutions (12), (13) have a small width of the temperature wave fronts and, correspondingly, the deformation rate compared to with the sample length ($\Lambda \ll L$). Then the average plastic deformation rate over the whole length (0,L) can be expressed approximately as

$$\bar{\dot{\varepsilon}}(t) = \frac{1}{L} \int_0^L [\dot{\varepsilon}(x-ct) + \dot{\varepsilon}(x+ct)] dx \approx [\dot{\varepsilon}(\theta_3)l_r + \dot{\varepsilon}(\theta_1)(L-l_r)]/L,$$
(15)

where the softening zone width l_r moves at the speed dl_r/dt . In a stationary case (c = 0, $\overline{\dot{\varepsilon}}(t) = \dot{\varepsilon}_0$) the width of plastic deformation zone l_r is determined easily from (15):

$$l_r = L \frac{\dot{\varepsilon}_0 - \dot{\varepsilon}(\theta_1)}{\dot{\varepsilon}(\theta_3) - \dot{\varepsilon}(\theta_1)}.$$
(16)

Let us consider the case when $\sigma \approx \sigma_c$. In this case, the share of randomly generated propagating thermal pulses (formed on the boundary or inside of the material) is small enough and does not lead to a noticeable change of the integral in (14). For this reason, no macroscopic changes of the load σ occurs. However, if σ exceeds σ_c slightly, then the softening effect takes place, as the deformation zone is continuously expanded and the value of the integral in (14) increases. According to (14) this reduces the load σ to a stable value σ_c .

There may be a situation when this tuning occurs with some delay and then, at $\sigma \approx \sigma_c$, it is possible a damped pulsating mode of the zone of plastic deformation softening and changing of the load σ .

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The transverse plastic zone l_r with elevated temperature, which is formed under these conditions, allows multiple characters. Instead of one large plastic deformation zone, there may be several smaller zones with the same total "width". The location and number of such zones are determined by the initial conditions.

Thus, since, in general, the width of the plastic deformation zone l_r is the value, which is adjusted to the specified conditions of crystal deformation, then the described autowave mechanism determines also the process of localization of high-temperature domains of plastic deformation in the cross-section of the sample in the form of either a neck or separate deformation bands.

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INVESTIGATION OF MULTISCALE MECHANISMS OF DYNAMIC DEFORMATION AND FRACTURE OF 1565 ALUMINUM ALLOY UNDER PLANE COLLISION AND HIGH-VELOCITY PENETRATION

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Abstract. High strength 1565 aluminum alloy was tested within impact velocity range of 250-750 m/s in two schemes of shock loading: (i) under uniaxial strain conditions and (ii) in high-velocity penetration. The combination of load regimes allows the different stages of multiscale structure formation to be retraced. The intensity of macro-meso momentum exchange is found to be responsible for both resistance to spallation and high-velocity penetration. The overall impact velocity region is found to be subdivided by three sub-regions of different mechanisms of dynamic straining and scales. The strength behavior of material differs for different regions of impact velocities. Within impact velocity regions where the resistance to penetration increases, the spall strength decreases. The transition from one scale level to another is shown to be realized through the excitation of velocity oscillations at the mesoscale.

Keywords: aluminum alloy, spallation, high-velocity penetration, multiscale deformation, macro-meso momentum exchange, velocity oscillations

1. Introduction

Mechanics of dynamic deformation and fracture is developed in two approaches. The traditional mechanics grounded on the continuum approach deals with the representative volume and the concept of "point" for the effective elastic-plastic features inside the representative volume so the properties of individual dislocations and other defects are not essential. The basic mathematical apparatus for macroscale is the traditional apparatus of continuum elasticity, the theory of plasticity and creep. Various continuum approaches are being considered to address these issues, some of which are discussed in publications of Makarov [1,2], Baer and Trott [3], Briant [4], and Nesterenko [5]. As for the dynamic deformation and fracture, recent monograph of Kanel [6] can be considered as a total for this direction.

Further development of the mechanics of deformed solid supposes the incorporating of multiscale mechanisms of deformation and fracture. A critical issues of this study: (i) direct transition from atom-dislocation scale to macroscale is impossible [7,8]; (ii) microstructural investigations, even extremely of high scientific level, reflect the state of the structure in post-shocked specimens, which does not coincide with its state during the straining [9]. The

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concept of mesoscale has been suggested in 80-th in two scientific schools simultaneously but of different approaches. Tomsk's school supposes the formation of mesostructure in form of synergetic transition. As Makarov [1,2] points out, the shocked system evolves under loading so that its microstructure is capable of self-organizing into definite deformation regions – mesoparticles. The scientific school of Saint-Petersburg (Phys-Tech. Institute of A.F. Ioffe) proceeds from the physical mechanisms of mesostructure formation, specifically, as collectivization of polarized dislocation structure [10].

The first problem herein is how to describe a transition from one scale to another. Hard coupling between dynamic variables at the macroscale and atom-dislocation scale doesn't work. Specifically, well-known Eshby's formula [11]

$$\Delta \rho \equiv \rho_{ik}^+ - \rho_{ik}^- = -\frac{1}{b} e_{ijl} \frac{\partial \varepsilon_{jk}}{\partial x_i},$$

which links a crystal curvature (macroscopic scale) and density of dislocations (microscale) can be used only for perfect crystals. Here ρ_{ik}^+ and ρ_{ik}^- are the densities of positive and negative dislocations, *b* is the value of Burgers-vector, ε_{ik} is the component of deformation.

Adequate description of high-strain-rate processes is thought to be a combination of deterministic and statistical approaches. This means that instead of hard coupling, the sought transition must incorporate statistical variables which could provide a flexible linkage between neighbor scales.

According to another Saint-Petersburg's school, the shock-induced meso-structures are speculated to be nucleated in the form of short-living (150-200 ns) single-sign dislocation groups which in their scale belong to mesoscale-1 [12,13]. In turn, the process of nucleation and propagation of dislocation groups results in particle velocity fluctuations which are registered in the form of particle velocity distribution.

In parallel, the well-known scientific school of Sandia Laboratory (USA) performed a series of shock-wave experiments under uniaxial strain conditions with line-VISAR registration. These experiments reveal the large-scale velocity fluctuations at the mesoscale-2 (50-500 μ m) for tantalum [14] and boron ceramics [15,16]. Specifically, these experiments reveal a direct coupling of the particle velocity distribution with the mechanism of spallation. Two-scale simulation of shock-wave propagation with taking into account the particle velocity distribution at the mesoscale has been conducted in [17,18]. The significant result of the simulation is a discovery of threshold particle velocity at which the material transits into a structure unstable state whilst the mechanism of dynamic deformation changes from uniform to turbulent.

As a rule, the investigations both theoretical and experimental, devoted to multiscale dynamic deformation deal with the shock-wave propagation initiated by loading under uniaxial strain conditions, which, however, cannot reveal the full picture of the dynamic deformation process. In contrast, the presented paper is devoted to studying the mesostructure formation in combined experiments. A critical step in having an efficient picture of multiscale processes is the parallel tests in two schemes of shock loading. The first scheme is the test under uniaxial strain conditions and the second scheme is the high-velocity penetration of elongated rigid rod. In the second scheme of shock tests, the impactor faces two mechanisms of resistance: (i) forehead resistance of plane nose of impactor and (ii) friction resistance of the lateral region of the rod. In shock tests under uniaxial strain condition, the target suffers only forehead resistance. A comparison of results in both schemes allows the role of macromeso momentum exchange in multiscale deformation and fracture to be revealed.

2. Experimental technique

Shock tests under uniaxial strain conditions were conducted with a one-stage light gas gun of 37 mm barrel diameter. Plane targets were the discs of 52 mm in diameter and 7 mm thick. Data on dynamic strength of the material, including dynamic yield limit, spall strength, and threshold of structural instability are inferred from the temporal profiles of the free surface velocity, $u_{fs}(t)$, which are registered with the velocity interferometer. In Figure 1 the qualitative pattern for three random positions of wavefront in the heterogeneous medium is presented. The dotted lines correspond to the mean shock front position whereas meander lines present the random positions of separate pieces of the shock front. In this situation, the shock wave can be considered as a superposition of three modes of motion: (i) *mode-1* is the mean motion of plane shock front, (ii) *mode-2* is the fluctuative motions of separate pieces of mesoscale-1 relatively averaged motion of mesoscale-2 and (iii) *mode-3* is the fluctuative motions of separate pieces of the shock front.



 $(1) D_{ms1} + D_{ms2} + (2) D_{ms1} + D_{ms2} + (3) D_{ms1} + D_{ms2}$

Fig. 1. Qualitative pattern of velocity-space configurations of shock front for different relations between velocity dispersions at mesoscale-1 and mesoscale-2

The random motions of shock front pieces are quantitatively characterized by the velocity variance D (square root of the particle velocity dispersion). The interference technique allows both the mean particle velocity, u_{fs} , and particle velocity variance, D_{ms1} , to be registered in real-time [19,20]. Typical free surface velocity profile $u_{fs}(t)$ and particle velocity variance profile D(t) for 1565 aluminum alloy are presented in Fig. 2. The free surface velocity profile characterizes a temporal history of mean particle velocity of dynamically deformed medium whereas the velocity variance $D_{ms1}(t)$, is a quantitative characteristic of scattering the particle velocity at the mesoscale.

For the steady shock waves, the particle velocity variance is maximum in the middle of the plastic front and decreases to zero to the top of the front. The measured with the interference technique value of the velocity variance characterizes an intensity of relaxation processes at the mesoscale-1. This means that to the top of the plastic front the relaxation processes at the mesoscale-1 are completed and transition to mesoscale-2 occurs.



Fig. 2. Free surface velocity profile, $u_{fs}(t)$, and velocity variance profile, D(t), at the impact velocity of 431 m/s

One of the important characteristics of multiscale dynamic deformation is the *defect of* particle velocity. It is determined in tests under uniaxial strain conditions as a difference between the velocity of the impactor and free surface velocity at the plateau of compressive pulse, $\Delta u_{def} = (U_{imp} - U_{fs}^{max})$ (Fig. 2). This characteristic provides the quantitative data on momentum exchange between macroscale and mesoscale.

The second dynamic characteristic which reflects a transition of material into a structure-unstable state is the *threshold of structural instability* U_{in} . It characterizes the beginning of shock-induced structural heterogenization of material. This characteristic can be obtained upon the series of the free surface velocity profiles registered under uniaxial strain conditions over the impact velocities range. The value of the free surface velocity $U_{fs} = f(U_{imp})$ at which the velocity defect begins to increase drastically is defined as the *threshold of structural instability*, U_{ins} . This characteristic has previously been introduced in [21-24]. It has been shown that material changes its structural state at the impact velocities which are higher than the threshold of structural instability. The threshold strain rate for such a kind of transition is determined for copper, steels, beryllium, aluminum alloys, and other materials.

Lastly, the third dynamic strength characteristic determined in tests under uniaxial strain conditions is the *spall strength* σ_{sp} which is often determined in the form of the so-called pull-back velocity, *W* at the back front of the compression pulse [25]. It should be noticed on the principal specifics of our experiments under uniaxial strain conditions. The laser beam

spot of interferometer focused on the free surface of the target is of the order of 50-70 μ m. This means that the free surface profiles registered in our experiments reflect the response of only a single structural element of mesoscale-2 (see Fig. 1). The total response of target on impact can be obtained by averaging over the totality of mesoscale elements.

The high-velocity penetration tests were conducted with the same facility. To provide perpendicularity relatively plane target, the rod of 20 mm in length and 5 mm in diameter is mounted into polyvinyl carbonate sabot. The conditions for "*rigid rod and studied target*" are provided by using the high-strength 02Cr18Co9Mo5-VI maraging steel as a material for the rod. Typical penetration cavern in 1565 aluminum alloy target is shown in Fig. 3.





The tests under uniaxial strain conditions provide the information on the character of spall fracture whilst the penetration tests allow the evolution of microstructure depending on the impact velocity to be retraced. In our experiments, the post shocked targets cut along the impact direction and after polishing and etching investigated with the optical microscope Axio-Observier Z-1m.

The quasistatic characteristics of the material are provided in Table 1.

Alloy	Target thickness,	σ_b ,	$\sigma_{02},$	δ,		
	mm	MPa	MPa	%		
Al. 1565	7	363	221	15.8		

Table 1. Mechanical characteristics of 1565 aluminum alloy

3. Experimental results and analysis

Structural instability and spall strength. A series of shocks under uniaxial strain conditions within impact velocity range of 250-750 m/s was performed. In Figure 4 the dependence of the value of maximum free surface velocity U_{fs}^{max} for 1565 aluminum alloy is plotted as functions of impact velocity. The free surface velocity corresponding to change of the slope of dependence $U_{fs} = f(U_{imp})$ is accepted to be the threshold of the structural instability of material. The critical changes of the slope of curve happen at the impact velocities of 440 m/s and 625.5 m/s (indicated by dotted lines).



Fig. 4. Maximum free surface velocity U_{fs}^{\max} versus impact velocity

The second dynamic strength characteristic of materials registered in tests under uniaxial strain conditions is the spall strength. Whereas the threshold of structural instability characterizes the dynamic strength of the material under compression, the spall strength is the tensile strength characteristic.



Fig. 5. Spall strength (1) and maximum free surface velocity U_{fs}^{max} (2) versus impact velocity

In Figure 5 the dependencies of maximum free surface velocity U_{fs}^{max} and spall strength on the impact velocity are plotted together. The breaks at the curves happen at the identical impact velocities indicated with dotted lines This means that the internal processes responsible for multiscale dynamic deformation and strength for both regimes of loading are mutually related.

Structural instability threshold and high-velocity penetration. Resistance to high-velocity penetration is characterized, firstly, by the value of penetration depth, L, and secondly, by the slope of curve $L = f(U_{imp})$, namely: (i) the smaller penetration depth L, the higher resistance to penetration and (ii) the smaller the slope of curve $L = f(U_{imp})$, the higher the resistance to penetration.



Fig. 6. Maximum free surface velocity U_{fs}^{max} (1) and penetration depth L (2) versus impact velocity

In Figure 6 the dependencies of $U_{fs}^{max} = f(U_{imp})$ and penetration depth $L = f(U_{imp})$ on the impact velocity are plotted together. Within impact velocities from 241.9 m/s to 750 m/s the penetration curve suffers the breaks at the impact velocities of 440 m/s (position *B'*) and 625.5 m/s (position *C'*). The relation between the rate of change of structural instability threshold and rate of change of penetration depth can be summering as following:

1). Impact velocity region of 241.9-625.5 m/s: $\frac{dU_{\text{max}}^{AB}}{du} < \frac{dU_{\text{max}}^{BC}}{du}; \quad \frac{dL_{A'B'}}{du} < \frac{dL_{B'C'}}{du}.$ 2). Impact velocity region of 440-750 m/s: $\frac{dU_{\text{max}}^{CD}}{du} < \frac{dU_{\text{max}}^{BC}}{du}; \quad \frac{dL_{C'D'}}{du} < \frac{dL_{B'C'}}{du}.$

The inequality $\frac{dL_{A'B'}}{du} < \frac{dL_{B'C'}}{du}$ means that resistance to penetration decreases after an impact velocity of 440 m/s. Within the impact velocity region from 625.5 m/s to 750 m/s, after point *C*', an analogous inequality takes place: $\frac{dL_{C'D'}}{du} < \frac{dL_{B'C'}}{du}$, which means that

resistance to penetration after impact velocity of 625.5 m/s again increases. It may be concluded that the processes responsible for structural instability of material and high-velocity penetration are mutual related. The change of slope of curve $U_{fs}^{max} = f(U_{imp})$ correlates with the behavior of the defect of particle velocity Δu_{def} .



Fig. 7. Penetration depth L(1) and velocity defect $\Delta u_{def}(2)$ versus impact velocity

Resistance to high-velocity penetration and velocity defect. Figure 7 shows that the behavior of the velocity defect correlates with the behavior of penetration depth. The relations between the rate of change of velocity defect and rate of change of penetration depth can be summering as following:

1) Impact velocity region of 241.9-625.5 m/s: $\frac{d\Delta u_{A'B'}^{def}}{du} > \frac{d\Delta u_{B'C'}^{def}}{du}$, $\frac{dL_{AB}}{du} < \frac{dL_{BC}}{du}$. 2) Impact velocity region of 440-750 m/s: $\frac{d\Delta u_{C'D'}^{def}}{du} > \frac{d\Delta u_{B'C'}^{def}}{du}$. $\frac{dL_{CD}}{du} < \frac{dL_{BC}}{du}$.

Within the upper region of impact velocities CD, the resistance to penetration increases. It should be noted that 1565 aluminum alloy has been specially created for working at high-velocity region of dynamic loadings. The beaks for both curves happen at identical impact velocities (indicated with vertical dotted lines).

Spall strength, resistance to high-velocity penetration, and velocity variance. It is thought to be very interesting to compare the spall strength and resistance to penetration behavior for different regions of impact velocities. In Figure 8 the penetration depth curve $L = f(U_{imp})$ for 1565 alloys is plotted together with the dependence for spall strength $W= f(U_{imp})$. A comparison of curves shows that the correlation between processes really exists. Dependence $W= f(U_{imp})$ based on tests under uniaxial strain conditions suffers two

breaks: at the impact velocities of 440 m/s and 625.5 m/s. The dependence of penetration depth $L = f(U_{imp})$ also suffers two breaks: at the impact velocities of 440 m/s and 608 m/s. The critical change of slope for penetration dependence happens at the velocity where the break for dependence $W = f(U_{imp})$ occurs (dotted lines in Fig. 8). Such behavior of curves evidences the common mechanism of structure behavior in tests under uniaxial strain conditions and high-velocity penetration. The breaks at the high region of impact velocities in both loading schemes also happen at close impact velocities: 625.5 m/s in-plane tests and 608 m/s in penetration tests. This means that both breaks are of the same nature.



Fig. 8. Spall strength, W, (1), velocity defect, ΔU_{def} , (2) and velocity variance, D, (3) versus impact velocity

Now let us consider a correlation between spall strength behavior and resistance to penetration over the impact velocity regions: 1) *Penetration*:

a) Impact velocity region 241.9 - 625.5 m/s: $\frac{dL_{AB}}{du} < \frac{dL_{BC}}{du}$. b) Impact velocity region 440 - 750 m/s: $\frac{dL_{CD}}{du} < \frac{dL_{BC}}{du}$. 2) Spallation: a). Impact velocity region 241.9 - 440 m/s: $\frac{dW_{A'B'}}{du} < 0$. b) Impact velocity region 440 - 625.5 m/s: $\frac{dW_{A'B'}}{du} \approx 0$. Investigation of multiscale mechanisms of dynamic deformation and fracture of 1565 aluminum alloy under plane...

c) Impact velocity region 625.5 - 750 m/s: $\frac{dW_{A'B'}}{du} < 0$.

Within impact velocity region of 241.9 - 625.5m/s, the slope of penetration depth curve changes at point *B'*: $\frac{dL_{A'B'}}{du} < \frac{dL_{B'C'}}{du}$, which means that the resistance to penetration within impact region *A'B'* of the curve (2) is higher as compared to that for piece *B'C'*. At the same time, the spall strength within the same impact velocity region shows the opposite trend. Within the piece *AB* the spall strength decreases from 137.8 m/s to 117.3 m/s. After point *B*, within piece *BC*, $\frac{dW_{BC}}{du} \approx 0$, which means that spall strength is approximately constant. The critical changes in both curves happen at an impact velocity of 440 m/s. The analogous situation is seen after the second critical impact velocity of ~ 625.5 m/s - within piece *C'D'* the slope of penetration curve (2) decreases: $\frac{dL_{C'D'}}{du} < \frac{dL_{B'C'}}{du}$, i.e. the resistance to penetration within region *C'D'* increases whereas $\frac{dW_{CD}}{du} < 0$, which means that spall strength in this region of strain rates decreases.

Thus, within impact velocity range of (241.9 - 750) m/s the strength behavior of 1565 aluminum alloy in two schemes of shock loading turns out to be opposite – when resistance to penetration increases, the spall strength decreases.

In Figure 8, besides the spall strength and penetration depth, the dependence for velocity defect on the impact velocity is provided. In our experiments, the mean particle velocity, u, and velocity variance, D_{ms1} , are registered in the form of temporal profiles (see Fig. 2). Independent measuring the impact velocity allows three shock-wave characteristics to be determined in real-time. The breaks at curves are seen to occur at identical impact velocities. The spall strength is seen to decrease when velocity defect increase (regions A'B' and C'D'). At the same time, the spall strength is *practically constant* when the velocity defect remains constant.

Such a kind of behavior of spall strength can be explained from the position of macromeso energy and momentum exchange which is described by the following equation [26]:

$$\Delta u_{def} = -\frac{1}{2} \frac{\partial D^2}{\partial u} \,. \tag{1}$$

The left-hand side of this equation, the velocity defect, characterizes the momentum which transferred from macroscale to mesoscale. This transference is realized due to a change of the mesoparticle velocity dispersion, D^2 . Eq. (1) can be written in the form

$$\Delta u_{def} = -D \frac{dD / dt}{du / dt}.$$
(2)

When the rate of change of the velocity variance equals to rate of change of mean particle velocity.

$$\frac{dD}{dt} = \frac{du}{dt},\tag{3}$$

the velocity defect equals velocity variance:

$$\Delta u_{def} = -D \,.$$

This situation corresponds to the equilibrium regime of multiscale dynamic deformation and corresponds to the middle region of impact velocities B'C' in Fig. 8. In the case of

(4)

uniaxial straining, the deformations at the macroscale and mesoscale equal, respectively, Eq. (2) can be written in the terms of strain and strain rate:

$$\Delta \varepsilon_{def} = -\varepsilon_{ms} \frac{d\varepsilon_{ms} / dt}{d\varepsilon_{mc} / dt}.$$
(5)

Here $\Delta \varepsilon_{def}$ is an additional macroscopic deformation resulted from the interscale momentum exchange, $d\varepsilon_{ms}/dt$ is the strain rate at the mesoscale, and $d\varepsilon_{mc}/dt$ is the strain rate at the macroscale. When

$$d\varepsilon_{mc} / dt = d\varepsilon_{ms} / dt \tag{6}$$

all change of deformation at the macroscale resulted from interscale momentum exchange is determined by the value of deformation at the mesoscale $\Delta \varepsilon_{def} = -\varepsilon_D$. In shock experiments, the directly registered characteristics are the free surface velocity, u_{fs} velocity defect, Δu_{def} , and velocity variance, *D*. At the same time, the physical meaning of the processes may be understood from Eq. (6) which implies the equality of local strain rate and macroscopic strain rate. As distinct from the macroscopic strain rate, the local strain rate cannot be directly determined in dynamic experiments. Therefore, Eq. (4) can serve as a reliable feature for the equality of local and macroscopic strain rates.

The meso-macro energy exchange can explain a non-monotonous behavior of spall strength depending on the strain rate. The power balance at the spalling zone can be written in the form:

$$\frac{1}{2}\rho C_{p}u^{2} = \frac{1}{2}\eta \frac{(u + \Delta u_{def})}{h}u.$$
(7)

Here ρ is a density of the material, C_p is the velocity of the shock wave, η is dynamic viscosity of deformed material and u is the particle velocity. The left-hand side of Eq. (7) characterizes the power which is brought into the spalling zone from the shock wave. The right-hand side of the equation describes the loss of power due to the normal rupture of material under tension at the spalling zone and reflects a motion of spall surfaces in opposite directions. As particle velocity is current changes owing to meso-macro energy exchange mechanism the mean particle velocity for this item includes the velocity defect Δu_{def} , and the total strain rate at the spalling zone equals:

$$\frac{d\varepsilon_1}{dt} = \frac{u + \Delta u_{def}}{h},\tag{8}$$

where h is the width of the spalling zone. From (7) and (8) one obtains

$$h = \left(\frac{\rho C_0}{\eta} - \frac{\Delta u_{def}}{h} \frac{1}{u}\right)^{-1}.$$
(9)

Time for spallation can be determined as

$$\tau_f = \frac{h}{u} = \left(\sigma - \eta \frac{\Delta u_{def}}{h}\right)^{-1},\tag{10}$$

where $\sigma = \rho C_p u$. Eq. (10) can be rewritten in the form:

$$\left(\sigma - \eta \frac{\Delta u_{def}}{h}\right)\tau_f = 1.$$
(11)

Generalization of this equation

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$$\int_{0}^{\tau_{f}} \left(\sigma - \mu \frac{\Delta u_{def}}{h} \right) dt = 1$$
(12)

can be considered as a *dynamic fracture criterion* that takes into account the meso-macro momentum exchange. In this equation, the value σ has a meaning of the spall stress which characterizes the resistance of the material to spallation. It is seen that spall stress decreases when the velocity defect increases.

4. Microstructural investigations

The initial structure of 1565 aluminum alloy contains elongated grains, i.e. texture (Fig. 9a). To understand the multiscale mechanisms of strength behavior of alloy in different regions of impact velocities it was thought to be appropriate to compare the microstructural data for different regions of impact velocity with the dependencies of penetration over the same regions. The overall region of impact velocities in accordance with Fig. 8 is subdivided into three sub-zones.



Fig. 9. Initial structural states of 1565 aluminum alloy (*a*), micro shears, and fault structures in post shocked specimen (*b*)

The main feature of post-shocked specimens is the presence of numerous micro shears of 3-10 µm length oriented along the shock direction. The micro shears are nucleated owing to mass velocity pulsations at small impact velocities. Theoretical [12,13] and experimental [4] investigations of multiscale mechanisms of dynamic deformation show that the behavior of mesostructure under dynamic loading can be characterized by the presence of short-living pulsations of particle velocity. The motions of mesostructural elements in form of single-sign dislocation groups create the short-living mass velocity pulsations of $\Delta t \approx 150-200$ ns duration. The velocity interferometer registers the particle velocity distribution in form of velocity variance D. In the case of 1565 aluminum alloy, the maximum value of velocity variance at the mesoscale-1 equals $D = 4.5 \cdot 10^3$ m/s (see Fig. 2), from where the mean displacement equals:

 $L = D \cdot \Delta t = 4.5 \times 10^3 \cdot 2 \times 10^{-7} = 9 \times 10^{-4}$ cm.

In their dimensions, the displacements belong to mesoscale-1 (1-10 μ m). The decreasing the distance to the bank of cavern density of micro shears increases.

Another structural element proper to high-velocity penetration is the so-called fault structures at the bank of the cavern. In Figure 9b a complex morphology of fault structure is presented – inside each cell a family of shear bands is incorporated.



Fig. 10. Three regions of lateral structure in 1565 aluminum alloy target after penetration

In Figure 10 the three states of structure for different regions of impact velocity are provided. Within the regions *AB* and *CD*, the specific feature of post shocked specimens is the presence of regular fault structures at the bank of the cavern and uniform deformation picture inside the region *BC*. The width of the region occupied by fault structures depends on impact velocity: within region *A* the width of the fault structure zone equals 7-12 μ m whereas at the regions for high-velocity penetration curve (Fig. 8) shows that resistance to penetration at these regions increases. Within region *BC* where the regular faults are absent, the post-shocked structure is uniform whilst the resistance to penetration decreases. From the point of view of resistance to penetration, the 1565 aluminum alloy turns out to be more preferable at the upper region of impact velocities decreases (see Fig. 8).

5. On the resonance excitation of mesoscale

In the light of the above experimental results, three questions arise: (i) what is the physical mechanism responsible for nucleation of fault structures, (ii) what parameters of shock wave determine the dimensions of fault structures, (iii) what is the physical mechanism for transition from one scale to another. To answer the questions we consider propagation of plane shock wave in a relaxing medium.

In the case of a steady shock wave, two important relationships have previously been found. The first of them ties the particle velocity variance, *D*, and strain rate [26]:

$$D = R \frac{\partial \varepsilon(t)}{\partial t} . \tag{13}$$

Here *D* is the velocity variance which is the quantitative characteristic of the intensity of the particle velocity chaotic pulsations in dynamically deformed solid, $\frac{d\varepsilon}{dt}$ is the strain rate and *R* is the proportionality coefficient. An analogous relationship is known to exist in turbulence where the intensity of turbulent pulsations is proportional to particle acceleration [27].

Eqs. (1), (13) determine the character of coupling between macroscopic and mesoscopic scales of dynamic straining. We use Eqs. (1) and (13) for a description of the response of relaxing medium on shock loading.

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In the case of one-dimensional propagation of shock wave, the balance equations for momentum conservation and medium continuity take the form

$$\rho u_t - \sigma_x = 0; \tag{14}$$

$$u_x - \mathcal{E}_t = 0. \tag{15}$$

The constitutive equation for a relaxing medium introduced by Duvall [28] and Taylor [29]:

$$\sigma - \rho C_l^2 \varepsilon = -2\mu \varepsilon^p \tag{16}$$

$$\sigma_{c} - \rho C_{i}^{2} \varepsilon_{c} = -F \,. \tag{17}$$

Here C_l is the longitudinal sound velocity, μ is the shear modulus, and the relaxation function

$$F = 2\mu \frac{\partial \varepsilon^p}{\partial t}$$
(18)

is determined through the plastic strain rate which, in turn, is determined by Orowan's equation for density and velocity of dislocations $\frac{d\varepsilon^p}{dt} = bN_dV_d$. As distinct from Duvall-Taylor approach, in the present investigation the stress relaxation in the dynamically deformed medium is accepted to be realized only through the motion of elementary carriers of deformation at the mesoscale. Dislocations and other carriers of the deformation of atomdislocation scale provide the formation and motion of mesoparticles whereas the mesoparticles play a role of self-consistent carriers of deformation. In this situation, the stress

$$\frac{\partial \varepsilon^{p}}{\partial t} = \frac{1}{C_{l}} \frac{\partial (\Delta u_{\partial e \phi})}{\partial t}.$$
(19)

The advantage of such an approach is that the relaxation model doesn't incorporate the parameters of dislocations, such as density and velocity of dislocations which cannot be controlled under conditions of dynamic straining. As distinct from the dislocation structure, defect of particle velocity can be registered in real-time (see Fig. 2). In this case, the relaxation function takes the form:

$$F = \frac{2\mu}{C_{t}} \frac{\partial (\Delta u_{def})}{\partial t}.$$
(20)

The equation system (14) - (17)) can be reduced to second-order differential equation

$$\rho \varepsilon_{tt} - \sigma_{xx} = 0. \tag{21}$$

Substitution of (1) and (13) into (19) yields:

relaxation is determined only by the velocity defect:

$$\frac{\partial \varepsilon^{p}}{\partial t} = \left(R^{2} / C_{l}^{2} \right) \frac{\partial^{2} \varepsilon}{\partial t^{2}}.$$
(22)

Then Eq. (21) is reduced to:

$$\varepsilon_{tt} - \rho C_l^2 \varepsilon_{xx} - 2 \left(\mu R^2 / \rho C_0^2 \right) \varepsilon_{xxtt} = 0.$$
⁽²³⁾

For the case of the steady propagation of shock wave, the single variable $\zeta = x - C_p t$ can be used. Eq. (23) takes the form:

$$(C_l^2 - C_p^2)\varepsilon_{\varsigma\varsigma} + 2\left(\mu R^2 / \rho C_l^2\right)\varepsilon_{\varsigma\varsigma\varsigma\varsigma} = 0.$$
⁽²⁴⁾

Exchanging $\varepsilon_{ss} = \psi$ leads to the equation for an oscillator:

$$(C_l^2 - C_p^2)\psi + 2(\mu R^2 / \rho C_l^2)\Psi_{\varsigma\varsigma} = 0.$$
⁽²⁵⁾

The frequency of oscillations equals

$$\omega = \frac{1}{2} \frac{\rho C_l^2 (C_l^2 - C_p^2)}{\mu R^2}.$$

Physically, the oscillatory regime of shock wave propagation is a sequence of *positive* back coupling provided by the Eqs. (1) and (13) which are used for locking the balance equations (14)-(17). The positive back coupling between macroscale and mesoscale is realized through the particle velocity dispersion and rate of its change.

As noted above, in our experiments the size of the laser spot of the interferometer (50-70 μ m) at the free surface of the target corresponds to mesoscale-2 (50-500 μ m) (see Fig. 1), so the experimental technique allows to registers: (i) the mean motion of single structural element of mesoscale-2 as a whole and (ii) the fine structure of shock wave including the high-frequency oscillations at the mesoscale-2. The temporal resolution of experimental diagnostics (0.6-1.0 ns), allows registering the fine structure of plastic wave including the high-frequency oscillations at the mesoscale-2. Where observed, the oscillations are excited at the top of the plastic front. Figure 11 demonstrates the velocity oscillations in 7 mm 1565 aluminum alloy target loaded at the impact velocity of 636.5 m/s. The oscillations are seen at the impact velocities which are higher than the threshold of structure unstable transition, U_{inst} . The space period of oscillations equals ~ 50 μ m, which coincides with the mean size faultstructures (40-50 µm). Thus, while the mesoscale-1 structures are nucleated owing to particle velocity pulsations, the fault-structures of mesoscale-2 are initiated due to resonance interaction of mesoscale-1 structures with the plastic front oscillations, which, in turn, result from positive back coupling between mesoparticle velocity dispersion (mesoscale) and velocity defect (macroscale).

Although oscillations are initiated due to the interaction of stochastic features of dynamically deformed structure in form of particle velocity dispersion, the transition itself happens due to swinging the high-frequency oscillations of mesostructure. Thus, it should be underlined that the macro-meso structural transition is not a direct transition from the chaotic motion of structural elements to translation motion of the next scale level as "noise-induced transition" [30]. This transition is thought to be realized through the oscillation regime of straining at the mesoscale. The oscillatory regime of dynamic deformation is found in shockwave experiments with copper, Armco-iron, steels, and other materials. The example of oscillations in shock loaded 1565 aluminum alloy is provided in Fig. 11.

Below the dimensions of fault-structures are calculated for regions AB and CD. The experimental free surface profiles are used for the calculation of parameters of shock waves. Region AB

- 1. Impact velocity $U_{imp} = 335$ m/s.
- 2. Velocity variance D = 22 m/s.
- 3. Velocity of plastic front $C_p = 5.478 \cdot 10^5 \text{ cm/s}.$
- 4. Longitudinal sound velocity $C_l = 6.387 \cdot 10^5 \text{ cm/s}.$

5. Strain rate
$$\frac{d\varepsilon}{dt} = 7.79 \cdot 10^5 \,\mathrm{c}^{-1}$$

- 6. Shear modulus $\mu = 2.7 \cdot 10^{11} \frac{dyn \cdot cm}{sek^2}$. 7. Density $c = 2.7 \cdot 10^{11} \frac{dyn \cdot cm}{sek^2}$.
- 7. Density $\rho = 2.7 \text{ g/cm}^3$.

(26)





From Eq. (1) $R = \frac{D}{d\varepsilon/dt} = 28 \cdot 10^{-4} cm$ and from Eq. (26) $\omega = 2.35 \cdot 10^8 s^{-1}$ or $f = \omega/2\pi = 0.374 \cdot 10^8 s^{-1}$ which corresponds to period of oscillations $T = \frac{1}{f} = 2.672 \cdot 10^{-8} s$. Then the space period of cell-structures in region *AB* equals: $\lambda = T \cdot U_{imp} = 2.672 \cdot 10^{-8} s \cdot 3.35 \cdot 10^4 cm/s = 8.95 \cdot 10^{-4} cm$. The obtained value for space period of oscillations coincides with the dimensions of fault-structures shown in Fig. 10*a*. *Region CD*

1. Impact velocity $U_{imp} = 653.7$ m/s.

2. Velocity variance D = 52 m/s.

- 3. Velocity of plastic front $C_p = 5.66 \cdot 10^5 \text{ cm/s}$.
- 4. Longitudinal sound velocity $C_l = 6.387 \cdot 10^5 \text{ cm/s}.$
- 5. Strain rate dε/dt = 5 ⋅ 10⁶ s⁻¹.
 6. Shear modulus μ = 2.7 ⋅ 10¹¹ dyn ⋅ cm/sek².
 7. Density ρ = 2.7 g/cm³. From Eq. (1) R = D/dε/dt = 10.36 ⋅ 10⁻⁴ cm and from Eq. (26) ω = 1.84 ⋅ 10⁸ s⁻¹ or f = ω/2π = 0.29 ⋅ 10⁸ s⁻¹ which corresponds to the time period of oscillations T = 1/f = 2.35 ⋅ 10⁻⁸ s. Then the dimension of fault-structures in region CD equals λ = T ⋅ U_{imp} = 2.35 ⋅ 10⁻⁸ ⋅ 6.637 ⋅ 10⁴ = 47 ⋅ 10⁻⁴ cm. The obtained value for space period of oscillations coincides with the dimensions of fault-structures for region CD shown in Fig. 10c.

6. Conclusions

Shock tests of 1565 aluminum alloy in two schemes of loading reveal the difference in mechanisms and scales of mesostructure formation depending on the scheme of shock loading and strain rate. Formation of fault-structures increases the resistance to high-velocity penetration. At the upper region of impact velocities, 1565 aluminum alloy reveals the increased resistivity to penetration.

Within impact velocity range of 250 - 750 m/s the strength behavior of alloy proves to be opposite – when resistance to penetration increases, the spall strength decreases.

The defect of particle velocity plays a role of a control parameter in the dynamic deformation of the material. It defines the transition from one scale to another.

The transition from one structural scale to another is realized through the excitation of mesoscale oscillations resulted from the back coupling between deformation processes at the macroscale and mesoscale.

The maximum dynamic strength is realized in the impact velocity range where the velocity defect equal to the velocity variance.

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STUDY OF THE DEFORMATION AND FRACTURE OF ZIRCONIUM ALLOYS UNDER DYNAMIC LOADING

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Abstract. The main objective of the present work is the experimental and theoretical investigation of the mechanical properties of the zirconium alloys E110 and E635 in a wide range of strain rates $(10^{-4} \div 3 \cdot 10^3 \text{ c}^{-1})$ and at different temperatures $(20^{\circ}\text{C} \div 350^{\circ}\text{C})$. The strain rate and temperature dependencies of deformation diagrams and strength characteristics under tension and compression have been received using the experimental study. The investigated materials have shown sensitivity to strain rate and temperature. Experimental data have been used to identify some LS-DYNA's material models.

Keywords: experimental investigation, strain rate, model, nuclear energy, dynamics, temperature, flow stress, plastic strain, ultimate strain

1. Introduction

The nuclear industry and energy have special requirements for the materials used. Conventional steels do not pass on safety indicators. Special alloys based on zirconium (Zr) have been developed for this industry. Zirconium is one of the key structural metals in nuclear energy; it is the main component of the alloys used to make the shell of the fuel elements of nuclear reactors. Zirconium alloys have a fairly high corrosion resistance with respect to water and steam and a relatively small cross-section for absorption of thermal neutrons. These alloys favorably differ from pure zirconium in the best mechanical properties. For example, alloy E110 is used as a structural material for the components of the fuel assembly. Currently, this material is the main material for the casings of the fuel rods, spacing grids, and in some cases the guide channels, for PWR (Pressurized water reactor) type reactors. Preservation of high ductility by E110 alloy in combination with corrosion resistance ensures the fuel assemblies' operability to high burnup.

In the new generation reactors, it is assumed that conditions will cause higher stresses in the shells and more intense oxidation processes. In this regard, it is relevant to search for alternative alloys not only for the casings of fuel elements, but also for structural elements of a fuel assembly, such as guide channels, a central pipe, and corners of a rigid frame capable of providing the required fuel resource.

Recently, a multicomponent alloy E635 has been widely used as a material for fuel assemblies of the water-moderated reactor with a capacity of 1000 MW.

Study of the deformation and fracture of zirconium alloys under dynamic loading

During the transport and technological operations such as fuel movement, loading/unloading of fuel, situations may arise that are accompanied by dynamic influences. To obtain reliable estimates of numerical modeling, it is necessary to use deformation models and strength criteria corresponding to the problem being solved. In dynamics problems, it is important to take into account the strain rate influence on the material characteristics. Extensive experimental research is required to build mathematical models describing this effect.

Despite the widespread use of zirconium alloys in nuclear power engineering, as well as the importance of studying the dynamic properties of alloys based on zirconium, there are very little data on this. Investigations of the mechanical characteristics of the metal alloy E110 were carried out in [1]. In this study, the behavior of a zirconium alloy was studied under shock-wave loading conditions. The authors determined the spall strength at strain rates of 10^5 - 10^6 s⁻¹ using laser interferometers VISAR and POV. At shock compression pressures of above 10.6 GPa it was obtained a three-wave structure of the compression pulse. According to the authors, this effect is associated with polymorphic transformations α - ω . In [2] the dynamic characteristics of the MA-15-Ti magnesium alloy were determined using the Kolsky method. Zirconium is a structure modifier in this alloy and it significantly improves physical and mechanical properties. There are few studies [3-7], which are devoted to the study of the dynamic mechanical properties and microstructural features of deformation in the adiabatic shear bands of amorphous zirconium-based alloys at strain rates about 10³ s⁻¹. For the investigated alloys an increase in the strength characteristics with increasing strain rate is noted, microstructural features of deformation are revealed and the mechanisms of formation of adiabatic shear bands are studied. In [8-13] the dynamic properties of ceramics based on zirconium are investigated using the Kolsky method and its modifications. Dynamic diagrams of deformation under a uniaxial stress state, as well as strength and deformation properties under uniaxial strain, were obtained.

The present work is devoted to the determination of the strain rate and temperature dependences of the deformation curves and ultimate plasticity characteristics of E110 and E635 zirconium alloys.

2. Test specimens

Specimens of two zirconium alloys E110 and E635 were subjected to quasistatic and dynamic tests. The chemical composition of these alloys is given in Table 1.

Denotation	Mass content, %						
	Zr	Nb	Sn	Fe	0	impurities	
E110	Base	0.9-1.1	-	0.05	0.1	0.18	
E635	Base	0.9-1.1	1.1-1.5	0.3-0.5	0.1	0.15	

Table 1. The chemical composition of tested alloys

The compression test specimens were in the form of cylinders with dimensions $\emptyset = 16 \text{ mm } L_0 = 8 \text{ mm}$ for static tests and $\emptyset = 10 \text{ mm } L_0 = 5 \text{ mm}$ for dynamic tests. For tensile tests, samples with threaded heads had the dimensions of the working part: $\emptyset = 5 \text{ mm}$, $L_0 = 15 \text{ mm}$ for static tests and $\emptyset = 5 \text{ mm}$, $L_0 = 10 \text{ mm}$ for dynamic tests.

3. Test methods

Static compression and tensile tests of the specimens at temperatures of $+ 20^{\circ}$ C and $+ 350^{\circ}$ C were carried out on a ZwickRoell Kappa 50 DS experimental setup with a maximum loading force of ± 600 kN. The measuring equipment included a class 1 force sensor in accordance with ISO 7500-1 and a high-precision displacement meter built into the movable beam of the

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machine, with an accuracy of positioning of the beam in a predetermined position of not more than $\pm 2 \mu m$. To obtain the elastic modulus *E* of the materials, we used a high-precision high-temperature extensometer RMA-12 / V7-1 (resolution 0.1 μm) installed on the working part of the sample and allowing to determine the elastic modulus at normal and elevated temperatures. The testing machine is equipped with a MAYTEC-HT 080/1 heating device.

Compression and tensile tests in the dynamic range of strain rates $(5 \ 10^2 - 5 \ 10^3 \ s^{-1})$ at temperatures +20°C, +200°C, and +350°C were carried out using the Kolsky (or Split Hopkinson Pressure Bar) method [14] and its modifications [15-17]. The following formulas can be used to calculate stress, strain, and strain rate in a specimen based on recorded pulses in the measuring bars:

$$\sigma_s(t) = \frac{EA}{2A_s^0} \varepsilon_1(t), \tag{1}$$

$$\varepsilon_{s}(t) = \frac{c}{L_{0}} \int_{0}^{t} \varepsilon_{2}(\theta) d\theta, \qquad (2)$$

$$\dot{\varepsilon_{s}}(t) = \frac{c}{L_{0}} \cdot \varepsilon_{2}(t). \qquad (3)$$

Here E – elastic modulus of the measuring bar, A – measuring bar's cross-section area, C – sound speed in the measuring bar, L_0 and A_s^0 – initial length and initial cross-section area of the specimen.

Instead of the $\varepsilon_1(t)$ and $\varepsilon_2(t)$, one of three expressions can be substituted, respectively:

$$\epsilon_{1}(t) = \begin{cases} \epsilon^{I}(t) + \epsilon^{R}(t) + \epsilon^{T}(t) \\ 2 \cdot (\epsilon^{I}(t) + \epsilon^{R}(t)) \\ 2 \cdot \epsilon^{T}(t) \end{cases}$$
(3)

$$- \text{ for strain calculation:} \\ \epsilon_{2}(t) = \begin{cases} \epsilon^{I}(t) - \epsilon^{R}(t) - \epsilon^{T}(t) \\ 2 \cdot (\epsilon^{I}(t) - \epsilon^{T}(t)) \\ -2 \cdot \epsilon^{R}(t) \end{cases}$$
(4)

Further, from the obtained parametric dependences $\sigma_s(t)$, $\varepsilon_s(t)$ and $\dot{\varepsilon}_s(t)$ time is excluded, and a deformation diagram $\sigma_s(\varepsilon_s)$ of a specimen with a known dependence $\dot{\varepsilon}_s(\varepsilon_s)$ is constructed. During the test, using a strain gauge on measuring bars, a loading stress (strain) impulse is recorded. The shape, amplitude, and duration of this impulse are set by choosing the length, material, and velocity of the striker which is accelerated in the barrel of the gas gun. In addition, stress (strain) pulses reflected from the specimen and transmitted through it are recorded, which are the "responses" of the material to the applied load and allow constructing a dynamic diagram of the test specimen.

An experimental setup that implements the SHPB method includes a pneumatic loading device (gas gun with a caliber of 20 mm) with a control system, a complex of measuring and recording equipment, and replaceable sets of bars made of steel or aluminum alloy with a diameter of 20 mm for testing under various conditions. In the present investigation bars made of high-strength steel with a yield strength of about 2000 MPa are used. The bars are fixed and centered in textolite plain bearings, which allow adjustment of their relative position with the help of adjusting elements to ensure alignment of the bars with each other and with the striker. The strain is measured using small-base strain gauges glued to the lateral surface of the bars at a considerable distance from the specimen. Moreover, to compensate for bending vibrations in the bars and increase the amplitude of the useful signal in the working sections, 4 strain gauges connected in series are glued. To study the behavior of materials at elevated temperatures, a miniature tube-type furnace is used. It warms the ends of the measuring bars with a sample located between them. An XC thermocouple welded to the side

surface of the sample was used to control the temperature of the specimen. At test temperatures up to +350°C any correction of the formulas and the method of processing experimental information was not performed, since at such temperatures, there are no noticeable changes in the elastic characteristics of the material of the bars (elastic wave velocity and elastic modulus).

4. Test results

The deformation diagrams at static compression and tension of the E110 and E635 alloys were constructed at temperatures $T = 20^{\circ}$ C and 350°C. Three samples were tested at each temperature, and the results were averaged.

Dynamic tests at high strain rate tension were carried out using the Nicholas scheme [16]. Four conditions were implemented in terms of strain rate: 1000, 1500, 2000, and 2800 s⁻¹ as well as three conditions in terms of temperature: +20, +200, and $+350^{\circ}$ C. In each loading condition, five specimens were tested to determine the scatter characteristics of the experimental data.

The compression schemes were used to obtain strain curves. The tensile schemes were used to determine the ultimate fracture characteristics.

Figure 1 illustrates the effect of the strain rate on the strain curves of the E110 alloy. Dynamic curves have larger initial yield strength and the angle of the plastic part of the curve. In the strain rate range from 850 to 2400 s⁻¹, the effect of strain rate hardening is weakly expressed.



Fig. 1. Strain rate influence on strain curves. E110 alloy

The left side of Fig. 2 illustrates the effect of temperature on the strain curves of E110 alloy. Dashed lines are static curves. The solid lines are the dynamic curves, obtained at strain rate \sim 1500 s⁻¹. The corresponding temperatures in Celsius degree are shown next to the each line. The right part of Fig. 2 shows slices of curves at different plastic strain levels (the corresponding plastic strain values are shown next to the each line). Dashed lines are static curves. The solid lines are the dynamic curves. If we analyze the results, it turns out that in the static region the influence of temperature is more pronounced. This can be seen by the slope of the curves on the right part of Fig. 2.

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Figure 3 shows the deformation curves of the E635 alloy at different strain rates. It can be noted that this material has a higher resistance to deformation than the E110 alloy.

Figure 4 illustrates the effect of temperature on E635. The same effect is observed as in the case of alloy E110.



Fig. 2. Temperature influence on strain curves. E110 alloy



Fig. 3. Strain rate influence on strain curves. E635 alloy



Fig. 4. Temperature influence on strain curves. E635 alloy

Study of the deformation and fracture of zirconium alloys under dynamic loading

Based on the shape of the specimens fractured in tension the ultimate plastic strains were determined using the formula:

$$\varepsilon_p^f = ln \frac{1}{1 - \frac{D_0^2 - D^2}{D_0^2}}.$$
(5)

Here D_0 – initial diameter of the specimen's cross section, D – diameter of the fractured specimen's cross-section in the neck.

The obtained data will be illustrated in the section «Model identification».

5. Model identification

To use in the numerical simulation, the obtained data must be turned into a mathematical model. So, the experimental surfaces were approximated by analytical functions.

The Johnson-Cook model is widely used to describe the dynamic behavior of viscoplastic materials. The mathematical formulation for the dependence of the radius of the yield surface on the strain, strain rate, and the temperature is formulated as follows [18,19]:

$$\sigma = (A + B \cdot \varepsilon_p^n) (1 + C \cdot \ln \dot{\varepsilon}_p^*) (1 - T^{*m}).$$
(6)
Here $T^* = \frac{T - T_0}{T_m - T_0}$, ε_p – equivalent plastic strain, $\dot{\varepsilon}_p^* = \dot{\varepsilon}_p / \dot{\varepsilon}_0$ – dimensionless plastic

strain rate, $\dot{\varepsilon}_0 = 1.0 \text{ s}^{-1}$, T_0 and T_m – room (or reference) temperature and melting temperature respectively. Five material constants are determined empirically: *A*, *B*, *n*, *C* μ *m*.

In addition to the classical, linear in the logarithm of strain rate multiplier

 $1 + C \cdot \ln(\dot{\varepsilon}^*),$ (7) other options exist to take into account the influence of the strain rate on the flow stress: - model of Hub-Kang [20]:

$$1 + C \cdot \ln(\dot{\varepsilon}^{*}) + C_{2} \cdot \ln(\dot{\varepsilon}^{*})^{2}, \qquad (8)$$

$$- \text{ model of Cowper-Symonds [21]:}$$

$$1 + \left(\frac{\dot{\varepsilon}^{*}}{c}\right)^{\frac{1}{p}}, \qquad (9)$$

$$- \text{ model of Allen-Rule-Jones [22]:}$$

 $(\dot{\varepsilon}^*)^C$.

Approximation independent material characteristics for E110 and E635 alloys are shown in Table 2.

1 1		
Property	Value	Dimension
Density, p	6600	kg/m ³
Young's modulus, E	95	GPa
Poisson's ratio, v	0.34	
The melting temperature, T _m	2106	K
T ₀	293	K
Specific heat, c _p	0.24	kJ/kg/K

Table 2. E110 and E635 properties

The disadvantage of the model is that the various effects are independent of each other. Thus, due to the multiplicative formulation, the temperature softening is the same for statics and dynamics, which does not allow us to describe the effect obtained earlier.

You can either focus on static data and well describe the effect of temperature in statics. In this case, the dynamic curves at different temperatures are poorly described (left side of Fig. 5). On the other hand, we can approximate dynamic curves well and get a poor description of static temperature softening (right side of Fig. 5).

(10)

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In Figure 5 dotted lines correspond to experimental curves, solid ones – to the mathematical model. Blue color indicates data at room temperature, orange – at temperature 200°C, and red – at temperature 350°C. Parameters of the mathematical model for static and dynamic temperature softening cases are given in Tables 3 and 4.

Table 5. Johnson-Cook parameters. ETTO, focus on state temperature softening						
Α	324	MPa				
В	3684	MPa				
n	1.324					
С	0.032					
m	0.36					

Table 3. Johnson-Cook parameters. E110, focus on static temperature softening

Table 4. Johnson-Cook	parameters. E	E110, focus o	on dynamic ten	perature softening
	•	,	2	

А	325.4	MPa
В	3756	MPa
n	1.34	
С	0.032	
m	0.73	



Fig. 5. E110 data approximation by the Johnson-Cook equation

In addition, the modified Johnson-Cook model was considered [6]: $\sigma = \sigma_A + B \cdot e^{-(\beta_0 - \beta_1 ln\dot{\epsilon})T} + A \cdot \varepsilon^n \cdot e^{-(\alpha_0 - \alpha_1 ln\dot{\epsilon})T}.$ Here σ_A , B, β_0 , β_I , A, n, α_0 , α_I – model's parameters. (11)

This model has more parameters but allows describing more complex effects. It can be seen from Fig. 6 that this model allowed us to approximate the experimental data with sufficient accuracy. Modified Johnson-Cook parameters for E110 and E635 alloys are shown in Table 5.



Fig. 6. Data approximation by the modified Johnson-Cook equation for E110 (left) and E635 (right)

E110	E635	
0	0	MPa
507	730	MPa
0.0014	0.0013	
6.4·10 ⁻⁵	5.9·10 ⁻⁵	
6512	8956	MPa
1.3	1.36	
0.0022	0.0022	
0.00013	6.43·10 ⁻⁵	
	E110 0 507 0.0014 6.4·10 ⁻⁵ 6512 1.3 0.0022 0.00013	$\begin{array}{c c c c c c c c c c c c c c c c c c c $

The obtained strain rate and temperature dependence of the ultimate plastic strain were approximated by the model:

$$\varepsilon_p^f = D_1 \cdot (1 + \dot{\varepsilon})^{D_4} \cdot \left(1 + D_5 \cdot \frac{T - T_0}{T_m - T_0}\right).$$
(12)

Parameters of approximation are given in Table 6.

Tabl	e 6	The	ultimate	plastic	strain	approx	imation	narameters
1 401	0.	Inc	unimate	prastic	Suam	uppion	mation	parameters

	E110	E635
D ₁	0.17	0.22
D_4	0.181	0.1
D ₅	5.83	3

Figure 7 illustrates the dependence of the ultimate plastic strain on strain rate and temperature. Markers correspond to experimental data obtained at different temperatures. The solid line corresponds to the mathematical model. It can be noted that the ultimate strain increases slightly with increasing strain rate and significantly increases with temperature rise.

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Fig. 7. Ultimate plastic strain for E110 (left) and E635 (right)

Figure 8 illustrates the approximation of the temperature dependences of the fracture strain for the studied alloys. It can be noted that the E635 alloy is fractured at lower values of plastic strain. The temperature has a greater effect on the ultimate characteristics of the E110 alloy.



Fig. 8. Temperature dependence of ultimate plastic strain for E110 (left) and E635 (right) and its approximations

6. Conclusions

As a result of the investigation of deformation of alloys E110 and E635 under compression and tension in a wide range of strain rates and temperatures from 20°C up to 350°C, mechanical characteristics are obtained in the form of deformation diagrams. It is noted that the mechanical behavior of the investigated alloys is sensitive to the strain rate and temperature. Obtained data is approximated by the modified Johnson-Cook model reasonably well. E635 alloy has a higher resistance to deformation than the E110 alloy but is fractured at lower values of plastic strain. The temperature has a greater effect on the ultimate characteristics of the E110 alloy than on the E635 alloy. As a result of the study, the mathematical models of the deformation and strength criteria are constructed which can be used in the development of digital copies of nuclear engineering designs.

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THE INFLUENCE OF TURMERIC MICROPARTICLES AMOUNT ON THE MECHANICAL AND BIODEGRADATION PROPERTIES OF CORNSTARCH-BASED BIOPLASTIC MATERIAL: FROM BIOPLASTIC LITERATURE REVIEW TO EXPERIMENTS F. Triawan^{1*}, A.B.D. Nandiyanto^{2**}, I.O. Suryani¹, M. Fiandini², B.A. Budiman³

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Abstract. The purpose of this study was to investigate the effects of turmeric microparticles amount on the mechanical and biodegradation properties of cornstarch-based bioplastic material. To produce the bioplastics, several steps were done sequentially: (1) dissolving a mixture of cornstarch, glycerol, and acetic acid in aqueous solution; (2) adding turmeric microparticles with a specific amount (i.e., 0.50; 0.75; 1.00; 1.50% (w/w)); (3) homogenizing the mixture at temperature of 60°C; (4) molding process; and (5) drying process to get a solid bioplastic. Experimental results showed that the addition of turmeric microparticles could change the bioplastics strength as well as its biodegradability, while too much amount of turmeric may result in high strength but low biodegradability.

Keywords: bioplastics, biodegradation, cornstarch, turmeric, mechanical properties

1. Introduction

Plastics have been widely used in many fields of applications (e.g., mulch films, greenhouse, construction materials, packaging material, etc.) because of their low cost, ease of manufacture, versatility, and resistance to water [1]. During the last 10 years, world plastic production has been reported to reach 359 tons in 2018. Amount of plastic waste continues to increase over the years and is considered to cause serious environmental problems. Plastic is mostly made from synthetic polymers (i.e., polypropylene, polystyrene, and poly (vinyl chloride)) derived from petrochemicals, which are difficult to degrade by microbes in the environment [1]. Usually, the degradation of these materials takes time up to 1,000 years to decompose in landfills by breaking the carbon chain [2].

Efforts have been made to overcome the problems arising from plastic waste. However, these efforts create new issues in the environmental and health [2]. The accumulation of plastic waste greatly disrupts the circulation of air to and from the ground because plastic materials generally have high barrier properties to O_2 and CO_2 permeability [3]. Burning plastic waste produces harmful substances such as dioxins, furans, and benzopyrene (a poisonous gas), causing cancer and damage the immune system[4]. In contrast, recycling plastic waste is very expensive and less effective.

To create a sustainable environment and prevent the harmful effects of environmental problems caused by plastic waste, the production of bioplastics has received a lot of attention [5]. Bioplastics are environmentally friendly plastics made from renewable polymer materials or biomass such as starch, vegetable oils, fruit waste, lignin, cellulose, and animal origin materials such as proteins and lipids [6]. The resulting bioplastics become biodegradable plastics, which are considered efficient in replacing the use of synthetic plastics. Starch is one of the most promising materials for the fabrication of bioplastics, mainly because it is easily degraded, inexpensive, abundant, and renewable [7].

The fabrication of starch-based bioplastics has been successful and widely developed. The most recent reports on the synthesis of bioplastics are represented in Table 1. However, when using bioplastic from starch without a reinforcing agent, the resulting bioplastic interactions still have disadvantages, such as not being resistant to water and low mechanical properties [8]. To overcome this problem, in the fabrication of bioplastics, other biopolymer additives are needed to improve the mechanical properties of the bioplastic. Reporting on bioplastics with additional reinforcing agents is essential for understanding the further development of bioplastics, including knowing what additives are compatible with pure bioplastics. Table 1 shows the results of bioplastic synthesis researches that have been done previously. Those research topics are usually focusing on enhancing the mechanical properties of the bioplastics.

One of the potential reinforcing agents is turmeric. Turmeric also gives an advantage in providing a yellow color to the final product. Here, the purpose of this study was to investigate the effect of the number of turmeric microparticles on the mechanical properties and biodegradation of cornstarch-based bioplastics. Turmeric was chosen as an additional reinforcing agent because there is an antimicrobial activity potential as an antimicrobial plastic and its water-insoluble nature resulting in a water-resistant bioplastic [9]. The addition of turmeric microparticles may improve the mechanical properties because it has extraordinary interfacial interactions in the polymer. In addition, bioplastic fabrication with turmeric as a reinforcing agent has not been widely reported. This information is critical to bring benefits to the further development of bioplastic.

2. Material and Method

Preparation of bioplastic. In this study, we used micron-sized cornstarch as a basis for the bioplastic materials. Several chemicals used in the experiment were acetic acid (25%), glycerol (95%), and distilled water. For the reinforcing agent, turmeric (*Curcuma Litonga*) was sliced, washed with water to remove impurities, and dried to remove water at 60°C using an electric furnace at atmospheric pressure. Then, the dried turmeric was put into a saw-milling process to transform it into powder form with a rotation speed at 18,000 rpm. To get a homogenous milling process, the saw-milling process was done three times, in which each milling has proceeded in 5 minutes. Detailed information about the preparation of curcumin and the apparatuses are explained in our previous studies [10,11].

Fabrication of bioplastics with the addition of turmeric was done through the following steps. In the initial stage, cornstarch, acetic acid, and glycerol were mixed with a composition ratio of 3:1:3. Then, the mixture was added specific size of turmeric powder 0.50; 0.75; 1.00; and 1.50% (w/w), and stirred manually until homogeneous. Simultaneously, with the manual mixing process and process gelatinization, the mixture was heated at 60°C for 30 minutes using an electrical heater to obtain a viscous product. The viscous product was molded and dried at room temperature for more than 24 hours until it forms a solid yellow film.
Table 1. Reports	on the synthesis of biopiasi		
Type of	Raw material	Results	Ref.
carbohydrate			
Cassava starch	Cassava starch, kaolin,	The bioplastic with addition kaolin	[12]
	and metakaolin	decreases young's modulus. However,	
		bioplastic with the addition metakaolin	
		increases Young's modulus from 19 to	
		25 MPa.	
	Fresh tilapia bones,	The best bioplastic with addition 2%	[13]
	modified tapioca flour,	chitosan and 5% gelatin concentration	
	chitosan, gelatin, 6%	with value tensile strength 19,05 MPa,	
	hydrochloric acid (HCl),	percent elongation 28.33% and	
	1% acetic acid	degraded in the soil for 14 days	
	(CH ₃ COOH), glycerol,		
	distilled water		
	Potassium persulfate	Compared without cellulose, bioplastic	[14]
	(KPS), palmitic acid,	with cellulose had the good tensile	
	and dimethyl sulfoxide	strength	
	(DMSO), Ferrous		
	ammonium sulfate		
	(FAS) hexahydrate,		
	cellulose, tapioca starch,		
	and citric acid		
	Cassava starch,	The bioplastic with the addition of 4%	[15]
	precipitated calcium	PCC optimizes tensile strength and	
	carbonate (PCC), and	increases thermal stability	
	glycerol		
	Cassava starch, sugar	6% of SPF gave best tensile strength	[16]
	palm fiber (SPF),	and young's modulus up to 20.7 and	
	distilled water, and	1114.6 MPa	
	plasticizer		
	Tapioca starch, NaNO ₃ ,	The concentration of 15% GO has the	[17]
	H_2SO_4 , KMnO ₄ ,	highest tensile strength of 3.92 MPa,	
	distilled water, H_2O_2 ,	elongation of 13.22%, and modulus	
	and glycerol	young of 29.66 MPa.	51.01
Sago starch	Chicken feather,	The addition of the reinforcement (lime	[18]
	Natrium Hydroxide	juice) effectively improve the tensile	
	(NaOH), Chloride Acid	strength	
	(HCI), sago starch,		
	glycerol, and lime juice		F101
	Sago starch, glycerol,	The concentration of CMF 15% has the	[19]
	NaOH, KOH, NaCl O_2 ,	highest tensile strength of 10,23 MPa.	
	acetic acid, and H_2SO_4	However, compared bioplastic with	
		CMF, bioplastic without CMF was	
XX71 (1 (more rapidly degraded	[00]
wheat gluten	wheat gluten, Fish	Compared without fish, bioplastic with	[20]
	waste (<i>Lates calcalifer</i>),	iisn nad nign tensile strength (6.5-	
	water, and grycerol	(.5 Fa) and good dispersion.	

Table 1. Reports on the synthesis of bioplastic

Table 1. (continue) Reports on the synthesis of bioplastic

	b) Reports on the synthesis	or orophastic	
Type of	Raw material	Results	Ref.
carbohydrate			
Cornstarch	Biopolymer	The addition of natural fibers (cotton,	[21]
	(cornstarch), glycerol,	jute, hair, and wool) increase tensile	
	de-ionized water, 5%	strength	
	acetic acid solution,		
	natural fibers like		
	cotton, jute, hair, and		
	wool.		
	Cornstarch, rice straw,	The addition of the reinforcement	[22]
	sodium hydroxide,	(cellulose nanocrystal) improves the	
	sodium hypochlorite,	tensile strength and young's modulus.	
	cellulose nanocrystal	However, the percent elongation of	
	(CNC), glycerol,	bioplastic decreases	
	sulfuric, acid, and acetic		
	acid		
	Cornstarch, glycerol,	The bioplastic tensile strength was	[23]
	white vinegar, titanium	increased from 3.55 to 3.95 MPa with	
	dioxide nanoparticles	the addition of TiO ₂ . It also increases	
	(TiO ₂) as reinforcing	the decomposition temperature with	
	agents	homogeneous morphology and viewer	
		cracks.	
	cornstarch (CS),	Compared without eggshell, bioplastic	[24]
	distilled water, eggshell	with eggshell improved the tensile	
	powder (ESP), and	strength, elongation et break, and water	
	glycerol	vapor	
	Cornstarch, polylactide,	Cornstarch decreased the thermal	[25]
	lysine diisocyanato,	stability of bioplastic. LDI increased	
	(LDI), and glycerol	the temperature of thermal degradation	
		(compared to bioplastic without LDI)	
		and decreased biodegradability. LDI	
		allowed a homogeneous surface	
		morphology	
Banana starch	Banana starch was	Bioplastics with the addition of 3%	[26]
	derived from green	ZnO increase the tensile strength up to	
	banana, glycerol	36 MPa. On the contrary, an elongation	
	purchased, chitosan, de-	and swelling percentage decrease with	
	acetylation, ZnO	increasing concentration of ZnO	
	powder, NaOH, glacial		
	acetic acid		
Cassava peel	Cassava peel, sorbitol,	MCC increases the tensile strength of	[27]
	and microcrystalline	bioplastic. It was reported that the	
	cellulose (MCC)	addition of 6% MCC has the highest	
		tensile strength. However, it decreased	
		elongation, density, and water	
		absorption.	

		of otoplastic	D.C
Type of	Raw material	Results	Ref.
carbohydrate			
Potato starch	Sodium hypochlorite,	Compared with bioplastics chitosan,	[28]
	glycerol, acetic acid	bioplastic with eggshell improved	
	chitosan (shrimp shells)	tensile strength and good	
	potato starch, and	biodegradability	
	eggshells		
Bamboo	Bamboo	Tensile strength of bioplastics with	[29]
	(Dendrocalamus asper),	optimal conditions at 5% of	
	cellulose, toluene-	microfibrils and 3% of potassium	
	alcohol solvent.	chloride	
	potassium chloride, and		
	hydrogen peroxide		
Tamarind seed	Tamarind seed	Bioplastic with the addition of	[30]
Tamarina seed	microcrystalline	Microcrystalline cellulose optimization	[50]
	cellulose ethanol	machanical properties	
	NaOH and glugarel	meenamear properties	
	NaOII, and gryceroi		
Jackfruit seed	Jackfruit seeds, Cocoa	The ratio of bioplastic starch with the	[31]
starch	pod husk distilled water	addition of microcrystalline cellulose to	[0-]
(Artocarpus	(H ₂ O) Sodium	have the best mechanical properties is	
hotoronhyllus)	Hydroxide (NaOH)	8.2 It possesses 0.637 MPa tensile	
neieropnyiius)	Sodium Humochlorita	strength and an extension of 7 04%	
	(NaOCI) A sid Chlorida	strength and an extension of 7.04%.	
	(NaOCI), Acid Chioride		
	(HCI)		5001
Avocado seed	Avocado seed,	The ratio of bioplastic avocado seeds	[32]
	microcrystalline	with the addition of microcrystalline to	
	cellulose, glycerol,	have the best mechanical properties is	
	hydrochloric acid,	7:3. It possesses 2.74 MPa tensile	
	potassium hydroxide,	strength and an extension of 3.61%.	
	Sodium hypochlorite,	The Bioplastic surface morphology is	
	sugar palm fibers, and	uneven and hollow	
	water		
Durian seed	Durian seeds, ultrapure	The mechanical properties test result of	[33]
	water, chitosan, acetic	bioplastic from durian seeds are still far	
	acid (0.10%) , and lime	from the standard when it is compared	
	water	with the moderate bioplastic. It has a	
		tensile strength of 0.1158 MPa while	
		the standard has an elongation of	
		2.1875% and Young's modulus of	
		4.1515 MPa.	

Table 1. (continue) Reports on the synthesis of bioplastic

Physicochemical properties. The prepared bioplastic was characterized using a Digital Microscope (BXAW-AX-BC, China) to analyze the chemical structure and particle morphology, respectively. To support the analysis, we conducted characterizations using a Fourier Transform infrared (FTIR-4600, Jasco Corp., Japan) to the prepared bioplastic.

Mechanical properties. The compression test was performed using 313 Family Universal Test Machine with a loading rate of 1 mm/sec at 24°C and humidity of 10%. The samples were tested for the compression test having a variable dimension, as shown in

(1)

Table 2. Before the test was carried out, the samples were measured using a Vernier caliper, and the compression plate was coated with Vaseline jelly as the lubricant to reduce the friction effect. Data collected from compression tests such as the load-displacement curves and the stress-strain curves were evaluated from each sample to analyze its mechanical properties, i.e. Young's modulus and ultimate strength.

Bioplastic with specific amount turmeric, % (w/w)	Dimension, cm
0.50	2×2×0.6
0.75	2×2×0.6
1.00	1.5×1.5×0.5
1.50	1.5×1.5×0.5

1 auto 2. Samples unitensity	Table 2	Sampl	es di	mensio
------------------------------	---------	-------	-------	--------

The following formula can be used to process the raw data from the compression test for further analyses:

(1) Ultimate compressive strength (S_{ucs}) is defined as the maximum force that can be held in the sample when being compressed before the material is broken. The ultimate compression strength can be calculated by dividing maximum stress (F_M ; N) with the cross-section area of the specimen (A; mm²)) as shown in Eq. (1) [34].

$$S_{ucs} = \frac{F_M}{A}.$$
(2) Young's modulus (E) is a mechanical property that measures the stiffness of elements of the stiffness of the stiff

(2) Young's modulus (E) is a mechanical property that measures the stiffness of elastic deformation of the specimen under a given load. Young's modulus can be obtained from the slope of the stress-strain since defines the relationship between stress (σ) and strain (ε) of material deformation in the linear elasticity regime. Young's modulus can be determined using Eq. (2) [34].

$$E = \frac{\sigma_2 - \sigma_1}{\varepsilon_2 - \varepsilon_1},$$
(2)

where ε_1 and ε_2 are the condition of relative elongation, and σ_1 and σ_2 are the stress that occurs at ε_1 and ε_2 , respectively. The method of observing the slope-strain of the sample for defining Young's modulus is adopted since the slope of the sample can be directly observed as a function of the material deformation (strain).

Biodegradability. The biodegradability tests were conducted by slicing the prepared bioplastics with sizes of about $5 \times 5 \times 5$ mm and then immersing them into ultrapure water. The weight losses of the sample were measure at the interval time of two days. In line with this test, during the immersing process, it was also visually observed the change of color. Detailed information about the biodegradability test is reported in our previous study [35].

3. Results and Discussion

Figure 1 is a photograph of a bioplastic fabrication with the addition of the amount of turmeric. The addition of turmeric gives the bioplastic end product its yellow color. The amount of turmeric added affects the physical condition of the bioplastic, where the bioplastic with a higher amount of turmeric causes the bioplastic to crack (see Figs. 1 (a) 0.50; (b) 0.75; (c) 1.00; and (d) 1.50% (w/w)).

To clarify the bioplastic structure, a microscope analysis was conducted (See Fig. 2). The results in Figs. 2(a) and (b) are the appearances of the micron-sized cornstarch and turmeric powder that has been prepared. Micron-sized cornstarch is a white crystal, solid and dense. Turmeric powder is a yellow color, heterogeneous surface, and agglomerate. Figure 2(c), (d), (e), and (f) are bioplastics with addition of specific amount of turmeric of 0.50; 0.75; 1.00; and 1.50% (w/w), respectively. Bioplastics with the addition of a higher amount of turmeric have a more heterogeneous surface and agglomerates, making them more brittle and

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stiffer. Figure 2(g) is the appearance of the bioplastic after being immersed for two weeks in water. The color of the bioplastic starts to change from yellow to brownish-yellow. It can be seen that after two weeks of immersion, cracks are found due to the swelling phenomenon. Figure 2(h) is the appearance of the bioplastic after being immersed for four weeks in the water in which fungi grow significantly.



Fig. 1. Photograph image of cornstarch-based bioplastics with the addition specific amount turmeric (a) 0.50; (b) 0.75; (c) 1.00; and (d) 1.50% (w/w)



Fig. 2. Microscope image of sample: (a) micro-sized cornstarch, (b) agglomerated turmeric powder, (c-f) bioplastic with specific amount turmeric ((c) 0.50; (d) 0.75; (e) 1.00; and (e) 1.50% (w/w)), (g) bioplastics after two weeks immerged in water and (h) fungi bioplastic after four weeks immerged in water

To confirm the phenomenon during the immersion process, Fig. 3 shows the results of the FTIR analysis of as-prepared bioplastics, bioplastics immersed for two weeks in water, and the surface of the bioplastic samples immersed for four weeks. Data were then compared with the standard FTIR analysis [36]. The as-prepared bioplastic results were identified at wavelengths 1022, 1647, and 3280 cm⁻¹. A comparison of FTIR peaks for bioplastics before and after two weeks of immersion in water confirms that biodegradability in water is simply a dilution of the outer components of the bioplastic. The reaction between water and bioplastics involves a dilution process and does not interfere with complicated reactions. We also found that in the FTIR spectra of bioplastics after four weeks of immersion, the absorption peak

experienced a decrease in intensity, indicating degradation that changed the chemical structure of bioplastics due to fungal activity.



Fig. 3. FTIR analysis results of as-prepared bioplastic, 2-week immerged bioplastic in water, and fungus on the 4-week immerged sample

A biodegradability test of bioplastic samples with different turmeric amounts was carried out by immersion method [35]. It was evaluated by analyzing the mass of the bioplastics as a function of days. Table 3 shows the results of the bioplastic reduction performed for two weeks. The analysis showed that the sample with 0.50% (w/w) of turmeric had the best biodegradability, which was indicated by a weight loss of 86% for two weeks. The possible weight loss during 2-week immersion is because the bioplastics' outer surfaces were diluted in water, which was confirmed by the identical FTIR patterns. This result is different for 2-week immersion bioplastic, in which the mass loss was followed by the appearance of fungus (see Fig. 2(h)) and fungus chemical structure (see Fig. 3). The present bioplastics were made from cornstarch, making microorganisms to break the polymer chain easily inside the bioplastic shower than that of bioplastic made from starch without additional curcumin [36]. The main reason is that the curcumin creates an antimicrobial agent, slowing the growth of microbes in degrading the bioplastic.

Figure 4 is a two-dimensional illustration model of particle crack during mechanical testing. The blue square and yellow circle represent the cornstarch and turmeric particle, respectively. The amount of turmeric added to the bioplastic fabrication process directly affects the mechanical and physical properties of the bioplastic. Due to the nature of a crack, the initiated crack propagates toward the turmeric particles because of the relatively low stiffness than cornstarch (see Fig. 4(a)) [38]. Furthermore, the bonding between cornstarch and turmeric is relatively low and easy to break [39]. This means the addition of turmeric particles are quite a lot, a polymerization between turmeric particles might occur, resulting in a higher stiffness of polymerized turmeric particles (see Fig. 4(c)). As a consequence, the initiated crack tends to avoid the polymerized turmeric particles. To confirm these phenomena, compressive test for different turmeric amount was conducted.

Table 3. Weight loss bioplastics with the addition of a specific amount of turmeric during the immersion process

0.50%	Days	Initial	Initial	Mass after	Mass loss,	Decay
(w/w)	-	Dimension,	mass,	Immersion,	wt%	dimension,
		cm^2	g	g		g/cm ²
	1	1.316	0.150	0.113	24	0.030
	2	1.311	0.093	0.043	55	0.039
	4	1.120	0.107	0.037	66	0.063
	6	1.254	0.133	0.040	71	0.075
	8	1.181	0.153	0.040	74	0.096
	10	1.283	0.143	0.027	81	0.092
	14	1.460	0.143	0.020	86	0.088
0.75%	Days	Initial	Initial	Mass after	Mass loss,	Decay
(w/w)		Dimension,	mass,	Immersion,	wt%	dimension,
		cm ²	g	g		g/cm ²
	1	1.089	0.130	0.087	33	0.040
	2	1.364	0.127	0.077	40	0.039
	4	1.203	0.140	0.067	53	0.070
	6	1.071	0.147	0.057	61	0.085
	8	1.214	0.133	0.050	63	0.069
	10	0.939	0.107	0.037	66	0.075
	14	1.145	0.0133	0.037	73	0.086
1.00%	Days	Initial	Initial	Mass after	Mass loss,	Decay
(w/w)		Dimension,	mass,	Immersion,	wt%	dimension,
		cm ²	g	g		g/cm ²
	1	1.106	0.147	0.090	39	0.052
	2	1.146	0.143	0.080	44	0.055
	4	0.887	0.127	0.063	50	0.071
	6	1.070	0.133	0.053	60	0.076
	8	1.038	0.140	0.053	62	0.085
	10	1.103	0.153	0.053	65	0.095
	14	1.101	0.143	0.043	70	0.093
1.50%	Days	Initial	Initial	Mass after	Mass loss,	Decay
(w/w)		Dimension,	mass,	Immersion,	wt%	dimension,
		cm ²	g	g		g/cm ²
	1	1.378	0.137	0.103	24	0.025
	2	1.006	0.120	0.063	48	0.065
	4	1.192	0.110	0.047	57	0.057
	6	1.168	0.127	0.047	63	0.072
	8	1.276	0.123	0.043	65	0.063
	10	1.433	0.130	0.043	67	0.061
	14	1.249	0.130	0.040	69	0.075



Fig. 4. Illustration progression cracking of bioplastic for (a) low density of turmeric, (b) high density of turmeric, and (c) high density of turmeric with polymerization

Figure 5 shows the plot of stress-strain data of the bioplastic sample from the compression test. Refer to Fig. 4, it can be observed that the stress-strain curve of each sample shows a similar trend by showing the elastic deformation region and followed by the ultimate stress (peak stress). The observation will be focused on the ultimate strength as it represents the maximum compression force per unit cross-section area that the sample can survive before breaking up.

To observe the ultimate strength of each sample, the stress-strain plot was particularly limited to the strain of 0.6 and stress of 2250 kPa, as presented in Fig. 6. The ultimate strength values can be then determined as shown in Table 4. The ultimate strength values of samples of 0.50; 0.75; and 1.00% (w/w) were 1059.0; 941.2; and 375.8 kPa, respectively, showing a decreasing trend of strength with increasing turmeric addition. It decreased because the turmeric particle has low stiffness and low bonding strength with cornstarch. As a result, it fastens the crack propagation and resulting in lower compressive strength. However, sample 1.50% (w/w) shows a different behavior of having the ultimate strength of 1957.0 kPa. It might be due to the high turmeric content in the material, which increased the potency of turmeric particles to do the polymerization process (see Fig. 4(c)), causing a higher stiffness. The high stiffness can resist crack propagation inside the bioplastics. This behavior was then confirmed by observing Young's moduli values of each bioplastic sample under compressive load.



Fig. 6. Stress vs strain of bioplastic samples limited at strain 0.6 and 2250 kPa, respectively

Bioplastic with the addition of specific amount turmeric, %	Ultimate strength,
(w/w)	kPa
0.50	1059.0
0.75	941.2
1.00	375.8
1.50	1957.0

Table 4. Ultimate strength of bioplastic samples

The amount of turmeric affects the stiffness of the sample as the higher turmeric amount may lower the intermolecular bonding that results in a heterogeneous sample structure. It causes the stiffness of the material to decrease. This is related to fiber interaction [40] and polymerization [35]. As the result, the measured Young's modulus decreased with increasing turmeric content. These phenomena are shown in Fig. 7, in which the slope of the stress-strain curve of each sample represented Young's modulus. Based on the plot, Young's moduli of bioplastic samples of 0.50; 0.75; and 1.00% (w/w) were concluded to be 13090, 13000, and 7500 kPa, respectively (see Table 5). However, the bioplastic sample with a turmeric amount of 1.50% (w/w) showed a different trend of having two peaks. It may be correlated with the polymerization of between turmeric particles in the sample (see Fig. 4(c)), therefore the rupture characteristics affect the instability during the compression test including the stress-strain curves [41]. Hence, the stress-strain curve showed different trends of having two peaks of the slope.



Fig. 7. Slope of stress-strain curves vs. strain of bioplastic specimens

The influence of turmeric microparticles amount on the mechanical and biodegradation properties of...

Bioplastic with specific amount turmeric,	Young's Modulus,
% (w/w)	kPa
0.50	13090
0.75	13000
1.00	7500
1.50	22083

Table 5. Ultimate strength of bioplastic samples

5. Conclusion

The present work investigated biodegradability and the mechanical properties of cornstarchbased bioplastic materials by incorporating the effect of turmeric microparticles number. Based on FTIR analysis, the bioplastic soaked in water for two weeks does not demonstrate any chemical reactions, which means the dissolving process mainly causes the loss of bioplastic weight. In contrast, the bioplastic left for four weeks shows a chemical reaction caused by fungi activity. From the compressive test results, it was revealed that, for turmeric of from 0.50 to 1.00% (w/w), increasing the turmeric amount resulted in decreasing the ultimate strength value. This was likely due to the bonding between cornstarch and turmeric particles relatively weak. Furthermore, the low Young' modulus was recorded as the number of turmeric particles is high. It indicates the turmeric particles has lower rigidity than the cornstarch matrix. Due to the nature of the cracks, which always propagate to particles having lower rigidity, the bioplastic will crack more easily for higher turmeric particles. Thus, in the range of turmeric of 0.50 to 1.00% (w/w), the highest ultimate strength and highest Young's modulus of bioplastic sample were achieved by sample 0.50 (w/w) i.e. 1059 and 13090 kPa, respectively. However, different phenomena appeared for turmeric of 1.50%, in which the ultimate strength and Young's modulus drastically increase i.e. 1957 and 22083 kPa, respectively. The turmeric particles are sufficient to create polymerization which causes the rigidity of turmeric particles to increase significantly. Thus, the crack propagates slowly in the bioplastic. The determination of turmeric amount in creating the cornstarch-based bioplastic is essential to assure the mechanical properties and biodegradability are as designed.

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SIMULATION OF INVERSE HALL-PETCH RELATION IN NANOCRYSTALLINE CERAMICS BY DISCRETE DISLOCATION DYNAMICS METHOD

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Abstract. A theoretical model of plastic deformation of nanocrystalline ceramics in the region of small grain sizes is proposed. In the framework of the model, deformation is described as the combined action of grain boundary sliding and emission of lattice dislocations from triple junctions of grain boundaries. Using the method of discrete dislocation dynamics we obtained an inverse Hall-Petch relation, which qualitatively coincides with the experimentally measured dependences of microhardness in nanocrystalline ceramics with extremely small grain sizes.

Keywords: discrete dislocation dynamics, inverse Hall-Petch relation, ceramics, yield stress, hardness

1. Introduction

The high strength and hardness of nanocrystalline ceramics make them good candidates for use in various industries, including electronics, optics, and power engineering [1-6]. Usually, the microhardness of ceramics obeys the Hall-Petch relation, which predicts a linear dependence between microhardness and the inverse square root of the grain size [7-9]. At the same time, several research groups [10-16] have demonstrated an inverse Hall-Petch relation (i.e., a decrease in microhardness with a decrease in grain size) in various nanocrystalline ceramics at grain sizes below a certain critical value. At the same time, the authors of Refs. [17,18] recently succeeded in synthesizing superstrong nanocrystalline MgAl₂O4 and ZnAl₂O₄ ceramics, which demonstrated the direct Hall-Petch relation down to grain sizes of 7 and 10 nm, respectively. The reason for these contradictory results is not yet clear, and for their explanation, it is necessary to understand the processes of plastic deformation occurring in nanoceramics.

Molecular dynamics simulations [16,19,20] and experiments [16,21] have demonstrated the important role of deformation processes associated with grain boundaries (for example, grain boundary sliding and grain rotations), as well as processes of intragranular dislocation plasticity and formation of shear bands. In these works, a transition was observed from predominantly intragrain plasticity to grain boundary mediated deformation processes with a decrease in the grain size. The processes of plastic deformation in nanocrystalline ceramics, as well as the direct and inverse Hall-Petch relation for such materials, were also studied in theoretical works [12,22,23]. Authors of Refs. [12,22] utilized phenomenological composite models, which do not take into account any physical mechanisms of plastic deformation. In a recent theoretical work [23], the transition from intragranular dislocation plasticity to sliding along grain boundaries was considered. As a result, the authors of [23] were able to explain the existence of both direct and inverse Hall-Petch dependences in nanocrystalline ceramics with very small grain sizes. At the same time, the assumptions of the model [23] about thermally activated sliding along grain boundaries, predicting a significant dependence of the microhardness on the strain rate, could not explain the observed [15] weak dependence of the microhardness on the strain rate in nanocrystalline MgAl₂O₄ ceramics.

At present, there is no universal physically substantiated model explaining the presence of the inverse Hall-Petch relation in nanocrystalline ceramics, together with other experimental data. In this work, we propose a model of plastic deformation of nanocrystalline ceramics realized via grain boundary sliding in combination with the emission of lattice dislocations from the regions of grain boundaries adjacent to triple junctions. To calculate the yield stress within the framework of this model and explain the inverse Hall-Petch relation for nanocrystalline ceramics, we will use the method of discrete dislocation dynamics, which is briefly described in the next section.

2. Discrete dislocation dynamics method: brief description

Discrete dislocation dynamics (DDD) is a common method for describing the motion of dislocations, which makes it possible to clearly track the positions of individual dislocations and calculate the accumulation of plastic deformation in a material. In this work, we propose a simple two-dimensional model, which in the future can be extended to the three-dimensional case in a fairly obvious, albeit time-consuming way. In the framework of two-dimensional DDD, edge dislocations are modeled as point sources of deformation, characterized by the Burgers vector **b**. The dislocations are assumed to be straight and infinitely long in the direction perpendicular to the model plane. The force \mathbf{F} acting on a dislocation is given by the well-known expression (the Peach-Koehler force [24]):

 $\mathbf{F} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \times \boldsymbol{\xi}$,

(1)

(2)

(3)

where σ is the tensor of elastic stresses created by all dislocations and the externally applied load, and ξ is the unit vector specifying the direction of the dislocation line. The dislocation velocity **v** can then be determined using the law of motion [25]:

$$\mathbf{v} = \mathbf{M} \cdot \mathbf{F}$$

where \mathbf{M} is the mobility tensor. In the simple case considered here, when dislocations are able to move only in one slip plane (which is typical for fcc structures), the tensor \mathbf{M} is given by the expression:

$$\mathbf{M} = m_{e} \left(\mathbf{I} - \mathbf{n} \otimes \mathbf{n} \right),$$

where m_g is dislocation mobility constant, **I** is the identity matrix, **n** is the vector normal to the slip plane of the dislocation. The time dependence of the dislocation position $r_i(t)$ in its slip plane is found as a result of the iterative process:

$$r_i(t + \Delta t) = r_i(t) + v_i(t)\Delta t, \qquad (4)$$

where $v_i(t)$ is the dislocation velocity **v** projection on the glide direction and Δt is the time step. Tracking all dislocation positions we can easily calculate the total plastic strain accumulated in the material at any given time.

Within the framework of the DDD approach, two main mechanisms are usually introduced: (1) nucleation of dislocations and (2) annihilation of dislocations. In the twodimensional approach, the nucleation of dislocations is described by randomly placing point dislocation sources of the Frank-Read type. When triggered, such a source generates a pair (dipole) of dislocations of opposite signs, equidistant from the source and spaced from each other at a certain (specified) distance l_s . Nucleation occurs when the effective shear stress at the source exceeds the specified critical value τ_s (source power). The distance l_s is, in fact, the equilibrium distance between two dislocations under the action of shear stress τ_s , and these quantities are related to each other by the known expression:

$$\tau_s = \frac{Gb}{2\pi(1-\nu)} \frac{1}{l_s},\tag{5}$$

where G is the shear modulus and v is Poisson's ratio. Annihilation of dislocations is implemented by removing any pair of dislocations of opposite sign that approach each other at a given (small) distance.

3. Simulation of grain boundary sliding and emission of dislocations from triple junctions of grain boundaries

Commonly the method described above is used to model dislocation plasticity, which is realized via glide of lattice dislocations. However, it is possible to use this method to describe the mechanism of grain boundary sliding. This mechanism is represented (see, for example, [26]), similarly to lattice slip, as the nucleation and slip of grain boundary dislocations along the grain boundary planes. Within the framework of DDD, grain-boundary dislocations are similar to lattice dislocations (except for the magnitude of the Burgers vector).



Fig. 1. A model of grain boundary sliding and emission of lattice dislocations from grain boundary triple junctions

A schematic depiction of the grain boundary deformation model is shown in Fig. 1. Consider a fragment of a nanocrystalline structure under the action of external shear stress. The material is assumed to be elastically isotropic and consists of identical hexagonal grains of size *d*. To simulate grain boundary sliding, we will place the source of grain boundary dislocations on one of the grain boundaries. Since the Burgers vector of grain-boundary dislocations is much smaller than the lattice one, such a source is activated at lower applied stress as compared to the sources of lattice dislocations. Therefore, grain boundary sliding is at first carried out relatively easily until the emitted dislocations begin to accumulate on some obstacle. The main and most important obstacle to the movement of dislocations is the triple junctions of grain boundaries. Their role is especially important in nanocrystalline structures due to the small grain size. In this work, we will not consider the mechanisms of overcoming

barriers by dislocations, i.e., the transfer of plastic shear through a triple junction to neighboring grain boundaries. Consequently, under the action of the applied voltage, the source will successively emit dipoles of grain-boundary dislocations (see Fig. 1), characterized by the Burger's vector, until a sufficient amount of them is accumulated to "lock" the source. Emission and sliding of grain boundary dislocations cause plastic shear along the grain boundary.

As a result of the source's operation, a double pile-up of grain-boundary dislocations is formed at the grain boundary, pressed against the triple junctions. As is known from the theory of dislocations [24], such pile-up is a stress concentrator and the area of the triple junctions are characterized by increased elastic stresses. Consequently, triple junctions can act as sources of heterogeneous nucleation of dislocations, which is regularly observed in molecular dynamics simulations [27,28]. In this work, we will also consider triple junctions as sources of lattice dislocations, activated in the stress field of grain-boundary dislocations pile-ups.

Within the framework of the DDD approach, the process of emission of lattice dislocations from triple joints is simulated by the following method. Near the triple junction where grain-boundary dislocations are accumulated, at a given short distance we place a virtual source of lattice dislocations (see Fig. 1). It is a virtual source in the sense that there is actually no actual Frank-Read source at this point. In reality, a lattice dislocation is emitted as a result of the splitting of the head grain-boundary dislocation of the pile-up. However, such a process is inconvenient to describe within the framework of the DDD formalism. Thus we place an ordinary dislocation source in the vicinity of the triple junction. In this case, the length, and, consequently, the power of the source (see formula (5)), will be determined by the distance to the nearest grain boundary from the dislocation source. The only difference between this source and the standard Frank-Read source is that we do not set a fixed sliding plane for it, but we check it for operation in all possible sliding planes that exist in the material being modeled. As a result of the activation of this source, one of the dislocations remains near the triple junction, and the second goes into the grain body. The dislocation remaining in the triple junction effectively "locks" the source, so the triple junction can emit only one dislocation.

Summing up, the modeled process in this work is presented as follows (Fig. 1). The applied stress activates the source of grain boundary dislocations (marked as \times) in the center of one of the grain boundaries, causing the intergranular slip. Grain-boundary dislocations accumulate at the triple junction, which leads to stress concentration in the vicinity of the triple junction. This, in turn, can lead (if the stress is high enough) to the activation of the source of lattice dislocations (\times) and the nucleation of one lattice dislocation near the triple junction, and the emission of another lattice dislocation into the grain body.

4. Results and discussion

Following the approach outlined in the previous paragraphs, we simulated plastic deformation in a nanocrystalline material using the example of MgAl₂O₄ ceramic bulk material characterized by the following value of parameters. For this, we used the model system shown in Fig. 1 and subjected to shear stress τ . We placed the source of grain-boundary dislocations exactly in the center of the grain boundary and set the distance $l_s = 2$ nm, the Burgers vector of lattice dislocations equal to b = 0.3 nm [23], and grain-boundary dislocations – $b_{gb} = b/10$. The virtual source of lattice dislocations was placed at a distance of 2 nm from the triple junction exactly on the grain boundary line. We defined possible lattice slip systems as follows. We assumed that a grain has six possible slip planes defined by an angle $\varphi = n\pi/3$ (where *n* is an integer) relative to a randomly specified orientation $0 \le \theta < \pi/3$ of the grain itself (relative to the reference coordinate system). Since in this work we are interested in the inverse Hall-Petch dependence, we simulated a material with very small grain size, in which there are no sources of lattice dislocations in the volume of grains (except for virtual sources near triple junctions).

Figure 2 shows the calculated dependences of the plastic shear strain on the applied stress τ for different grain sizes. The dependences clearly show a strain jump corresponding to the moment of emission of a lattice dislocation from a triple junction. Translating shear into tensile deformation, we also calculated the dependence of the conventional tensile yield stress $\sigma_{0,2}$ on the grain size (Fig. 3). Figure 3 clearly demonstrates the inverse Hall-Petch dependence in the range of grain sizes from 10 to 50 nm – an increase in the yield stress with an increase in the grain size.



Fig. 2. Shear strain γ dependence on applied shear stress τ for various grain sizes of nanocrystalline MgAl₂O₄ ceramic



Fig. 3. Yield stress $\sigma_{0,2}$ dependence on the grain size d of nanocrystalline MgAl₂O₄ ceramic

It should be noted that the simplified nature of the model does not allow obtaining realistic absolute values of the yield stress that coincide with the experimental data. While our simulations estimate yield stress at the level of 0.01-0.02G (which for MgAl₂O₄ ceramic with

 $G \approx 100$ GPa gives ~1–2 GPa), the experimental data on microhardness measurements in nanocrystalline ceramics [10-16] reports typical values of $H_v = 20-30$ GPa, which translates (using standard phenomenological relation $H_v = 3\sigma_{0.2}$) to yield stress of the order of 6–10 GPa. So our data significantly underestimate yield stress (microhardness). The discrepancy in absolute values of calculated and measured yield stress is most likely attributed to the lack of certain deformation mechanisms specific to MgAl₂O₄ ceramic in our model. For example, it is possible that the transfer of plastic shear through a triple junction to neighboring grain boundaries, grain rotation, and GB amorphization might play a significant role. Also, choice of model parameters (such as dislocation mobility and source strength) might be improved.

At the same time, the qualitative nature of the dependences coincides with the experimental data on microhardness measurements in nanocrystalline ceramics [10-16]. Further research is planned to improve the proposed model.

5. Conclusion

Thus, in this work, we have proposed a theoretical model of deformation of nanocrystalline ceramics, which describes the inverse Hall-Petch relation in the region of small grain sizes. The model was verified by the method of discrete dislocation dynamics. The results of the model showed a qualitative agreement with the experimental data. We can conclude that grain boundary sliding combined with intragrain plasticity seems to reasonably explain the experimental observations.

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SYNTHESIS OF METALLIC COMPOSITE BASED ON IRON FRAME AND SIC NANOSTRUCTURES AND ITS STRENGTH PROPERTIES

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Abstract. The article discusses a new approach to the synthesis of metallic composite materials based on nanostructuring of a metal frame (on the example of iron) by SiC nanostructures (10-50 nm). Optimal conditions are established for the nano-SiC coating on the porous Fe surface during sequential chemisorption of $Cl_2Si(CH_3)_2$ and CH_4 molecules from the gas phase. The resulting composite possesses enhanced strength in comparison with the best steel samples although the residual porosity (up to 5%) of Fe matrix is still preserved after pressing.

Keywords: composite, metallic framework, iron, disperse phase, SiC, ultimate strength

1. Introduction

One of the crucial tasks of modern materials science is the development of new composites with improved functional properties [1]. The importance of an interdisciplinary approach to this task should be noted [2-4]. The structural organization of matter is one of the key problems of natural science. This is because the questions of the matter organization at different levels are studied by physics, mechanics, chemistry, and biology. Establishing physical and chemical parameters that control the properties of artificially ordered nanostructures materials based on them is one of the most important areas of world research. From the physical mesomechanics point of view, chemical nanostructuring of materials leads to new objects with multi-level organization, which is necessary for a more correct approach to the study (experimental and theoretical) of structural transformation at the nanoscale level [2-6].

Iron- or aluminum-based composites are important materials for a wide range of structural applications. An enhancement of the mechanical properties of iron- or aluminum-based composites can be realized by creating a nanoscale structure with high uniformity and well-formed intergranular boundaries [2,7].

Known metal composites fabrication techniques [1,2] cannot give a uniform distribution of the dispersed phase in the bulk matrix. The lack of uniform distribution prevents the achievement of the maximal mechanical properties of the composite [6].

We have developed a new approach to the synthesis of composites based on the processes of three-dimensional nanostructuring (reinforcement) of the matrix frame with a dispersed nanophase [8-11].

Metal matrix nanostructuring involves the distribution of nano-carbide in the bulk porous matrix. The product is a composite material comprising an iron metallic frame reinforced (permeated) with silicon carbide (SiC)-based nanostructures with improved strength. The purpose of this work was to establish the conditions for obtaining SiC nanolayers on the nanodispersed porous Fe powder surface. In fact, the composite formation process includes 3 main stages:

1. Fabrication of Fe matrix with a pre-defined porosity;

2. Surface modification of prepared porous Fe matrix with SiC (10-50 nm) nanostructures.

3. Pressing and sintering to produce a massive (non-porous) Fe/SiC nanocomposite.

2. Materials and Methods

Chemicals. The chemicals were obtained from commercial suppliers: SiCl₄ (99,6%), (Alfa Aesar), CCl₄, Cl₂Si(CH₃)₂. (Sigma-Aldrich), FeCl₂·4H₂O, NaOH (Merck), and CH₄ (gaseous) (Lengaz).

Methods. The powder phases were identified by powder XRD using Bruker D2 Phaser diffractometer with a cobalt anode.

The morphology of samples was studied with the scanning electron microscope (Zeiss Merlin) operated at 10-15 kV in In-lens, SE2, and EDS modes. The magnifications from 300 up to 600 000 (spatial resolution 1 nm) were used.

The Mössbauer spectra were recorded at the constant acceleration in combination with the use of a multichannel Nuclear Data Instruments ND 60 analyzer. In our work, we used a ⁵⁷Co radiation source that decays to ⁵⁷Fe.

Specific surface (S_{sp}) of the samples were determined using BET model of nitrogen adsorption. From specific surface values S_{sp} , the average size of powder particles can be evaluated according to the equation $d_{av} = 6/(\rho S)$, where ρ is substance density.

The ultimate strength (σ_b) was determined on the AG-50kNXD desktop testing machine (Shimadzu) at the Resource Center for innovative composite materials technologies of St. Petersburg State University.

Iron nanoparticles fabrication. As it is known, with a decrease in grain size, the strength increases while maintaining plasticity. The effect of low-temperature and high-speed superplasticity is manifested, and physical properties changes are observed.

In order to obtain Fe NPs of high dispersion, it is necessary to use the precursors that could be reduced at a possibly lower temperature [1]. So, we selected the way via amorphous iron oxide-hydroxide FeOOH as intermediate.

FeOOH was synthesized by precipitation from $FeSO_4 \cdot 7H_2O$ using NaOH in distilled water.

Final precipitate washed with distilled water and dried at 120°C for 5 h.

Fe nanopowders were obtained by subsequent FeOOH (1 g) reduction in a quartz tube furnace with nichrome heaters at 400°C for 90 min. Hydrogen (\geq 99.99% pure) was used as the reductant. The rate of the H₂ supply was 2–5·10⁻⁶ m³/s. As a result, we produced Fe nanoparticles denoted as [Fe]_aH.

Iron nanoparticles compaction. $[Fe]_aH$ (particle size of 60 nm) was uniaxially compacted in a cylindrical mold (internal diameter 15 mm; the height of the compact 5-7 mm).

Optimized pressing conditions were suggested after pre-experiments: powder weight 9g, height of the resulting sample h = 4.96 mm, diameter = 15 mm, $\rho = 4.60$ g/ml. The pressure of 200 MPa loaded during 60 s, maintained for 180 s, then unloaded during 30 s.

The compacts' density was determined by hydrostatic weighing with an accuracy of 2 %.

These conditions provide Fe samples with 20-30% residual porosity. This is proved to be sufficient for further surface chemical reactions.

ALD deposition of SiC. SiC dispersed phase on Fe was produced by ALD [12-18] in a flow-type reactor. The ALD technique is based on alternating chemical reactions of low molecular weight reagents on the surface. As a result of each reaction cycle, new carbide unit was added chemically bonded to the support. Depending on the number of such cycles, layers of the various thickness are synthesized. The chemical composition of the samples was determined by photocolorimetry for silicon and chemical analysis for carbon, based on burning the sample in oxygen and gas chromatographic determination of carbon in CO and CO_2 .

Stream of dry helium was used both to provide an inert atmosphere and to assist the removal of gaseous by-products from the reactor. The synthesis temperature was 200-500°C.

It's important that when storing, $[Fe]_aH$ is covered by the surface oxide layer of varying thickness. The composition of the oxide layer (usually 3-5 nm thick) is not stable and varies depending on storage conditions and other factors. So, it was necessary to purify Fe surface from the oxide layer before deposition. For this purpose, we used surface standardization. According to the developed approach, at this stage, metallic Fe particles were chlorinated to form =Fe-Cl groups on the surface:

 $[Fe]_{a}H + CCl_{4} \rightarrow [Fe]_{a}-Cl + HCl\uparrow$.

In this way we cleaned the surface from undesired functional groups.

Next, Fe powders (~80 nm) were pressed together with SiC nanostructures and sintered to produce a non-porous composite. Fe/SiC powders uniaxially compacted in a cylindrical mold (internal diameter of 15 mm, the height of the compacts 5-7 mm) at a pressure of up to 500 MPa, holding under pressure for 180 seconds.

Finally, Fe/SiC samples were sintered in a tube furnace. To achieve the lowest porosity, composites were sintered in H_2 atmosphere at 950°C for 2 hours with preheating the press from 700 to 950°C for 1 h.

3. Results and Discussion

TEM images for FeOOH particles are shown in Fig. 1. FeOOH particles showed the presence of aggregates with a length of \leq 50 nm. S_{sp} for FeOOH is found to be 198 m²/g from the nitrogen sorption experiment.



Fig. 1. Electronic microphotographs of FeOOH samples

Comparing the size of iron nanoparticles for FeOOH samples reduced at different temperatures, it follows that an increase in the reduction temperature of FeOOH samples from 400 to 550°C leads to an increase in the size of metallic iron particles.

The effect of reduction conditions on the phase composition, structure, and dispersion of resulting Fe powder was studied. Analysis of Fe powders by Mössbauer spectroscopy after reduction for 90 minutes at a temperature of 400°C and after reduction for 60 minutes in the temperature range of 450-550°C, showed that the samples contain only α -Fe (Fig. 2).



					Se	extets					
#	G(Lorentz.)	A1(r.un.)	A2(r.un.)	A3(r.un.)	Γ1(mm/s)	Γ2(mm/s)	Г3(mm/s)	IS(mm/s)	QS(mm/s)	Heff(mm/s)	%
1	1.000+/- 0.000	-0.067+/- 0.001	-0.049+/- 0.001	-0.027+/- 0.001	0.322+/- 0.005	0.298+/- 0.007	0.307+/- 0.011	0.000+/- 0.001	-0.004+/- 0.002	32.904+/- 0.009	99.0

Fig. 2. Mössbauer spectrum of Fe sample obtained from FeOOH dried at 120°C and reduced by H_2 at 400°C

The experimental specific surface areas and the calculated average sizes of dispersed Fe particles are listed in Table 1. An increase of reduction temperature from 400 to 550°C leads to a decrease in S_{sp} of metallic Fe from 8.4 to 2 m²/g. Further, FeOOH reduction at 400°C for 90 minutes was used for the experiments.

Table 1. Specific surface area and the average size of Fe particles after reduction at different temperatures

Starting material	S_{sp} , m^2/g	Reduction temperature, °C	S_{sp} , m^2/g	d _{av} , nm
FeOOH	150	400	8.4	90
heated at		450	6.6	115
120°C		500	3.7	200
		550	2.1	380

To create a nanostructured material, it is necessary at the first stage to obtain a metal matrix with a certain porosity.

The pressure varied from 50 MPa to 300 MPa. The pressing time ranged from 30 seconds to tens of minutes. The loading and unloading time varied from seconds to minutes.

(1)

(2)

(3)

(4)

(5)

The following mode was selected to get a Fe matrix with residual porosity 20-30%. For Fe NPs, applying a pressure of 200 MPa for 60 seconds, holding under pressure for 180 seconds, unloading for 30 seconds, powder weight -9 g. Residual porosity is required for surface chemical reactions on the pore surface of Fe NPs.

The synthesis of SiC nanostructures on the porous iron matrix surface. SiC nanostructures on the porous Fe matrix surface were ALD-synthesized based on a series of successive surface reactions with functional groups on the surface. An important feature of ALD nanolayers is the absence of nucleation under certain synthetic conditions, which allows tuning the functional properties of the product more finely.

The synthesis included the following sequence of operations:

1. Porous Fe particles (1 g) were exposed to CCl_4 vapors at 350°C to remove the oxide layer (reaction 1).

2. Chlorinated samples underwent direct treatment by vapors of silicon-containing CH_3SiH for attaching silicon-carbon groups to the Fe particles surface (reaction 3).

3. Alternatively, the chlorinated sample was first converted to methylated one by methane treatment at 500°C (reaction 2). After that, the methylated sample reacted with $Cl_2Si(CH_3)_2$ (reaction 4).

 $[Fe]_{a}H + CCl_{4} \rightarrow Fe]_{a}-Cl + HCl\uparrow,$

 $[Fe]_{a}-Cl+CH_{4}\rightarrow [Fe]_{a}-CH_{3}+HCl\uparrow,$

 $[Fe]_a$ -Cl + CH₃SiH \rightarrow $[Fe]_a$ -CH₂SiH + HCl \uparrow ,

 $[Fe]_a-CH_3 + Cl_2Si(CH_3)_2 \rightarrow [Fe]_a-HC = Si(CH_3)_2 + 2HCl\uparrow$,

 $Fe]_{a}-HC=Si(CH_{3})_{2}+Cl_{2}Si(CH_{3})_{2}\rightarrow [Fe]_{a}-HC=Si(CH_{3})_{2}-HC=Si(CH_{3})_{2}+2HCl.$

Reaction (3) resulted in the substitution of Cl by silicon-carbon groups. Since methylsilane is thermally stable up to 400°C, this reaction was performed in the range of 300-400°C. However, in this range, the replacement of Cl with silicon-carbon groups was not effective enough – ca. 40% (according to the Cl content in the product).

At the same time, methylation (reaction 2) and subsequent reaction with $Cl_2Si(CH_3)_2$ is found to give almost 100% replacement.

Based on these results, we further used reaction (4). Chemical analysis of modified Fe suggested that the Si and Cl content reaches a maximum at 400°C. The amounts of reacting silicon and chlorine on the sample remain approximately constant, with the Cl/Si ratio 2.4–2.6. Above 450°C the silicon content significantly decreases. Further increase of SiC nanolayer thickness is performed using reaction (5).

The reaction product comprises the Fe particles surface with silicon-carbon tails $HC=Si(CH_3)_2$ covalently bound to surface $-CH_3$ groups.

As a result of this work, Fe/SiC samples with varied SiC content were synthesized (Table 3).

Sample No.	Cycles number	SiC content (wt%)	Sample composition
1	-	-	100% Fe
2	1	1.5	95.5% Fe + 1.5% SiC
3	2	3	97% Fe + 3% SiC
4	5	8.5	91.5% Fe + 8.5% SiC
5	10	15.5	84.5% Fe+ 15.5% SiC
6	16	25.5	74.5% Fe + 25.5 % SiC

Table 3. Composition of Fe/SiC samples

Figure 3 shows the XRD pattern of sample No. 6 (SiC content 25.5 wt. %) that confirms the presence of α -Fe and SiC peaks.



Fig. 3. XRD pattern of a Fe/SiC (25.5 wt%) sample after heating at 900°C

It is found that in the range of 700-800°C, SiC is in a partially amorphous state, while higher heating temperatures (900°C and more) leads to the formation of polycrystalline SiC. Based on XRD data, the average size of SiC crystallites after heating at 700-800°C is found to be ~ 2 nm, and at 900°C is ~ 6 nm.

Pressing and sintering of iron coated with hardening SiC nanostructures. Bulk nanocrystalline materials are of high interest because their structural and functional properties differ significantly from those of coarse-grained analogues [9,19].

Nanocrystalline materials are usually obtained by powder metallurgy, crystallization from an amorphous state, and severe plastic deformation. Features of nanocrystalline materials (grain size, a significant amount of interfaces, porosity, and other structural defects) depend on the preparation methods and have a significant impact on their properties.

The optimal conditions to achieve the best strength of non-porous compacts were analyzed, namely, the temperature and duration of sintering and pressing, intermediate temperature exposures, and the sintering medium (argon or hydrogen).

The pressure of 0.05 to 1.1 GPa was applied. A further increase in pressure does not lead to a significant increase in the compact density. At pressures of up to 0.5 GPa, the nanopowders compacted much less intensely than coarse particles. The loading time was varied from 1 to 23 minutes, the exposure duration under load ranged from 1 to 3 minutes, the duration of unloading was 2-4 minutes. The results of powder pressing show that loading for more than 15 minutes leads to the absence of cracks in the samples. Increasing the holding time under load from 1 to 3 minutes also leads to similar results.

To achieve the lowest porosity, compacts must be sintered in H_2 at 950°C for 2 hours with preheating of the press from 700 to 950°C for 1 h. This mode of sintering allowed to increase the density of the bulk sample (porosity is reduced to 5%). Sintering at a temperature above 1000°C did not improve the residual sample porosity.

Figure 4 depicts the nanowire formation on the α -Fe NPs surface. A SiC nanolayer of a predetermined thickness is formed on the surface of α -Fe nanoparticles. During the pressing and sintering stages, the pore walls of α -Fe NPs with a SiC nanolayer move towards each other. As a result, the SiC nanolayers are combined, and finally, a SiC nanowire is formed that permeates the entire α -Fe volume as a "frame within a frame" structure.



Fig. 4. Formation of the silicon carbide nanowires in the bulk nanocomposite on α-Fe: a) initial α-Fe with selected pore segment designated as B; b) pore segment on the walls of which the SiC nanolayer grows; c) SiC layers shift during pressing; d) merged SiC in the pore after compaction and sintering

Strength properties of metallic composites based on iron and silicon carbide strengthening nanomodifiers (Fe/SiC). The mechanical properties of nanomaterials depend significantly on the grain size. At the big grain sizes, an increase of the strength and hardness with decreasing grain size is due to the appearance of additional grain boundaries that are obstacles to dislocation motion. For small nanoscale grains, a strength increase is due to the low density of existing dislocations and the difficulty of new dislocations formation.

Strength data of Fe/SiC samples are presented in Fig. 5. For comparison, also the strength properties of the best grades of steel according to [20] are shown.

The ultimate strength of the obtained Fe/SiC composites is comparable to the properties of the best grades of steel, which contain a high percentage of alloying additives. Thus, it is evident that the formation of Fe/SiC composite using the surface structuring is a promising tool for obtaining new-generation composites.



Fig. 5. The ultimate strength of a) Fe-based composites with SiC dispersed phase (this work); b) known steels in comparison with best sample composite

4. Conclusion

The authors offered the structuration of an iron-based metal matrix with carbide nanolayers, which results the composite with a "frame within a frame" structure. A synthesis has been developed of SiC nanolayers on the porous surface of Fe matrix during sequential chemisorption of CH_4 and $Cl_2Si(CH_3)_2$ molecules from the gas phase.

The conditions are established for pressing and sintering a Fe bulk material with nanosilicon carbide to obtain a composite with minimal residual porosity and improved strength.

The ways of adjustment of metal materials strength using structuring the metal matrix (on the example of iron) with SiC are discussed.

The proposed approach can also be used to create analogous composites based on an

aluminum frame with improved mechanical properties and is implemented via a nanosized material with a high degree of uniformity.

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QUASI STATIC AND FLEXURAL MECHANICAL PROPERTY EVALUATION OF BASALT/FLAX REINFORCED COMPOSITES K. Arun Prasath^{1*}, V. Arumugaprabu¹, P. Amuthakkannan², K. Naresh³, M.S. Muthugopal¹, M. Jeganathan¹, R. Pragadeesh¹

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Abstract. Basalt fiber is one of the best reinforcing materials and satisfies all the needs of a composite material. Flax is predominately used natural fiber which has better mechanical and sudden load shock-absorbing properties. The general-purpose polyester resin in one an excellent binding agent which equally distributes the load along the direction of applications. To understand the mechanical properties of the natural and synthetic fiber of these flax/basalt fiber combinations is essential to reduce the usage of synthetic fibers. In this paper, the maximum tensile strength was found on the combination of pure 10 layers of basalt and it was about 185MPa. The maximum flexural strength absorption was seen in the combination of 10 layers of basalt fiber composite about 190MPa. The maximum impact energy was absorbed by composite D, the alternative layers of basalt and flax fiber composite. SEM analysis shows with matrix cracking, and fiber twist was seen, this is because of the improper mixing of the fiber and matrix also seen in the composites.

Keywords: basalt fiber, flax fiber, polyester resin, quasi-static mechanical behavior, tensile test, impact test

1. Introduction

Flax fiber is a food crop cultivated in cooler regions of the world. It is mainly used in textile industries. They have good mechanical properties and also shock-absorbing properties. Basalt is a dark-colored, fine-grained, igneous rock composed mainly of plagioclase and pyroxene minerals. It most commonly forms as an extrusive rock, such as a lava flow. The cost of the basalt fiber was found to be comparatively cheaper than that of carbon fiber and this basalt/flax combination shows better static and dynamical properties [1]. The combination of hybrid composite is of flax and basalt powder. It comprises of 10 layers of flax fiber and basalt fiber. The mechanical properties of flax fiber and basalt fiber combination possess better results. The fabrication of those composites was made from a compression molding technique which is responsible for achieving some better results. It was found the addition of flax layers increased the amount of energy absorption [2]. The combination of a hybrid combination of carbon and basalt fiber has better tensile strength were found. The materials included were carbon and basalt along with epoxy resin Vacuum bagging process is the process used to fabricate the composite. The testing included are hardness, tensile, and thermal conductivity tests. The carbon/basalt fiber seemed to have better mechanical properties orientation at the angle of 90 degrees than 45 degrees [3]. The combination of hybrid composite is of glass and Kevlar yarns. The effect of homogeneous and hybrid

external patches in weave was noted in the woven glass fibers. The composite fabrication with glass and Kevlar yarns and the matrix material used here is epoxy resin. The better result of the provides the repair applications of the Kevlar mainly as polar fibers [4]. The combination of the basalt and epoxy resin shows better characteristics and mechanical properties, while assorted with the short basalt fiber composites. The better shear and mechanical properties were seen, by increasing the basalt content in the composite improve the strength of the composite [5]. The tensile behavior of the woven basalt fiber composites possesses a high strain rate. Basalt dry fabric was the material used here and the resin was used with the epoxy composites. The testing of quasi-static and dynamic testing results with better results and impact applications [6]. The glass fiber and basalt fiber composite and their mechanical behavior were in comparison. The composite included increasing the percentage of glass fiber content in the composite. These composites showed better and increased tensile and shear strength than other combinations [7]. The combination of hybrid composite is of plain weave fabrics and composite sheet. At different strain rates of flax fiber-reinforced composites, the improved strain rate was noted [8]. The combination of hybrid composite is of flax/basalt fiber. With the topological approach in optimizing mechanical properties flax/basalt fiber hybrid composite. The flexural test, impact results shows that hybridization reduced the brittleness and offered good yield property, the internal damages of the composites studied with SEM [9]. The combination of hybrid composite has good environmental durability in the case of carbon/flax fiber hybrid composites. The tensile test and flexural test was done with hydrothermal treatment changes in surface morphology was studied with SEM analysis. The final result comprises, the addition of flax fiber improved the mechanical properties of the composites [10]. The hybrid combination of flax fiber and basalt fiber results with better bending strength and flexural test, the failure morphology was studied through SEM analysis. The increase in flax fiber as reinforcement in the composite increases the impact bending of the composites [11]. A thorough literature study shows that the combination of basalt and flax fiber possesses better mechanical properties. By nature, the hybridization of basalt and flax fiber offers a good bonding towards quasi-static (tensile and impact) and flexural mechanical studies for various applications.

2. Materials and Methods

The reinforcement material used here was woven flax and basalt fiber and matrix material as general-purpose polyester resin. The additives used were methyl ethyl ketone peroxide (MEKP) is an accelerator and cobalt napthalate as the catalyst. The flax fiber was purchased from vruksha fibers Guntur and the resin was purchased from vasavi Bala resins, Chennai. Composite prepared by varying the sequence of flax and basalt fiber. And the fabrication was done by compression molding technique with 100kgf/cm² pressure at room temperature for 3 hours.

3. Result and Discussion

In this chapter, the hybridization effect of bi-directional basalt/flax fiber and the morphological analysis for tensile, flexural, and impact properties are also discussed with scanning electron microscopy (SEM). The fiber was arranged with different stacking order and their mechanical properties are analyzed for further studies in this chapter.

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 Table 1. Composite type and specimen code

Specimen code	Flax/Basalt Stacking
А	10L of Flax
В	5L of Flax/ 5L of Basalt
С	2L F/2LB/2L F/2LB/2L F
D	2L B/2L F/2L B/2L F/2L B
Е	3L F/2L B/3 L F/2L B
F	4L F/2L B/2L F/2L B
G	3L B/2L F/3L B/2LF
Н	4L B/2L F/2L B/2L F
Ι	10L of Basalt



Fig. 1. Tensile strength analysis of flax/basalt fiber composite

Tensile Strength. The tensile strength of the material determines the maximum strength that the material withstand while pulling with some force. The tensile test was carried out with the ASTM D3039 standard and the dimension of the specimen about $200 \times 20 \times 3$ mm. The test was executed in the universal testing machine (UTM). This tensile test helps to study the ductile property of the material in various loading conditions. The tensile strength of the material depends on the like preparation of material, fabrication standard, and the temperature adopted for processing. The above table 1 shows the specimen code and different stacking of flax and basalt fiber composite. Figure 1 clearly, defines the tensile strength exhibited by different layers of flax and basalt fibers. The maximum tensile strength acquired by pure 10 layers of basalt fiber was good while compared to flax fibers. In the hybridization of basalt and flax fiber as alternate sequences, basalt as the first layer, and flax in the last seen in the composite F and G. These composites produce a better performance compared with other combinations of hybrids about 145MPa. Because the linear relationship between the fiber

arrangement and tensile modulus was good, increases the load-bearing capacity of the composite [6]. From the overall comparison, the hybridization of basalt/flax fiber shows better results compared with all other combinations except the pure basalt composite. This results in the combination of flax/basalt produce good tensile strength. However, the pure basalt layer can have performed.

Flexural Strength. The flexural test is also known as the modulus of rapture which denotes the property of the material resists the deformation bending. The flexural test was carried out on the universal testing machine (UTM) with a three-point bending fixture. The test was conducted with the standard of ASTM D790 with a dimension of 125×13×3 mm. This flexural strength of the composite represents the highest stress experienced within the reinforcement fiber to the matrix material. There is a better flexural energy capability was noted for basalt and flax fiber composite [7]. Figure 2 shows the flexural strength analysis of flax/basalt fiber composite. The maximum flexural strength absorption was seen in the 10 layers of basalt fiber composite about 190MPa, this is because the failure of the composite happens as a straight-line crack. This type of crack pattern does not experience a major failure in the composite, especially for basalt fiber composites [8]. The combination hybridization effect of basalt/flax alternate layers possess some better flexural results in the layering effect of the composite. In composite F, the alternate layers of basalt and flax fiber show some noted results about 140MPa. The flexural strength of the composites depends on the stress concentration and load absorbing capability of the composite. And the bonding of fibers with the matrix is also considered to be an important content while study about the flexural strength of the composite. As synthetic fiber basalt shows a better performance in this area also, reduce the usage of basalt fiber in the stack will be eco-friendly. The alternative sequence of basalt and flax fiber shows good strength compared with other combinations.



Fig. 2. Flexural strength analysis of flax/basalt fiber composite

Impact Strength. Impact strength determines the sudden load capability of the material and its related properties. In polymer composites, the impact strength was considered to be an important property of the material towards the fracture. The charpy impact test was examined with ASTM D256 with the specimen dimension of $65 \times 13 \times 3$ mm. The maximum impact energy was absorbed by composite D, the alternative layers of basalt, and flax fiber composite. The energy absorbed around 25J, this shows the hybrid application of basalt and

flax for various mechanical applications. The impact performance of basalt hybrid composite depends on the elastic modulus of the supportive reinforcement. However, the combination of flax reinforcement with basalt always has a high elastic modulus [9] than other fibers as reinforcement. The other combinations as 10 layers of pure basalt (composite A) and flax (composite I) type of composite do not show a better impact response compared to these hybrids. From the overall observations, the alternative layers of basalt and flax fiber composite produce a good impact strength towards the application of sudden load.



Fig. 3. Flexural strength analysis of flax/basalt fiber composite

Morphological Analysis. Morphological analysis is one of the general problem solving and provides a better solution for any of the approaches. In polymer composite, the morphological study helped to examined through microscopy for mechanical failures. Scanning Electron Microscope (SEM) is one type of technique to study the failure and factors responsible for the failure were studied with the electron microscope. The internal structure specimen was affected by cracks and holes, due to the application of mechanical loads. Figure 4 shows the SEM analysis of mechanical testing as tensile, impact, and flexural test of alternate layers of flax and basalt fiber composite, which shows better results compared to other combinations. Figure 4a shows the failure analysis of the tensile specimen, in that the matrix crack was noticed this is due to not proper bonding between the reinforcement and matrix responsible for this type of failure [10]. Figure 4b shows the SEM analysis of the flexural specimens, in that the fiber twist was seen this is because of the improper mixing of the fiber and matrix shows this type of internal failure observation. In the impact specimen fiber pull out and blow holes in between the fiber and matrix were noted [11]. This is the type of response that can observe only improper curing time of fabrication and blowholes for the bending of fibers which initiate the crack without the responses of the matrix in the time of application of load [12], shown in Fig. 4c as impact responses.


Fig. 4. SEM morphological analysis of flax/basalt fiber composite

4. Conclusion

- 1. The maximum tensile strength acquired by pure 10 layers of basalt fibers (composite I) around 185MPa, by nature the strength absorbing capability for basalt fiber was good while compared to flax fibers. In the hybridization of basalt and flax fiber as alternate sequences, basalt as the first layer, and flax in the last seen in the composite F and G.
- 2. The maximum flexural strength absorption was seen in the 10 layers of basalt fiber composite about 190MPa, this is because the failure of the composite happens as a straight-line crack. This type of crack pattern does not experience a major failure in the composite, especially for basalt fiber composites.
- 3. The alternate layers of basalt and flax fiber show some noted results about 140MPa.The flexural strength of the composites depends on the stress concentration and load absorbing capability of the composite.
- 4. The energy absorbed around 25J, this shows the hybrid application of basalt and flax for various mechanical applications. The impact performance of basalt hybrid composite depends on the elastic modulus of the supportive reinforcement.
- 5. The SEM analysis of the tensile specimen, in that the matrix crack was noticed this is due to not proper bonding between the reinforcement and matrix responsible for these types of failure. The fiber twist was seen this is because the improper mixing of the fiber and matrix shows this type of internal failure observation. In the impact specimen fiber pull out and blow holes in between the fiber and matrix were noted.
- 6. From the results obtained theoretically and experimentally, the combination of basalt and flax fiber composite shows better impact strength than other mechanical properties.

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This hybrid combination has the application in automobile and aircraft components with the replacement of metals.

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MODELING ANTIFRICTION PROPERTIES OF COMPOSITE BASED ON DYNAMIC CONTACT PROBLEM FOR A HETEROGENEOUS FOUNDATION

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Abstract. Based on the solution of the dynamic contact problem of vibration of a rigid punch on a heterogeneous half-space, taking into account friction in the contact area, the tribological properties of an oil-filled composite material with a microstructure are modeled. The microstructure of the base is taken into account in the framework of the Biot-Frenkel model. The boundary-value problem is reduced to the integral equation, its approximate solution is constructed, which describes contact stresses, tangential displacements. The dependencies of the friction forces on the microstructure of the composite, the viscosity of the fluid filling the pores, and the degree of phase interaction are investigated.

Keywords: dynamic contact problem with friction, oil-filled composite

1. Introduction

Currently, there is a considerable amount of concepts, hypotheses, and research on diverse friction and wear-related issues. Many attempts have been made to study the properties, structure, and state of the surface layers of tribological conjugations at the atomic and molecular levels. The core problem of surface engineering (for example, metal friction units) is the synthesis of coating technologies and materials with specified wear-resistant properties. The most remarkable result to emerge from our study [1] is that the methods of vacuum ionplasma treatment (PVD-method) and atomic modifications of diamond-like coatings (DLC) are the most appropriate among the wide array of methods aimed at hardening surface and improving tribological properties. However, along with increasing the strength properties of the materials, such technologies contribute to the formation of a damping layer with residual compressive stresses inside and a large number of stress micro-concentrators at the boundary with the main material. The above-listed aspects predetermine the formulation and solution of the dynamic contact problem, taking into account the friction forces on tribocontact. This problem is attracting an increasing interest due to the widespread application of polymer composite materials [2]. Recently, oil-filled nanocomposites, whose components are characterized with viscoelastic properties and the properties of viscous-fluid filler, have become extensively used in units and parts of tribotechnical purposes [3-5]. Constructing new composite materials with given physical and mechanical properties poses an actual, yet practically unexplored task to study the influence of dynamic effects that are caused by vibration on the antifriction properties of these materials. We undertook this study to investigate the patterns of changes in the stress-strain state of a composite material depending on its composition and dynamic loading conditions by solving a dynamic contact problem. The latest takes into account friction in the contact area for a base with a microstructure. The

equations of the heterogeneous Biot medium are used to describe the microstructure of a base consisting of an isotropic viscoelastic matrix and a filler fluid possessing the properties of a viscous amorphous liquid [6]. The mechanical properties of the matrix material were determined experimentally by nanoindentation. The change in the mechanical modules of the medium while varying porosity was studied by the differential scheme of the self-consistency method. It should be noted that contact problems in a quasi-static formulation for homogeneous viscoelastic media that simulate surface phenomena in tribology are considered in [7-9]. The properties of the contacting surfaces significantly affect the friction force. Much work on the influence of microgeometry of contacting surfaces on the friction force was carried out by [9]. Consideration of the base microstructure as a whole for contact stresses was presented in [10-12]. In these studies, contact problems in quasistatic and dynamic formulations were considered, and the microstructure of a heterogeneous medium was described in terms of the Biot-Frenkel model. In the study [12] a two-phase medium has been described as equivalent to a single-phase assuming that the velocities of solid and liquid phases are equal. The tribological properties of oil-filled composites were experimentally studied in [13]. Dynamic contact problems for elastic layered bases are presented in [14], including non-traditional for tribology formulations [15].

This paper outlines a new approach to the study of surface interaction in the contact area, taking into account the heterogeneity of the base within the model of two-phase Biot-Frenkel medium and dynamic effects. In this context, we tried to find out the dependencies of the friction forces on the composite microstructure, the viscosity of the pore-filling fluid, and the degree of phase interaction. Interestingly, the tribological process is also characterized by tangential displacements under the punch. The strength and wear resistance of the composite depends on the energy impact in the area of contact with friction. Moreover, it is necessary to take into account both normal and tangential displacements in the contact area.

2. Statement and solution of the contact problem for a heterogeneous half-space

The contact problem of oscillations of rigid flat punch on the surface of a heterogeneous halfspace under the action of a force applied to it, which varies in harmonic law, is considered. Let a two-phase medium consisting of a viscoelastic porous matrix-skeleton and fluid filling pores occupy a flat region $|x_1| < \infty$, $x_2 \le 0$. On the front impenetrable boundary of the heterogeneous medium, a rigid punch oscillates with frequency ω under the action of the force. The width of the rigid punch is 2a. Let that force be applied to the punch so as to ensure full contact with the surface. In the contact area $|x_1| \le a$, the normal and tangential stresses are connected by the Amonton-Coulomb law. To take into account the internal microstructure of the base, we use, as the most tested model, described by the equations of the heterogeneous two-phase Biot - Frenkel medium in terms of the displacements [6]: $A\nabla \cdot \nabla \mathbf{u} + 2N\nabla \nabla \cdot \mathbf{u} + O\nabla \nabla \cdot \mathbf{v} =$

$$= \rho_{11} \frac{\partial^2 \mathbf{u}}{\partial t^2} + \rho_{12} \frac{\partial^2 \mathbf{v}}{\partial t^2} + b \left(\frac{\partial \mathbf{u}}{\partial t} - \frac{\partial \mathbf{v}}{\partial t} \right),$$

$$Q \nabla \nabla \cdot \mathbf{u} + R \nabla \nabla \cdot \mathbf{v} =$$

$$= \rho_{12} \frac{\partial^2 \mathbf{u}}{\partial t^2} + \rho_{22} \frac{\partial^2 \mathbf{v}}{\partial t^2} - b \left(\frac{\partial \mathbf{u}}{\partial t} - \frac{\partial \mathbf{v}}{\partial t} \right),$$
(1)

 $A, N, Q, R, \rho_{11}, \rho_{12}, \rho_{22}$ are the mechanical characteristics of a two-phase medium [16], $e_{ij}, \varepsilon_{ij}, i, j = 1, 2$ are the strain tensors corresponding to displacement vectors of the solid phase $\mathbf{u}\{u_1, u_2\}$ and liquid phase $\mathbf{v}\{v_1, v_2\}, b = m^2 \eta k_o^{-1}$ and η, k_o – fluid viscosity and permeability, $\Gamma_{ij} = \sigma_{ij}^s + \delta_{ij}\sigma^f$, *i*, *j* = 1,2 is a full stress tensor acting on a poroelastic medium, $\sigma_{ij}^s = Ae\delta_{ij} + 2Ne_{ij} + Q\epsilon\delta_{ij}$ is a stress tensor acting on a viscoelastic skeleton, $\sigma^f = Qe + R\epsilon$ is a pore pressure. The viscosity of the composite matrix is taken into account in the framework of the model of frequency-independent internal friction. According to this approach, the shear modulus has the form $N(1+i\beta)$, where the value of β is proportional to the loss coefficient of a viscoelastic material [17] and can be determined experimentally [18]. As a result of this, a small complex component is present in the coefficients of equation (1) N, A, Q, R [19]. The oscillation mode is steady. Separate the time factor and the presentation will be carried out for the dimensionless amplitude values of the corresponding functions, while the linear dimensions are assigned to the half-width of the punch, and the stress to the shear modulus Nof the matrix. The boundary conditions in this case are:

$$u_{2}(x_{1},0) = v_{2}(x_{1},0), |x_{1}| < \infty,$$

$$\Gamma_{21}(x_{1},0) = \Gamma_{22}(x_{1},0) = 0, |x_{1}| > 1,$$

$$\Gamma_{21}(x_{1},0) = \mu\Gamma_{22}(x_{1},0), u_{2}(x_{1},0) = \delta, |x_{1}| \le 1,$$
(2)

where δ is the punch upsetting, μ is the coefficient of friction. The statement of the boundary value problem (1) – (2) closes the condition for the emission of waves at infinity. The contact pressure and horizontal displacement $u_1(x_1, 0)$ under the punch must be found. We represent the displacements in the form of two scalar and vector potentials. As a result, equations (1) are split into three wave equations, and the potentials correspond to three types of waves propagating in a heterogeneous medium:

$$\mathbf{u}(\mathbf{x}) = \nabla \left(L_1(\mathbf{x}) + L_2(\mathbf{x}) \right) + \nabla \times \Psi(\mathbf{x}),$$

$$\mathbf{v}(\mathbf{x}) = \nabla \left(m_1 L_1(\mathbf{x}) + m_2 L_2(\mathbf{x}) \right) + \nabla \times \Psi_1(\mathbf{x}), \ \mathbf{x} = (x_1, x_2),$$

$$\Delta L_j(\mathbf{x}) + \theta_j^2 L_j(\mathbf{x}) = 0, \ \theta_j = \zeta_j \vartheta, \ j = 1, 2,$$
(3)

 $m_i, \zeta_i, j = 1, 2$ are the roots of the following equation:

$$\begin{vmatrix} q_{12} & q_{11} \\ q_{22} & q_{12} \end{vmatrix} \zeta^{2} + \left(\begin{vmatrix} \gamma_{11} & \gamma_{12} \\ q_{12} & q_{22} \end{vmatrix} + \begin{vmatrix} \gamma_{22} & \gamma_{12} \\ q_{12} & q_{11} \end{vmatrix} \right) \zeta + \begin{vmatrix} \gamma_{12} & \gamma_{11} \\ \gamma_{22} & \gamma_{12} \end{vmatrix} = 0.$$

$$\begin{vmatrix} \gamma_{12} & \gamma_{22} \\ q_{12} & q_{22} \end{vmatrix} m^{2} + \begin{vmatrix} \gamma_{11} & \gamma_{22} \\ q_{11} & q_{22} \end{vmatrix} m + \begin{vmatrix} \gamma_{11} & \gamma_{12} \\ q_{11} & q_{12} \end{vmatrix} = 0,$$

$$\gamma_{11} = (\rho_{11} + ib / \omega) / \rho_{11}, \quad \gamma_{12} = (\rho_{12} - ib / \omega) / \rho_{11},$$

$$\gamma_{22} = (\rho_{22} + ib / \omega) / \rho_{11}, \quad \vartheta^{2} = \rho \omega^{2} a^{2} / N,$$

$$q_{11} = (A + 2N) / N, \quad q_{12} = Q / N, \quad q_{22} = R / N.$$

The vector potential satisfies the following equation: $\Delta \Psi(\mathbf{x}) + \theta_2^2 \Psi(\mathbf{x}) = 0.$

$$\theta_{3} = \zeta_{3} \vartheta, \ \zeta_{3} = (\gamma_{11} \gamma_{22} - \gamma_{12}^{2}) / \gamma_{22},$$

$$\Psi_{1}(\boldsymbol{x}) = -\gamma_{12} / \gamma_{22} \Psi(\boldsymbol{x}).$$

The velocities of longitudinal waves and shear wave are determined $V_i = \omega a / \theta_i$, i = 1, 2, 3.

After applying the Fourier transform with respect to the variable x_1 to Eqs. (1) – (3) we construct Green's matrices. Further, using the inverse Fourier transform, we obtain the relationship of displacements and stresses of a two-phase medium:

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$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{2\pi} \int_{\Upsilon} \boldsymbol{K}_{u}(\alpha, x_{2}) \mathbf{Q}(\alpha) e^{-i\alpha x_{1}} d\alpha,$$

$$\boldsymbol{v}(\boldsymbol{x}) = \frac{1}{2\pi} \int_{\Upsilon} \boldsymbol{K}_{v}(\alpha, x_{2}) \mathbf{Q}(\alpha) e^{-i\alpha x_{1}} d\alpha,$$

$$\mathbf{Q}(\alpha) = \int_{-\infty}^{\infty} \boldsymbol{q}(\boldsymbol{x}) e^{i\alpha x_{1}} dx_{1},$$

$$\boldsymbol{q}(\boldsymbol{x}) = \left\{ \Gamma_{21}(\boldsymbol{x}), \Gamma_{22}(\boldsymbol{x}) \right\}.$$
(4)
The circuit Υ is selected in accordance with the conditions of radiation of waves at

The circuit Υ is selected in accordance with the conditions of radiation of waves at infinity, $\mathbf{K}_{u}(\alpha, x_{2})$, $\mathbf{K}_{v}(\alpha, x_{2})$ are Green's matrices for skeleton and fluid displacements, respectively [20].

Satisfying the boundary conditions (2) in relation (4), we have obtained the integral equation with a difference kernel with unknown normal contact pressure:

$$\int_{-1}^{1} K(x_1 - \xi) q_2(\xi) d\xi = \delta_0, \ \delta_0 = \delta / a.$$
(5)

The kernel of the integral equation (4) has the form:

$$K(x_{1} - \xi) = \frac{1}{2\pi} \int_{Y} (\mu K_{21}(\alpha) + K_{22}(\alpha)) e^{i\alpha(x_{1} - \xi)} d\alpha,$$

$$K_{11}(\alpha) = \left(\left(2g_{3}s_{3} + \gamma_{13}(g_{01} - g_{02}) \right) \alpha^{2} + s_{3}(g_{2} - g_{1}) \right) / D(\alpha),$$

$$K_{12}(\alpha) = i\alpha \left(2g_{0} + 2(s_{1} - s_{2})\gamma_{13}\alpha^{2} + (\alpha^{2} + s_{3}^{2})g_{3} \right) / D(\alpha),$$

$$K_{21}(\alpha) = i\alpha \left(2g_{0} + \gamma_{12} / \gamma_{22}g_{1} + g_{2} \right) / D(\alpha),$$

$$K_{22}(\alpha) = (m_{1} - m_{2})s_{1}s_{2}\theta_{3}^{2} / D(\alpha),$$

$$D(\alpha) = 2\left(2g_{0} + \gamma_{13}g_{1} \right) \alpha^{2} + (\alpha^{2} + s_{3}^{2})(g_{2} - g_{1}),$$

$$g_{1} = \begin{vmatrix} g_{01} & g_{02} \\ s_{1} & s_{2} \end{vmatrix} , \quad g_{2} = \begin{vmatrix} g_{01} & g_{02} \\ m_{1}s_{1} & m_{2}s_{2} \end{vmatrix} , \quad g_{3} = \begin{vmatrix} s_{2} & s_{1} \\ (1 - m_{1}) & (1 - m_{2}) \end{vmatrix} , \quad g_{0} = (m_{1} - m_{2})s_{1}s_{2}s_{3},$$

$$g_{0i} = 2\alpha^{2} - \theta_{i}^{2} \left(q_{11} + q_{12} + (q_{12} + q_{22})(1 - m_{i}) \right), \quad i = 1, 2,$$

$$\gamma_{13} = 1 + \gamma_{12} / \gamma_{22}; \quad s_{k} = \sqrt{\alpha^{2} - \theta_{k}^{2}}; \quad k = 1, 2, 3,$$
where α is the Fourier transform parameter, the functions $K_{1}(\alpha)$, $i, i = 1, 2$, are elements of β_{1}

where α is the Fourier transform parameter, the functions $K_{ij}(\alpha)$, i, j = 1, 2 are elements of the Green's matrix (4) for a heterogeneous medium. The functions $K_{ij}(\alpha)$, i, j = 1, 2 have the following behavior at infinity:

$$\lim_{\alpha \to \infty} K_{ii}(\alpha) = d_{ii} / |\alpha|, \lim_{\alpha \to \infty} K_{ij}(\alpha) = (-1)^i d_{ij} / \alpha, \ i \neq j .$$

Next, we regularize the kernel (6) of the integral equation (5) to separate its logarithmic singularity. We use the function $d_{22} / \sqrt{\alpha^2 + R^2}$ as a regularizer of the kernel $K(x_1 - \xi)$ of the integral equation (5). This function coincides with the function $K_{22}(\alpha)$ at infinity and does not have poles in the complex plane. As a result, relation (6) has the form: $K(x_1 - \xi) = I_1(x_1 - \xi) + K_0(R|x_1 - \xi|) / \pi$,

$$I_{1}(x_{1}-\xi) = \frac{1}{2\pi} \int_{\gamma} L(\alpha) e^{i\alpha(x_{1}-\xi)} d\alpha,$$

$$L(\alpha) = \mu K_{21}(\alpha) + K_{22}(\alpha) - d_{22} / \sqrt{\alpha^{2} + R^{2}},$$
(7)

where $K_0(z)$ is zero-order Macdonald function. The integral $I_1(x_1 - \xi)$ in (7) is rapidly convergent. The choice of a parameter R >> 1 minimizes the contribution of integrals over $iR \le \alpha < i\infty, -iR \ge \alpha > -i\infty$ cuts [12]. The Macdonald function zero-order has the expression in the form of a series [21]:

$$K_0(z) = -I_0(z)\ln(\gamma z/2) + \sum_{m=0}^{\infty} \left(\frac{z}{2}\right)^{2m} \frac{\psi(m+1)}{(m!)^2}, \ \lim_{z \to 0} I_0(z) = 1,$$

where $I_0(z)$ is modified Bessel function of the first kind, γ is the Euler's constant. The logarithmic singularity in the explicit form in relation (6) is separated.

After regularization of the integral equation (5), the representation of the kernel (7) makes it possible to efficiently apply the numerical solution scheme based on the boundary element method. We choose the partition points x_{1i} , $i = \overline{1, N}$ that are uniformly distributed, with a step h = 2/N on a segment [-1+h/2, 1-h/2]. The function $q_2(x_1)$ is constant within each of the elements of the partition: $q_2(x_1)|_{x_{1i} < x_1 < x_{1i+1}} = q_2(x_{1i}) = q_i$, $i = \overline{1, N}$. The midpoints of the corresponding segments of the partition $[x_{1i}; x_{1i+1}]$, $i = \overline{1, N}$ are selected as nodes. As a result, the solution of the integral equation (5) reduces to a finite system of linear N- order algebraic equations with respect to unknowns q_i , $i = \overline{1, N}$. The system has a quasi-diagonal matrix and converges quickly:

$$\sum_{m=1}^{N} r_{mn} q_n = \delta_0, \quad m, n = 1, 2, ..., N,$$

$$r_{mn} = \begin{cases} I_1(x_{1m} - \xi_n) + \frac{\sqrt{2\pi}}{R} d_{22} sign(x_{1m+1} - \xi_n) \left(Erf(z_2) - Erf(z_1) \right) / h, & m \neq n \\ I_1(x_{1n} - \xi_n) + 2d_{22} Erf(\sqrt{hR/2}) / h, & m = n \end{cases}$$

$$z_1 = \sqrt{(x_{1m} - \xi_n)R}, \quad z_2 = \sqrt{(x_{1m+1} - \xi_n)R},$$

$$d_{22} = (m_1 - m_2)\theta_3 / d_g,$$

$$d_g = 2((\theta_1^2 + g_{01})m_2 - (\theta_2^2 + g_{02})m_1 - (\theta_2^2 - \theta_1^2 + g_{02} - g_{01})\gamma_{12} / \gamma_{22}),$$
(7)

where Erf(z) is probability integral [22]. The integral $I_1(x_{1m} - \xi_n)$ is calculated by integration over the contour Υ in the complex plane. The integration contour is selected in accordance with the radiation conditions so that the displacements of the surface of the heterogeneous half-space decrease with distance from the vibrating punch. This choice is made after finding the poles and branch points of the integrands in (7) and analyzing them when the internal friction of the medium tends to zero. Note that to analyze the rate of convergence of the process, the residual elements were estimated for the number of partitions N and 3N. Number of mesh elements chosen from the condition that the residual is less than 10^{-4} .

Horizontal movements under and outside the punch are determined through the elements of the Green's matrix of the heterogeneous medium $K_{11}(\alpha)$, $K_{12}(\alpha)$ and contact pressure:

$$u_{1}(x_{1},0) = \int_{-1}^{1} K_{1}(x_{1}-\xi)q_{2}(\xi)d\xi,$$

$$K_{1}(x_{1}-\xi) = \frac{1}{2\pi}\int_{\Upsilon} \left(\mu K_{11}(\alpha) + K_{12}(\alpha)\right)e^{i\alpha(x_{1}-\xi)}d\alpha.$$

Next, we perform the procedure for extracting a singularity in the function $K_1(x_1 - \xi)$, similar to the algorithm described above. Then we discretize the contact area and determine the tangential displacement under the punch, taking into account contact pressures determined from relation (7):

$$\begin{split} u_{1}(x_{1},0) &= \sum_{n=1}^{N} q_{n} \tilde{r}_{nm}, \quad m = \overline{1,N} \\ \tilde{r}_{mn} &= \begin{cases} I_{2}(x_{1m} - \xi_{n}) + \frac{\sqrt{2}\pi}{R} \mu d_{11} sign(x_{1m+1} - \xi_{n}) \left(Erf(z_{2}) - Erf(z_{1}) \right), & m \neq n, \\ I_{2}(x_{1n} - \xi_{n}) + \mu d_{11} Erf(\sqrt{hR/2}), & m = n, \end{cases} \\ d_{11} &= (g_{01}m_{2} - g_{02}m_{1} + (g_{01} - g_{02})\gamma_{12} / \gamma_{22}) / d_{g}. \end{split}$$

3. Results of computational experiments

In accordance with the above method, normal and tangential contact stresses, tangential displacements under the punch were determined. The calculations were carried out for the mechanical characteristics corresponding to a two-component composite material with a Phenylone-based matrix modified with a nano-additive (magnesium aluminum spinel) and cylinder oil-contained filler.

Correct determination of the mechanical characteristics A, R, Q, N of a Biot medium for a heterogeneous composite is a multi-stage problem. The values of Young's modulus E_s and Poisson's ratio v_s were determined during field experiments when compressing a Phenylone sample without a filler in a loading mode that provides purely elastic deformations of the sample [23]. Further, the mechanical properties of Phenylone and composites with a Phenylone matrix [24] were determined based on the nanoindentation method with the previously found Poisson's ratio. The next step was to study the effect of porosity on the bulk modulus drained porous medium K_b . The results obtained based on the self-consistent [25] scheme and generalized differential self-consistent scheme are compared. Note that at low porosity (m < 0.2), the relative error of the two calculation methods did not exceed 4%. Thus, the coefficients of equations (1) for the known bulk modulus of a viscoelastic matrix K_s , drained porous medium K_b , fluid K_f , and porosity m were calculated by the formulas [10].

The calculations were carried out with the following data: $K_s = 6.3$ GPa, $K_f = 2$ GPa, N = 2.29 GPa, $\rho_s = 1.2 \cdot 10^3$ kg/m³, $\rho_f = 0.93 \cdot 10^3$ kg/m³, $K_b(m = 0.05) = 5.32$ GPa, $K_b(m = 0.1) = 4.36$ GPa, $K_b(m = 0.15) = 3.40$ GPa, $K_b(m = 0.2) = 2.44$ GPa, $\omega = 50$ Hz.

The Phenylone has a low tendency to creep under the action of stresses [26] and the use of nano-additives to modify the composite matrix allows one to suppress relaxation processes. The viscosity of the composite matrix was taken into account in the framework of the model of frequency-independent internal friction. The calculations were carried out for the range $10^{-3} < \beta < 0.5 \cdot 10^{-1}$ [18]. The experimental determination of the coefficient of the interaction of phases, the permeability of the composite is a very laborious problem. We will rely on the known data for artificial media containing clay particles, they have a permeability coefficient in the range $10^{-14} < k_o < 10^{-10}$ [27], and the tortuosity of the pore channels corresponds to the case of spherical particles [28].

Particular attention was paid to the analysis of the effect of porosity on the magnitude of contact pressures. The distribution of the real part of normal contact pressure $\text{Re} q_2(x_1)$ with a

change in porosity *m* and fluid saturation of the base is shown in Fig. 1 for values $\mu = 0.2, \delta_0 = 1, \beta = 0.05, b = 0$.



Fig. 1. Influence of porosity of a heterogeneous base on the distribution of the real part of normal contact pressure

Moreover, the curve marked with a marker «*» corresponds to zero porosity. This curve was obtained based on the solution of the dynamic problem of punch vibrations in a similar formulation for the case of an equivalent elastic medium [12].

It is established that the dependence of normal and tangential contact stresses on the porosity of a heterogeneous base is non-linear. Note that the contact normal and tangential stresses are largely dependent on the porosity and mass fraction of the filler fluid. Moreover, the stress distribution over the contact area is asymmetric, which is also characteristic of contact problems of the theory of elasticity with allowance for the friction forces. It is important to note that for the case of dynamic loading, the influence of the coefficient of friction on contact pressures is more pronounced than in problems in a quasistatic formulation [7,10].

It should be noted that the parameter $b = m^2 \eta / k_0$ characterizing the interaction of the phases of the composite has a significant effect on contact pressures. With an increase in the viscosity of the fluid filling the pores and a decrease in the permeability coefficient of the porous elastic medium, the stress distribution under the punch changes, as illustrated in Fig. 2. This figure shows the distribution of the real parts of normal pressures under the punch, calculated with the same input data with increasing parameter η / k_0 .

It has been experimentally shown [29] that the increase in the vibration frequency induces the decrease in the contact stresses. The results of the numerical analysis also confirm the given fact [11]. The change in the amplitude of the friction force during the period of vibration plays a key role. The wear resistance of the composite depends greatly on the energy impact in the friction area, taking into account both the normal and tangential displacements in the contact area [11]. An increase in the vibration frequency leads to a decrease in the contact stresses per unit time; however, a large amount of energy is generated in the contact area. Figure 3 presents the plot of the tangential contact stresses for a *T*-period under punch vibrations affected by the applied force that varies according to the $P = P_0 \cos \omega t$ law for $\eta/k_0 = 0.01 \cdot 10^{10}$. The tangential contact stresses Γ_{21} during the vibration period change sign, while its amplitude delineates a flat figure, the area of which is proportional to the energy of the friction force. The above information makes it possible to predict the composite's wear resistance.



Fig. 2. The effect of fluid viscosity and permeability on the distribution of the real (left) part and imaginary (right) part of normal contact pressures



Fig. 3. Change in the tangential stresses during the vibration period T

4. Conclusions

Contact stresses and tangential displacements under the punch for a heterogeneous base depend not only on the friction coefficient in the contact area, but also substantially depend on the vibration frequency, porosity, permeability of the medium, and fluid viscosity. A change in the friction coefficient during vibration has a much greater effect on contact stresses than in a quasistatic problem when the punch moves. Based on the considered model, it is possible to evaluate the energy effect over a period of oscillation, on which the wear resistance of the composite material depends. In this case, it is necessary to take into account not only normal movements but also horizontal movements in the contact area. The studies that were performed allow us to find the optimal ratio of the mechanical properties of a composite material operating under dynamic loading.

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NUCLEAR GEOMETRY: FROM NITROGEN TO NEON

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Abstract. The nuclear geometry was developed by analogy with the fullerene geometry. On the basis of this geometric approach, it was possible to design the structure of nitrogen, oxygen, fluorine and neon isomers and their isotopes, which can be obtained by means of nuclear synthesis. The most stable nuclei can be classed into two groups: basic nuclei having equal number of protons and neutrons and isotopes having one or two more neutrons. The latter ensure their mechanical stability with respect to shear stresses, sending their electron to the external coat of mail created by the basic nuclei.

Keywords: fluorine, carbon, graph representation, isomer, isotope, neon, nitrogen, nuclear electron, nuclear geometry, nuclear reaction, nuclear synthesis, oxygen

1. Introduction

Earlier, by analogy with fullerenes, the nuclear geometry was designed. For hydrogen, deuterium, tritium and helium 3, we obtained a point, a linear and a plane structure respectively. Helium 4 has a tetrahedral symmetry. Three-fold symmetry prisms refer to lithium 6 and 7; four-fold ones are in correspondence with beryllium 8, 9, and 10; and five-fold symmetry prisms with boron 10 and 11. Carbon is an unusual element. It has four isomers of different symmetry: three-fold, six-fold and tetrahedral ones. The two stable and one half-stable isotopes of carbon inherit the structure of these isomers.

The geometric models of nuclei, developed by analogy with the fullerene geometry, allow explain why the nuclei have a definite number of stable isotopes and isotopes having a large half-decay period. Contrary to the usual "arithmetic approach", when the nuclear reactions are written down simply as, e.g. ${}^{12}C + {}^{4}He \rightarrow {}^{16}O$ or ${}^{16}O + {}^{4}He \rightarrow {}^{20}Ne$ [1], we have used the geometric approach, when the reactions are considered if the reacting nuclei are compatible from the geometric standpoint.

In this contribution I submit the geometric approach which explains not only the generation of nitrogen, oxygen, fluorine and neon but also that of their isotopes and isomers in the framework of one and the same unified modeling. It should be emphasized that we use, instead of this vague notion "nuclear isomerism" [1], the clear notion accepted for molecules, i.e. we accept that space isomerism of nuclei is the phenomenon which consists in the existence of nuclei having an equal mass number but different positions of the nuclear constituents in the space.

2. Isotopes of nitrogen and their isomers

There are two stable isotopes of nitrogen: $_7N^{14}$ (99.63 %) and $_7N^{15}$ (0.37%) [2]. This brings up the question: how to obtain them and their space isomers? It has stated above that the reacting nuclei should be compatible from the geometric standpoint. Using the previous experience, write down the nuclear reactions which are geometrically compatible:

$${}^{4}He + {}^{6}Li \rightarrow ({}^{4}He^{6}Li) + {}^{4}He \rightarrow {}^{14}N, \quad {}^{4}He + {}^{7}Li \rightarrow ({}^{4}He^{7}Li) + {}^{4}He \rightarrow {}^{15}N$$

They formally describe the formation of nitrogen isotopes. The reactions are written in line with the postulate by Svante August Arrhenius (1889) according to which a chemical reaction is a two-stage process. At first, there forms an intermediate compound and afterwards a usual chemical reaction is going on. Now we investigate this question more closely.

2.1. Joining a tetrahedron with a triangular prism. From the geometric point of view, the headline is in conformity with reaction ${}^{4}He + {}^{6}Li \rightarrow ({}^{4}He^{6}Li) \rightarrow {}^{10}B$ which is illustrated in Fig. 1. From the figure it follows that helium is almost completely dissolved in the boron structure formed. As for lithium, only three protons (from six) take part actually in the reaction. The reacting particles are specially marked in the figure; the protons are light pink balls, the new proton-proton bonds are lilac, the old bonds, which have to be destroyed, are shown using red dot lines. The graph representation of the reaction is shown in Fig. 2.



Fig. 1. Joining of a tetrahedron (α -particle) to a triangular-prism (${}^{6}Li$): *a*) separate tetrahedron and triangular prism; proton bonds (red lines), reacting protons (light pink spheres), neutral atoms (dark pink spheres), *b*) intermediate compound: old bonds to be destroyed (red dot lines), new bonds (lilac lines), *c*) semiregular heptahedron (${}^{10}B$)



Fig. 2. Graph representation of the nuclear reaction ${}^{4}He + {}^{6}Li \rightarrow {}^{10}B$. Embedding the graph of α - particle into the graph of lithium: *a*) separate graphs corresponding to a triangular prism (above) and to a tetrahedron (below), *b*) embedding, *c*) graph of tri-(tetra-penta)₃ polyhedron shown in Figure 1c. All notations are the same as before

To get a comprehensive idea of the fusion, one need to construct a tertion net and its graph. Since graph designing is simpler, we begin with it. There is no need to construct the graph of the tertion net *ab ovo*. One can take as a base the graph of the proton cell and put on its edges the tertions, and then to connect them (brown lines) (Fig. 3a). Removing the base, one receives the graph of the tertion net (Fig. 3b). Having this graph and the proton cell shown above (Fig. 1c), designing the tertion net becomes easier (Fig. 3c).

Nuclear geometry: from nitrogen to neon



Fig. 3. Electronic structure of boron ¹⁰B: *a*) graph of tertion net being constructed on the base of the proton-cell graph denoted by dot red lines; *b*) graph of tertion net; *c*) tertion net

2.2. Joining a tetrahedron with a semiregular heptahedron. By analogy with the previous procedure one can design reaction ${}^{4}He + {}^{10}B \rightarrow ({}^{4}He^{10}B) \rightarrow {}^{14}N$ which is illustrated in Fig. 4. One can see that helium is again completely dissolved in the nitrogen structure formed. As for boron, only three protons (from ten) take part in the reaction. The reacting particles are specially marked in the figure as before: the protons are light pink balls, the new proton-proton bonds are lilac, the old bonds, which have to be destroyed, are shown using red dot lines. The graph representation of the nuclear reaction is shown in Fig. 5. The tertion net and its graph are presented in Fig. 6.



Fig. 4. Joining of a tetrahedron to a heptahedron: *a*) separate tetrahedron (α -particle) and heptahedron (${}^{10}B$), *b*) intermediate compound, *c*) regular nonahedron (${}^{14}N$)



Fig. 5. Graph representation of the nuclear reaction ${}^{4}He + {}^{10}B \rightarrow {}^{14}N$. Embedding the graph of boron into the graph of α - particle: *a*) inversion graph of α - particle above and boron graph below, *b*) embedding, *c*) graph of tetra₆-hexa₃ nonahedron shown in Fig. 4c. All notations are the same as before



Fig. 6. Electronic structure of nitrogen ¹⁴N: a) graph of tertion net being constructed on the base of the proton-cell graph denoted by dot red lines; b) graph of tertion net; c) tertion net

2.3. *Embedding isotopy*. The reactions considered above ${}^{4}He + {}^{6}Li \rightarrow ({}^{4}He^{6}Li) \rightarrow {}^{10}B$ and ${}^{4}He + {}^{10}B \rightarrow ({}^{4}He^{10}B) \rightarrow {}^{14}N$ show the mechanism of obtaining the nucleus of nitrogen 14. If to replace in these reactions lithium 6 by lithium 7, i.e. to consider reactions ${}^{4}He + {}^{7}Li \rightarrow ({}^{4}He^{7}Li) \rightarrow {}^{11}B, {}^{4}He + {}^{11}B \rightarrow ({}^{4}He^{11}B) \rightarrow {}^{15}N,$

one can construct the nucleus of nitrogen 15. The structure of the reaction components is presented in Fig. 7. From the figure it follows that the proton cells become the body-centered ones. The most drastic changes are connected with the tertion nets and their graphs.



Fig. 7. Structure of the nuclear reaction; each column contains successively proton cell, tertion net and graph of the tertion net: a) lithium 7; b) boron 11; c) nitrogen 15

Nuclear geometry: from nitrogen to neon

2.4. Another isomer. Modeling the growth of fullerenes [3], we obtained two isomers of C_{14} , one having the shape similar to that of presented in Fig. 4c; the other is shown in Fig. 8 and corresponds to reaction $C_4+C_{10} \rightarrow (C_4C_{10}) \rightarrow C_{14}$. It should be emphasized that the second fullerene isomer was designed by the mechanisms which are typical for the fullerenes, but not for the nuclei. The question arises how to obtain the same shape for the nucleus of nitrogen 14 through the use of possible nuclear reactions only.



Fig. 8. C_{14} as joining cluster C_4 with cupola C_{10} ; Dark–red and light-blue balls are reacting and neutral atoms, respectively; solid and dot red lines are new covalent bonds

One has to approach the problem in stages. Fist of all it is necessary to set up a topological correspondence between the reacting constituents of the fullerene and those of the nucleus designed. Clear that cluster C₄ can be associated with α -particle and cupola C₁₀ with an intermediate nucleus ¹⁰B. Therefore the general problem is reduced to the problem how to obtain the intermediate nucleus ¹⁰B having the shape similar to cupola C₁₀.

One is inclined to think that there is the following chain of nuclear reactions (Fig. 9). At first, two alpha-particles combine forming a dimer (a). Then the dimer combines with another alpha-particle forming a linear trimer having one proton, which is slightly connected with the trimer through the use of only one bond (b). Similar to the interactions of electronic and atomic degrees of freedom [4], the interaction of tertions (they are not shown in the figure) and protons leads to internal rotation [5] of the slightly connected proton (c). This structure can fold up in three dimensions (d). During the process some inter-proton bonds are destroyed and there appear two split protons (e). Relaxation of the structure obtained creates the boron nucleus having three-fold symmetry (f). The reactions can be written as

 ${}^{4}He + {}^{4}He \rightarrow ({}^{4}He^{4}He) + {}^{4}He \rightarrow ({}^{4}He^{4}He) \rightarrow {}^{10}B + d.$



Fig. 9. Generation of boron-10 isomer: a) dimer formation, b) trimer formation with one slightly connected proton, c) internal rotation of the proton, d) folding and appearance of two new slightly connected protons, e) folding and splitting two new protons, f) heptahedron structure obtained after relaxation

2.5. Joining a tetrahedron with another heptahedron. Now it is possible to design another reaction ${}^{4}He + {}^{10}B \rightarrow ({}^{4}He^{10}B) \rightarrow {}^{14}N$ which is illustrated in Fig. 10. One can see that helium is again completely dissolved in the nitrogen structure formed. As for boron, now six protons (from ten) take part in the reaction. The reacting particles are specially marked in the figure as before: the reacting protons are light pink balls, the new proton-proton bonds are lilac, the old bonds, which have to be destroyed, are shown using red dot lines. The graph representation of the nuclear reaction is given in Fig. 11. The tertion net and its graph are presented in Fig. 12.



Fig. 10. Joining of a tetrahedron to a heptahedron: *a*) separate tetrahedron (α -particle) and heptahedron (${}^{10}B$), *b*) intermediate compound, *c*) base-truncated triangular bipyramid (${}^{14}N$)



Fig. 11. Graph representation of the nuclear reaction ${}^{4}He + {}^{10}B \rightarrow {}^{14}N$. Embedding the graph of boron into the graph of α - particle: *a*) inversion graph of α - particle above and boron graph below, *b*) embedding, *c*) graph of tetra₃-penta₆ base-truncated triangular bipyramid shown in Fig. 10c. All notations are the same as before

Nuclear geometry: from nitrogen to neon



Fig. 12. Electronic structure of nitrogen isomer ¹⁴N: *a*) constructing the graph of tertion net on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

2.6. *Embedding isotopy*. The reaction considered above ${}^{4}He + {}^{10}B \rightarrow ({}^{4}He^{10}B) \rightarrow {}^{14}N$ shows the mechanism of obtaining the nucleus of nitrogen 14. If to replace in that reaction boron 10 by boron 11, i.e. to consider reaction ${}^{4}He + {}^{11}B \rightarrow ({}^{4}He^{11}B) \rightarrow {}^{15}N$, one can construct the nucleus of another isotope of nitrogen 15 (Fig. 13).



Fig. 13. Structure of isotope ¹⁵N: a) proton cell; b) graph of the tertion net; c) tertion net

3. Isotopes of oxygen and their isomers

There are three stable isotopes of oxygen: ${}_{8}O^{16}$ (99.76 %), ${}_{8}O^{17}$ (0.04 %) and ${}_{8}O^{18}$ (0.20 %) [2]. As stated above, the reacting nuclei should be compatible from the geometric standpoint. Using our previous experience, write down the nuclear reactions which are geometrically compatible:

$${}^{12}C + {}^{4}He \to {}^{16}O, \quad {}^{13}C + {}^{4}He \to {}^{17}O$$
$${}^{8}Be + {}^{8}Be \to {}^{16}O, \quad {}^{8}Be + {}^{9}Be \to {}^{17}O, \quad {}^{9}Be + {}^{9}Be \to {}^{18}O$$

They formally describe the formation of oxygen isomers and isotopes. Now we investigate the reactions more closely.

3.1. Joining of a tetrahedron to a heptahedron. Reaction ${}^{4}He + {}^{12}C \rightarrow ({}^{4}He^{12}C) \rightarrow {}^{12}O$ is illustrated in Fig. 14. From the figure it follows that helium is almost completely dissolved in the carbon structure formed. As for carbon, only three protons (from six) take part actually in the reaction. The graph representation of the nuclear reaction is shown in Fig. 15. The tertion net and its graph are presented in Fig. 16.



Fig. 14. Joining of a tetrahedron to a heptahedron: *a*) separate tetrahedron (α -particle) and truncated tetrahedron (${}^{12}C$), *b*) intermediate compound, *c*) another truncated tetrahedron (${}^{16}O$)



Fig. 15. Graph representation of the nuclear reaction ${}^{4}He + {}^{12}C \rightarrow {}^{16}O: a)$ inversion graph of α - particle above and carbon graph below, b) embedding, c and c') graphs of tri₄-hexa₆-truncated tetrahedron shown in Fig. 14c. All notations are the same as before



Fig. 16. Electronic structure of oxygen isomer ¹⁶O: *a*) graph of tertion net constructed on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

3.2. *Embedding isotopy*. The reaction considered above shows the mechanism of obtaining the nucleus of oxygen 16. If to replace in that reaction carbon 12 by carbon 13, i.e. to consider reaction ${}^{4}He + {}^{13}C \rightarrow ({}^{4}He^{13}C) \rightarrow {}^{17}O$, one may obtain an isotope of oxygen 17 (Fig. 17).



Fig. 17. Structure of isotope ¹⁷O: a) Proton cell; b) Graph of the tertion net; c) Tertion net



Fig. 18. Joining of two cubes: *a*) separate cubes (beryllium) *b*) intermediate compound, *c*) square barrel-shape decahedron $\binom{^{16}O}{}$



Fig. 19. Fusion of two cubes as connection of their graphs: *a*) separate graphs (beryllium) *b*) intermediate compound, *c*) square barrel-shape decahedron (${}^{16}O$)



Fig. 20. Electronic structure of oxygen isomer 16 O: *a*) graph of tertion net (brown lines) constructed on the basis of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

3.4. Embedding isotopy. The reaction considered above shows the mechanism of obtaining the nucleus of another isomer of oxygen 16. Replace again in that reaction one

beryllium 8 by beryllium 9; then we obtain another isotope of oxygen 17 (Fig. 21). Replacing both beryllium 8 by beryllium 9, we have an isotope of oxygen 18 (Fig. 22).



Fig. 21. Structure of isotope ¹⁷O: a) Proton cell; b) Graph of the tertion net; c) Tertion net



Fig. 22. Structure of isotope ¹⁸O: a) proton cell; b) graph of the tertion net; c) tertion net

4. Isotopes and isomers of fluorine

There is only one stable isotope of fluorine, ${}_{9}F^{19}$ (100 %), and an unstable isotope having a comparatively large half-decay period being equal to 109.8 min., ${}_{9}F^{18}$ [2]. As we stated above, the reacting nuclei should be compatible from the geometric standpoint. Using the previous experience, write down the geometrically compatible nuclear reaction ${}^{12}C + {}^{6}Li \rightarrow {}^{18}F$. Consider the reaction more closely.

4.1. Joining of a triangular prism to a triangular barrel. The reaction is illustrated in Fig. 23. From the figure it follows that only three protons of lithium (from six) and three protons of carbon (from twelve) take part actually in the reaction. The graph representation of the nuclear reaction is shown in Fig. 24. The tertion net and its graph are presented in Fig. 16.



Fig. 23. Joining of a triangular prism to a triangular barrel: *a*) separate prism (lithium) and separate barrel (carbon) *b*) intermediate compound, *c*) (tri-penta₃)₂-hexa₃ polyhedron (${}^{18}F$)



Fig. 24. Embedding the graph of carbon into the graph of lithium: a) separate graphs, b) embedding, c) graph of (tri-penta₃)₂-hexa₃ polyhedron (fluorine)



Fig. 25. Electronic structure of fluorine isomer ¹⁸F: *a*) graph of tertion net constructed on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

4.2. *Embedding isotopy*. If to replace in that reaction lithium 6 by lithium 7 or carbon 12 by carbon 13, i.e. to consider reactions ${}^{7}Li + {}^{12}C \rightarrow {}^{19}F$ or ${}^{6}Li + {}^{13}C \rightarrow {}^{19}F$, one haso0n one and the same isotope of fluorine 19 (Fig. 26). It should be emphasized that, on the basis of previous results, the first reaction is more probable.



Fig. 26. Structure of isotope ¹⁹F: a) Proton cell; b) Graph of the tertion net; c) Tertion net

4.3. Joining of a triangular prism to a truncated tetrahedron. The reaction illustrates an example of nuclear special isomerism (Fig. 27). Here the number of reacting protons is increased from six to nine. 3. The figure obtained has the shape of a truncated triangular bipyramid. The graph representation of the nuclear reaction is shown in Fig. 28. The tertion net and its graph are presented in Fig. 29.



Fig. 27. Joining of a triangular prism to a truncated tetrahedron: *a*) separate prism (lithium) and separate truncated tetrahedron (carbon) *b*) intermediate compound, *c*) truncated triangular bipyramid (${}^{18}F$)



Fig. 28. Embedding the graph of carbon into the graph of lithium: *a*) separate graphs, *b*) embedding, *c*) graph of truncated triangular bipyramid (fluorine)

Nuclear geometry: from nitrogen to neon



Fig. 29. Electronic structure of fluorine isomer ¹⁸F: *a*) graph of tertion net constructed on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

4.4. *Embedding isotopy*. If to replace in reaction ${}^{12}C + {}^{6}Li \rightarrow {}^{18}F$ lithium 6 by lithium 7 or carbon 12 by carbon 13 one obtains one and the same isotope of fluorine 19 (Fig. 30). It should be emphasized that, on the basis of previous results, the first reaction is more probable.



Fig. 30. Structure of isotope ¹⁹F: a) proton cell; b) graph of the tertion net; c) tertion net

5. Isotopes of neon and their isomers

There are three stable isotopes of neon: ${}_{10}\text{Ne}^{20}$ (90.51 %), ${}_{10}\text{Ne}^{21}$ (0.27 %) and ${}_{10}\text{Ne}^{22}$ (9.22 %) [2]. The crucial question is how to obtain them and their space isomers in the framework of one and the same assumptions. Consider the nuclear reactions which are geometrically compatible.

5.1. Fusion of two pentagonal pyramids. The reaction is written as ${}^{10}B + {}^{10}Be \rightarrow {}^{20}Ne$. It is illustrated in Figs. 31, 32 and 33.



Fig. 31. Joining of two prisms: *a*) separate prisms (boron) *b*) intermediate compound, *c*) dodecahedron $\binom{20}{Ne}$



Fig. 32. Fusion of two prisms as connection of their graphs: *a*) separate graphs (boron) *b*) intermediate compound, *c*) dodecahedron (²⁰Ne)



Fig. 33. Electronic structure of neon isomer ²⁰Ne: *a*) graph of tertion net constructed on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

5.2. Two-stage reactions. The reactions can be written as ${}^{12}C + {}^{4}He \rightarrow {}^{16}O, {}^{16}O + {}^{4}He \rightarrow {}^{20}Ne.$

As it was shown, carbon 12 has several space isomers. Therefore there appear several space isomers of neon.

5.2.1. Joining two tetrahedrons with a hexagonal prism. Those two- stage reactions are illustrated in Figs. 34-35. The graph representation of the nuclear reactions is shown in Fig. 36. . The tertion net and its graph are presented in Fig. 37.



Fig. 34. Joining of a tetrahedron (α -particle) to a hexagonal prism (${}^{12}C$): *a*) separate tetrahedron and hexagonal prism; proton bonds (red lines), reacting protons (light pink spheres), neutral atoms (dark pink spheres), *b*) intermediate compound: old bonds to be destroyed (lilac dotted lines), new bonds (lilac lines), *c*) cupola of three-fold symmetry (${}^{16}O$)

Nuclear geometry: from nitrogen to neon



Fig. 35. Joining of a tetrahedron to a cupola: *a*) separate tetrahedron (α -particle) and cupola (${}^{16}O$), *b*) intermediate compound, *c*) tetra₃-penta₆-hexa₃ dodecahedron (${}^{20}Ne$)



Fig. 36. Embedding the graph of α -particle into the graph of carbon (a, b, c); embedding the graph of cupola into the graph of α -particle (d, e, f)



Fig. 37. Electronic structure of neon isomer ²⁰Ne: *a*) graph of tertion net constructed on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

5.2.2. Joining two tetrahedrons with a triangular barrel. Those two- stage reactions are presented in Figures 37-38. The graph representation of the nuclear reactions is shown in Fig. 39. The tertion net and its graph are illustrated in Fig. 40.



Fig. 37. Joining of a tetrahedron (α -particle) to a triangular barrel (${}^{l2}C$): *a*) separate tetrahedron and triangular barrel, *b*) intermediate compound, *c*) tri-(tetra-penta-hexa)₃ decahedron (${}^{l6}O$)



Fig. 38. Joining of a tetrahedron to a decahedron: *a*) separate tetrahedron (α -particle) and decahedron (${}^{16}O$), *b*) intermediate compound, *c*) (tetra-hexa)₆ dodecahedron (${}^{20}Ne$)



Fig. 39. Embedding the graph of α -particle into the graph of carbon (a, b, c); embedding the graph of oxygen into the graph of α -particle (d, e, f)



Fig. 40. Electronic structure of neon isomer ²⁰Ne: *a*) graph of tertion net constructed on the base of the proton-cell graph (dot red lines); *b*) graph of tertion net; *c*) tertion net

5.3. *Embedding isotopy*. If to replace in the previous reactions carbon 12 (hexagonal prism) by carbon 13 (body centered hexagonal prism), one obtains the isotope of neon 21 shown in Fig. 41. Replacing carbon 12 (triangular barrel) by carbon 14 (dimer embedded triangular barrel) leads to appearance of the isotope neon 22 (Fig. 42). It should be emphasized that here only the most probable reactions of the isotopes are considered.



Fig. 41. Structure of isotope ²¹Ne: a) proton cell; b) graph of the tertion net; c) tertion net



Fig. 42. Structure of isotope 22 Ne: a) proton cell; b) graph of the tertion net; c) tertion net

6. Discussion

As stated above, there are two stable isotopes of nitrogen, $_7N^{14}$ (99.63 %) and $_7N^{15}$ (0.37%), three stable isotopes of oxygen, $_8O^{16}$ (99.76 %), $_8O^{17}$ (0.04 %) and $_8O^{18}$ (0.20 %), only one

stable isotope of fluorine, ${}_{9}F^{19}$ (100 %), and three stable isotopes of neon, ${}_{10}Ne^{20}$ (90.51 %), ${}_{10}Ne^{21}$ (0.27 %) and ${}_{10}Ne^{22}$ (9.22 %) [2]. Consider the most stable isotopes: nitrogen ${}_{7}N^{14}$ (99.63 %), oxygen ${}_{8}O^{16}$ (99.76 %), fluorine ${}_{9}F^{19}$ (100 %), neon: ${}_{10}Ne^{20}$ (90.51 %) and neon ${}_{10}Ne^{22}$ (9.22 %). They can be classed into two groups: basic nuclei having equal number of protons and neutrons (Fig. 43) and isotopes having one or two more neutrons (Fig. 44).



Fig. 43. Protonic and electronic structure of basic nuclei: a) nitrogen, b) oxygen c) neon

It should be noted that the nuclei of the first group have several space isomers. By analogy with fullerenes, only such isomers were chosen which have the most probability of generation. What all the nuclei have in common is that their proton structure is stable with respect to mechanical shear stresses. At the same time basic nuclei of the second group are unstable with respect both shear stresses and thermal vibrations. However they acquire stability incorporating one or two neutrons. It is believed that the stability is ensured also by the coat of mail (tertion net) which becomes denser after the nuclei embed the extra neutrons.



Fig. 44. Protonic and electronic structure of isotopes: a) fluorine, b) neon

7. Summary

By analogy with fullerenes, the nuclear geometry has been designed. For nitrogen, oxygen, fluorine and neon the protonic and electronic structures both for basic isomers and their

isotopes were obtained. The most stable nuclei can be classed into two groups: basic nuclei having equal number of protons and neutrons and isotopes having one or two more neutrons. The latter ensure their mechanical stability with respect to shear stresses, sending their electron to the coat of mail created by the basic nuclei.

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NUCLEAR GEOMETRY: SODIUM, MAGNESIUM, ALUMINUM

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Abstract. The nuclear geometry has been developed by analogy with the fullerene geometry. On the basis of this geometric approach, it was possible to design the structure of sodium, magnesium and aluminum isomers and their isotopes, which can be obtained by means of nuclear synthesis. The most stable nuclei can be classed into two groups: basic nuclei having equal number of protons and neutrons and isotopes having one or two more neutrons. The latter ensure their mechanical stability with respect to shear stresses, sending their electron to the coat of mail created by the basic nuclei.

Keywords: aluminum, graph representation, isomer, isotope, magnesium, nuclear electron, nuclear geometry, nuclear reaction, sodium

1. Introduction

Earlier, by analogy with fullerenes, the nuclear geometry has been designed The geometric models of nuclei, developed by analogy with the fullerene geometry, allow explain why the nuclei have a definite number of stable isotopes and isotopes having a large half-decay period. Contrary to the usual "arithmetic approach", when the nuclear reactions are written down simply as in chemistry, the geometric approach was used when the reactions are considered, if the reacting nuclei are compatible from the geometric standpoint.

In this contribution I expand the geometric approach which explains not only the generation of sodium, magnesium and aluminum but also that of their isotopes and isomers in the framework of one and the same unified modeling. It should be emphasized again that I use, instead of the vague notion "nuclear isomerism" [1], the clear notion accepted for molecules, i.e. I accept that space isomerism of nuclei is the phenomenon which consists in the existence of nuclei having an equal mass number but different positions of the nuclear constituents in the space.

2. Isomers of sodium and their isotopes

There is only one stable isotope of sodium, ${}_{11}Na^{23}$ (100 %), and an unstable isotope having a comparatively large half-decay period being equal to 2.602 y, ${}_{11}Na^{22}$ [2]. Previously it was suggested that nuclei can be separated into two main types: basic nuclei having equal number of protons and neutrons and isotopes having one or two more neutrons. First consider simpler basic nucleus, ${}_{11}Na^{22}$ that can be obtained by two ways:

through the use of reaction $d + {}_{10}Ne^{20} \rightarrow {}_{11}Na^{22}$, and

by means of two-stage reaction ${}^{10}C + {}^{4}He \rightarrow {}^{16}O, {}^{16}C + {}^{6}Li \rightarrow {}^{22}Na.$

Consider the first reaction more closely.

2.1. Joining a dimer to a $(tetra-hexa)_3$ -penta₆ dodecahedron. The reaction is illustrated in Figs. 1, 2 and 3. Here a deuteron is incorporated into a basic nucleus of neon having three-fold symmetry. From Fig. 1 it follows that for neon only four protons from twenty take part

really in the reaction. They are specially marked in the figure; the protons are pinked, the new proton-protons bonds are lilac, the old bonds, which were destroyed, are shown using red dot lines. Here tertions are omitted.



Fig. 1. Attachment of deuteron to neon: *a*) separate particles; *b*) intermediate compound; *c*) sodium 22 Na after relaxation



Fig. 2. Graph representation of the nuclear reaction $d + {}_{10}Ne^{20} \rightarrow {}_{11}Na^{22}$. Embedding the graph of deuteron into the graph of neon: *a*) separate graphs corresponding to a dimer (at the left) and to a tetra₃-penta₆-hexa₃ dodecahedron (at the right); *b*) embedding, *c*) graph of the tetra-penta₁₀-hexa₂ triacaidecahedron shown in Fig. 1c. All notations are the same as before



Fig. 3. Electronic structure of sodium 22 Na: *a*) graph of tertion net being constructed on the base of the proton-cell graph (red dot lines; *b*) separate graph of tertion net; *c*) tertion net

2.2. Two-stage reaction. Now consider the two-stage reaction which is written above as ${}^{12}C + {}^{4}He \rightarrow {}^{16}O$, ${}^{16}O + {}^{6}Li \rightarrow {}^{22}Na$. The first stage is illustrated in Fig. 4 and consists in joining a tetrahedron with a hexagonal prism. Earlier this reaction was already analyzed as the fist stage for obtaining neon having the shape of tetra₃-penta₆-hexa₃ dodecahedron. The second stage is shown in Fig. 5. It consists in joining a triangular prism to a cupola of three-fold symmetry which was formed at the fist stage. The graph representation of the two-stage reaction is presented in Fig. 6.

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Fig. 4. Joining a tetrahedron (α -particle) to a hexagonal prism (${}^{12}C$): *a*) separate tetrahedron and hexagonal prism; proton bonds (red lines), reacting protons (light pink spheres), neutral atoms (dark pink spheres); *b*) intermediate compound: old bonds to be destroyed (red dot lines), new bonds (lilac lines); *c*) cupola of three-fold symmetry (${}^{16}O$)



Fig. 5. Joining a triangular prism to a cupola: *a*) separate prism (${}^{6}Li$) and cupola (${}^{16}O$), *b*) intermediate compound, *c*) tri-penta₉-hexa₃ triacaidecahedron (${}^{22}Na$)



Fig. 6. Graph representation of the two-stage nuclear reaction ${}^{12}C + {}^{4}He \rightarrow {}^{16}O + {}^{6}Li \rightarrow {}^{22}Na$. *a)* separate graphs corresponding to a tetrahedron (above) and to a hexagonal prism (down); b) embedding the graph of helium into the graph of carbon; c) graph of cupola oxygen; d) graphs corresponding to a triangular prism (above) and to a hexagonal cupola (below);

e) embedding the graph of oxygen into the graph of lithium; f) graph of sodium

Nuclear geometry: sodium, magnesium, aluminum

One additional remark is necessary. The final graph shown in Figure 6f reflects the three-fold symmetry of the sodium shape obtained. However we can consider this structure from another point of view. As noted above, the nuclei can be separated into two types: basic nuclei having equal number of protons and neutrons and isotopes having one or two more neutrons. Let's extend the classification. Among the basic nuclei we will recognize two subgroups: ideal (perfect) nuclei and imperfect ones. Similar to crystals, the perfect nuclei are highly symmetric. The imperfect nuclei have lost high symmetry and the loss is connected with structural defects. By analogy with crystals, one can consider the structure shown in Fig. 5f as a perfect classical dodecahedron by Plato which was spoiled by adding a defect in the form of an extra interstitial dimer. Following such approach developed for fullerenes [3] one defines such nuclei as having topological symmetry. The situation is illustrated in Fig. 7, where two graphs, corresponding with the shape shown in Fig. 5c, are presented. The graph at the left reflects the symmetry induced by an extra dimer, whereas the graph at the right emphasizes the topological symmetry.



Fig. 7. Two graphs of one and the same structure shown in Fig. 5c, reflecting different sides of symmetry: *a*) ordinary symmetry; *b*) topological symmetry

To gain a more penetrating insight into the electronic structure of imperfect nuclei, it is better to use topological symmetry. The tertion net and its graph, which are presented in Fig. 8, are designed through the use of topological symmetry.



Fig. 8. Electronic structure of sodium 22 Na: *a*) graph of tertion net being constructed on the base of the proton-cell graph (red dot lines); *b*) separate graph of tertion net; *c*) tertion net

2.3. Stability due to neutron embedding. Let's replace in the previous reactions neon 20 having the shape of a (tetra-hexa)₃-penta₆ dodecahedron by neon 21 (the same dodecahedron but body centered). Then there arises the isotope of sodium (²³Na) shown in Fig. 9. If to replace in the previous reactions carbon 12 (hexagonal prism) by carbon 13 (body centered hexagonal prism), there appears the isotope of sodium 23 shown in Fig. 10. It should be noted that in the first case additional tertions have the charge of ¹/₂ e, in the second case of ¹/₃ e. The

reasons are connected with the number of hexangular facets which incorporate the electrons of internal neutrons. So there leaves room for two isomers of sodium isotope, ²³Na.

Why the basic nuclei are unstable and the isotopes are stable? One can submit the following explanation. It is clear that any nucleus structure (proton cell) must be stable with respect to mechanical stresses which appear due to thermal vibrations of protons. It is assumed that the stability is insured by the coat of mail that dictates geometry of a proton cell. On the basis of the previous experience, one can envision that the coat of mail (tertion net), which ensures such stability, doesn't contain hexagons. The coat of mail of both basic isomers has the hexagons (Figs. 3 and 8). Embedding extra neutron eliminates the hexagons and does the coat of mail denser (Fig. 9 and 10). In its turn it leads to increasing stability and transforming the basic nuclei into the corresponding isotopes.



Fig. 9. Structure of isotope ²³Na: a) proton cell; b) graph of the tertion net; c) tertion net



Fig. 10. Structure of another isotope ²³Na: a) proton cell; b) tertion-net graph; c) tertion net

3. Isomers of magnesium and their isotopes

There are three stable isotopes of magnesium: ${}_{12}Mg^{24}$ (78.99 %), ${}_{12}Mg^{25}$ (10.00 %) and ${}_{12}Mg^{26}$ (11.01 %); beside there is an unstable isotope ${}_{12}Mg^{28}$, which has a reasonably small halfdecay period being equal to 21.07 hours [2]. The crucial question is again how to obtain them and their space isomers in the framework of one and the same assumptions. Previously it was suggested that the nuclei can be separated into two main types: the basic nuclei having equal number of protons and neutrons and the isotopes having one or two more neutrons. A better understanding can be gained if to begin with the basic nucleus, ${}_{12}Mg^{24}$ that can be obtained by various ways through the use of the most probable geometrically compatible reactions: ${}^{12}C + {}^{12}C \rightarrow {}^{24}Mg$, ${}^{8}Be + {}^{16}O + \rightarrow {}^{24}Mg$.
Nuclear geometry: sodium, magnesium, aluminum

3.1. Joining two hexagonal prisms. The reaction is illustrated in Figs. 11, 12 and 13. Here both configurations have six-fold symmetry. From Fig. 11 it follows that for each carbon only half protons take part in the reaction. They are specially marked in the figure; the protons are pinked, the new proton-protons bonds are lilac, the old bonds, which were destroyed, are shown using dotted lines. Here tertions are also omitted.



Fig. 11. Joining two hexagonal prisms: *a*) separate prisms (carbon); *b*) intermediate compound; *c*) regular penta₁₂-hexa₂ tettarecaidecahedron $({}^{24}Mg)$



Fig. 12. Graph representation of the nuclear reaction ${}_{6}C^{12} + {}_{6}C^{12} \rightarrow {}_{12}Mg^{24}$; embedding a graph of carbon into another: *a*) separate graphs corresponding to carbon nuclei; *b*) embedding, *c*) graph of the penta₁₂-hexa₂ polyhedron (${}^{24}Mg$)



Fig. 13. Electronic structure of six-fold symmetry magnesium 24 Mg: *a*) graph of tertion net constructed on the base of the proton-cell graph (red dot lines; *b*) separate graph of tertion net; *c*) tertion net

3.2. Joining a cube to a square barrel. The reaction is shown in Figs. 14, 15 and 16. Here both configurations have four-fold symmetry. From Fig. 14 it follows that for beryllium half protons take part in the reaction but for oxygen only four protons from sixteen do it. They are specially marked in the figure; the protons are pinked, the new proton-protons bonds are lilac, the old bonds, which were destroyed, are shown using dotted lines. Here tertions are also omitted.



Fig. 14. Joining a cube to a square barrel: *a*) cube (beryllium) at the top, barrel (oxygen) at the bottom; *b*) intermediate compound; *c*) regular tetra₂-penta₈-hexa₄ polyhedron of four-fold symmetry $\binom{24}{Mg}$



Fig. 15. Graph representation of the nuclear reaction ${}^{8}Be + {}^{16}O + \rightarrow {}^{24}Mg$; embedding the graph of oxygen into the graph beryllium: *a*) separate graphs corresponding to the nuclei; *b*) embedding, *c*) graph of the tetra₂-penta₈-hexa₄ polyhedron having four-fold symmetry (${}^{24}Mg$)



Fig. 16. Electronic structure of four-fold symmetry magnesium ²⁴Mg: *a*) graph of tertion net constructed on the basis of the proton-cell graph (red dot lines0; *b*) separate graph of tertion net; *c*) tertion net

3.3. Joining two truncated tetrahedra I. The reaction is illustrated in Figs. 17, 18 and 19. As a result we have obtained a basic nucleus of three-fold symmetry having equal number of protons and neutrons.



Fig. 17. Mirror-symmetry joining two truncated tetrahedra: *a*) separate tetrahedra (carbon); *b*) intermediate compound; *c*) regular tri₂-tetra₃-hexa₉ polyhedron of three-fold symmetry $({}^{24}Mg)$



Fig. 18. Graph representation of the nuclear reaction ${}_{6}C^{12} + {}_{6}C^{12} \rightarrow {}_{12}Mg^{24}$; embedding a graph of carbon into another one: *a*) separate graphs corresponding to carbon nuclei; *b*) embedding, *c*) graph of the tri₂-tetra₃-hexa₉ polyhedron of three-fold symmetry (${}^{24}Mg$)



Fig. 19. Electronic structure of three-fold symmetry magnesium ²⁴Mg: *a*) graph of tertion net being constructed on the basis of the proton-cell graph (red dot lines);
 b) separate graph of tertion net; *c*) tertion net

Joining two truncated tetrahedra considered refers to mirror reflection. However there is also rotatory reflection joining. This type is illustrated by the example of fullerenes. By analogy with the fullerenes consider the corresponding reaction.

3.3. Joining two truncated tetrahedra II. The reaction is shown in Figs. 20, 21 and 22.



Fig. 20. Rotatory-reflection joining two truncated tetrahedra: *a*) separate tetrahedra (carbon); *b*) intermediate compound; *c*) tri₂-penta₆-hexa₆ polyhedron of three-fold symmetry $({}^{24}Mg)$



Fig. 21. Graph representation of the nuclear reaction ${}_{6}C^{12} + {}_{6}C^{12} \rightarrow {}_{12}Mg^{24}$; embedding a graph of carbon into another one: *a*) separate graphs corresponding to carbon nuclei; *b*) embedding, *c*) graph of the tri₂-tetra₃-hexa₉ polyhedron of three-fold symmetry (${}^{24}Mg$)



Fig. 22. Electronic structure of three-fold symmetry magnesium ²⁴Mg: *a*) graph of tertion net being constructed on the base of the proton-cell graph (red dot lines);
 b) separate graph of tertion net; *c*) tertion net

Nuclear geometry: sodium, magnesium, aluminum

From the results obtained it follows that the basic nucleus magnesium 24 has few isomers having three, four and six-fold symmetry. Expanding the analogy, one can assume that the magnesium isotopes, having one, two or four internal neutrons, inherit also that symmetry.

3.4. One-neutron embedding isotopy. From the results obtained it may be concluded that magnesium isotopes ${}_{12}\text{Mg}^{25}$ having different symmetry can be formed by various ways. In the reactions described above

$$^{12}C + ^{12}C \rightarrow ^{24}Mg, \quad ^{8}Be + ^{16}O + \rightarrow ^{24}Mg,$$

here only basic nuclei having equal number of protons and neutrons are taken into attention. Let us replace one carbon 12 (hexagonal prism) with carbon 13 (body centered hexagonal prism) and beryllium 8 (cubic cell) with beryllium 9 (body centered cube), i.e. think over the reactions

$${}^{13}C + {}^{12}C \to {}^{25}Mg, \qquad {}^{9}Be + {}^{16}O + \to {}^{25}Mg.$$

In the first case we obtain the isotope of magnesium 25 having six-fold symmetry. It is shown in Fig. 23. In the second case replacing leads to appearance of the isotope magnesium 25 having four-fold symmetry, which is illustrated in Fig. 24. It should be emphasized that here only the most probable reactions with isotopes are considered.



Fig. 23. Structure of six-fold symmetry isotope ²⁵Mg: a) proton cell; b) graph of the tertion net; c) tertion net



Fig. 24. Structure of four-fold symmetry isotope ²⁵Mg: a) proton cell; b) graph of the tertion net; c) tertion net

From the results obtained, it follows also that in the first case the neutron decays into a proton and two negatively charged particles, having charge $\frac{1}{2}e$. In the second case the charge

is equal to $\frac{1}{4} e$. It was shown previously that the difference can be attributed to the Stark effect, if to associate splitting with symmetry of a nuclear cell and the number of hexagonal faces.

3.5. Two-neutrons embedding isotopy. Magnesium isotopes ${}_{12}Mg^{26}$ having different symmetry can be obtained by different ways: through the use of geometrically compatible reactions ${}^{13}C + {}^{13}C \rightarrow {}^{26}Mg$, rotatory reflection (Fig. 25) and mirror reflection (Fig. 26), and rotatory reflection one ${}^{12}C + {}^{14}C \rightarrow {}^{26}Mg$ (Fig. 27).



Fig. 25. Structure of three-fold mirror-symmetry isotope ²⁶Mg: a) proton cell; b) graph of the tertion net; c) tertion net



Fig. 26. Structure of isotope ²⁶Mg having three-fold rotatory reflection symmetry: a) proton cell; b) graph of the tertion net; c) tertion net



Fig. 27. Structure of isotope ²⁶Mg having six-fold symmetry: *a*) separate prisms; b) proton cell; c) core of the nucleus with the nearest cell protons and the binding tertions

Nuclear geometry: sodium, magnesium, aluminum

3.6. Four-neutrons embedding isotopy. Magnesium isotopes ${}_{12}Mg^{28}$ can be obtained through the use of the geometrically compatible reaction ${}^{14}C + {}^{14}C \rightarrow {}^{28}Mg$. The reaction is shown in Fig. 27. Here one runs into a new phenomenon. Up to now, when there were two internal neutrons, they were decomposed into protons and tertions by the external surroundings, the protons being tightly connected with the electronic coat of mail and maybe only slightly connected, if are connected at all, one another. Now it is seen that the internal protons form the core, they being tightly connected one another and slightly connected with the external electronic coat of mail (Fig. 28). Four internal neutrons give 12 tertions; 6 of them form the coat of mail of the core, 4 refer to the bonds connecting the core and the external proton cell and 2 are incorporated into the external coat of mail. All tertions have the charge $\frac{1}{3}e$; they are specially marked in emerald in Fig. 28.



Fig. 27. Structure of isotope ²⁸Mg having six-fold symmetry: *a*) separate prisms (carbon 14); b) proton cell; c) core of the nucleus with the nearest cell protons and the binding tertions



Fig. 28. Electronic structure of six-fold symmetry magnesium isotope 28 Mg: *a*) core tertion net (octahedron); *b*) binding tertion net (tetrahedron); *c*) tertion net of an external coat of mail

4. Isotopes of aluminum and their isomers

There is only one stable isotope of aluminum, ${}_{13}Al^{27}$ (100 %), and an 'unstable' isotope however having a very large half-decay period being equal to $7.2 \cdot 10^5$ y, ${}_{13}Al^{26}$ [2]. The latter is a basic nucleus having equal number of protons and neutrons. From the aforesaid, it follows that it is easier to consider at first a simpler basic nucleus. It can be obtained by several ways, but the simplest one is through the use of reaction $d + {}_{12}Mg^{24} \rightarrow {}_{13}Al^{26}$.

4.1. Incorporating a dimer into a penta₁₂-hexa₂ polyhedron. The reaction is illustrated in Figs. 29 and 30. Here a deuteron is incorporated into a basic nucleus of magnesium having six-fold symmetry. From Fig. 29 it follows that for magnesium only four protons from twenty four take part really in the reaction. They are specially marked in the figure; the protons are pinked, the new proton-protons bonds are lilac, the old bonds, which were destroyed, are not shown. Here tertions are omitted.



Fig. 29. Attachment of deuteron to magnesium: *a*) separate particles; *b*) intermediate compound; *c*) aluminum (²⁶Al) after relaxation



Fig. 30. Graph representation of the nuclear reaction $d + {}_{12}Mg^{24} \rightarrow {}_{13}Al^{26}$. Embedding the graph of deuteron into the graph of magnesium: *a*) separate graphs corresponding to a dimer (at the left) and to a penta₁₂-hexa₂ polyhedron (at the right); *b*) embedding, *c*) graph of the penta₁₂-hexa₃ polyhedron. All notations are the same as before

One can consider aluminum 26 obtained as a polyhedron having topological six-fold symmetry. At the same time it has ordinary three-fold symmetry as it shown in Fig. 31. The electronic structure corresponding to three-fold symmetry is illustrated in Fig. 32.



Fig. 31. Structure of aluminum 26 and its graph showing three fold symmetry



Fig. 32. Electronic structure of aluminum 26: *a*) graph of tertion net being constructed on the base of the proton-cell graph; *b*) separate graph of tertion net; *c*) tertion net

4.3. Neutron embedding. Let's replace in the previous reaction magnesium 24 having the shape of a penta₁₂-hexa₂-polyhedron by magnesium 25 (the same polyhedron but body centered). Then we obtain the isotope of aluminum $\binom{27}{Al}$ shown in Fig. 33. It should be noted that in this case additional tertions have the charge of $\frac{1}{3}e$. The reasons are connected with the number of hexangular facets which incorporate the electrons of an internal neutron.

Why the basic nucleus and the isotope are stable? One can suggest the following explanation. It is clear that any nucleus structure (proton cell) must be stable with respect to mechanical stresses which appear due to thermal vibrations of protons. Assume that the stability is insured by the coat of mail that dictates geometry of a proton cell. On the basis of the previous experience, we came to conclusion that the coat of mail (tertion net), which ensures additional stability, doesn't contain hexagons.



Fig. 33. Structure of isotope ²⁷Al: a) proton cell; b) graph of the tertion net; c) tertion net

5. Summary

By analogy with fullerenes, the nuclear geometry has been designed. For sodium, magnesium and aluminum, the protonic and electronic structures both for basic isomers and their isotopes were obtained. The most stable nuclei can be classed into two groups: basic nuclei having equal number of protons and neutrons and isotopes having one or two neutrons. The latter ensure their mechanical stability with respect to shear stresses, sending their electrons to the coat of mail created by the basic nuclei.

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(3)

MATERIAL BEHAVIOUR DURING A COMPLEX STRESS TEST OF THIN-WALLED, CYLINDRICAL SINGLE-CRYSTAL SPECIMENS

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Abstract. The von Mises and Hill yield criteria are commonly used when the stress-strain state of parts under complex loading conditions is calculated. However, those yield criteria are not suitable in some materials and do not reliably describe the inelastic behavior of the material under complex stress conditions. The development of a simple and accurate criterion of plastic flow is relevant. This paper presents the results of the yield criterion development for a single crystal nickel-based superalloy (ZhS32) based on the systematization of experimental data. Various types of stress state were realized during the experiment: tension, compression, torsion, as well as combinations of tension-torsion, compression-torsion.

Keywords: single-crystal, crystallographic orientation, anisotropy, stress-strain state, plasticity, yield strength, ultimate strength, complex stress test

1. Introduction

The complex geometric shapes of gas turbine engine parts and the loads acting on them lead to an inhomogeneous complex stress-strain state. The stress state can be estimated using the Lode-Nadai coefficient (1) [1,2] or the stress triaxiality factor (2) [3]:

$$\mu = 2 \frac{\sigma_2 - \sigma_3}{\sigma_1 - \sigma_3} - 1,$$
(1)

$$\eta = -\frac{\sigma_0}{\sigma_i} - 1,$$
(2)

where σ_1 , σ_2 , and σ_3 are the principal stresses, σ_0 is the mean stress among the normal stresses or hydrostatic pressures, and σ_i is the stress intensity.

When parameters (1) and (2) at the nodes of the finite element model (FEM) of a modern turbine blade are calculated, large areas of the blade cover a complex stress state. Fig. 1 shows the distribution histograms of the Lode-Nadai coefficient at the nodes of the FEM of the blades with convective and perspective cooling systems, respectively.

Many criteria can quantitatively evaluate the complex stress state and the complex strain state. These criteria apply to various types of materials [4-6]. One of the main yield criteria studied by engineers is the criterion of maximum shear stress or the Tresca criterion (3) [7,8]. The yield criterion is as follows: plastic strains in the material occur when the maximum shear stress reaches its critical value.

 $\sigma_1 - \sigma_3 = \sigma_Y$, where σ_Y is the yield strength. Material behaviour during a complex stress test of thin-walled, cylindrical single-crystal specimens



Fig. 1. Distribution histograms of the Lode-Nadai coefficient for the different blades

The next and most popular yield criterion is the von Mises criterion (4) [7,8]. This criterion is also called energetic because it is based on the potential energy of shape change. $\frac{1}{2}\sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_2 - \sigma_4)^2} = \sigma_{V_1}$ (4)

reduced stress. The reduced stress is the maximum among the normal components of the stress deviator.

$$max\{|\sigma_1 - \sigma_0|, |\sigma_2 - \sigma_0|, |\sigma_3 - \sigma_0|\} = \frac{2}{3}\sigma_Y.$$
(5)

Currently, many yield criteria have been developed based on the systematization of experimental data, such as Mohr, Pisarenko-Lebedev, Hill, and Tsai-Wu [9,10]. If a criterion based on the systematization of experimental data is used, determining its coefficients from tests is required [e.g., Mohr's criterion (6) or the Pisarenko-Lebedev criterion (7)].

$$\sigma_1 - \chi \sigma_3 = \sigma_{Y},\tag{6}$$

$$\chi \sigma_i + (1 - \chi) \sigma_1 = \sigma_Y,\tag{7}$$

where χ is the tensile/compressive yield strength ratio, σ_i – stress intensity.

Hill yield criterion is often used when stress-strain state calculations for anisotropic parts are performed.

$$F(\sigma_{x} - \sigma_{y})^{2} + G(\sigma_{y} - \sigma_{z})^{2} + H(\sigma_{z} - \sigma_{x})^{2} + 2L\tau_{xy}^{2} + 2M\tau_{yz}^{2} + 2N\tau_{zx}^{2} - \sigma_{y}^{2} = 0$$
(8)
where $F = \frac{1}{2} \left(\frac{1}{R_{x}^{2}} + \frac{1}{R_{y}^{2}} - \frac{1}{R_{z}^{2}} \right)$, $G = \frac{1}{2} \left(\frac{1}{R_{y}^{2}} + \frac{1}{R_{z}^{2}} - \frac{1}{R_{x}^{2}} \right)$, $H = \frac{1}{2} \left(\frac{1}{R_{z}^{2}} + \frac{1}{R_{x}^{2}} - \frac{1}{R_{y}^{2}} \right)$, $L = \frac{3}{2} \left(\frac{1}{R_{xy}^{2}} \right)$,
 $M = \frac{3}{2} \left(\frac{1}{R_{yz}^{2}} \right)$, $N = \frac{3}{2} \left(\frac{1}{R_{zx}^{2}} \right)$, where $R_{x} = \frac{\sigma_{x}^{Y}}{\sigma_{Y}}$, $R_{y} = \frac{\sigma_{y}^{Y}}{\sigma_{Y}}$, $R_{z} = \frac{\sigma_{z}^{Y}}{\sigma_{Y}}$, $R_{xy} = \sqrt{3} \frac{\tau_{xy}^{Y}}{\sigma_{Y}}$, $R_{yz} = \sqrt{3} \frac{\tau_{yz}^{Y}}{\sigma_{Y}}$, $R_{zx} = \sqrt{3} \frac{\sigma_{xx}^{Y}}{\sigma_{Y}}$, σ_{ij}^{Y} - yield stress values.

When calculations are carried out for single-crystal (SX) parts considering the cubic symmetry of mechanical characteristics, Hill yield criterion is simplified and transformed into (9).

$$\sqrt{(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + K_p(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2) - \sigma_Y} = 0,$$
(9)

where $K_p = 4 \frac{\sigma_{Y<001>}^2}{\sigma_{Y<011>}^2} - 1$, $\sigma_{Y<001>}$ – yield strength in <001> crystallographic direction, $\sigma_{Y<011>}$ – yield strength in <011> crystallographic direction. Further, it will become clear that in such formulation the criterion describes the material behavior worse than the Mises criterion. However, using the adjusted parameter ($K_p = 4 \frac{\sigma_{Y<011>}^2}{\sigma_{Y<111>}^2} - 1$, where $\sigma_{Y<111>}^2$ – yield strength in <111> crystallographic direction) it is possible to achieve good agreement between theoretical and experimental data.

Based on Schmid's law [11] crystallographic approach is widely used for the stressstrain state determination of SX blades. According to Schmid's law, octahedral or cubic slip systems are realized when plastic deformation of the crystal lattice occurs.

$$\min_{k}\{n_k\}[\sigma]\{l_k\} > \tau_0,\tag{10}$$

where $\{n_k\}$ – the normal direction to the slip plane, $[\sigma]$ – stress tensor, $\{l_k\}$ – slip direction, τ_0 – critical resolved shear stress.

A.S. Semenov proposed an approach [12] to generalize the crystallographic criterion using smooth dependences based on the Hill yield criterion (11).

$$\left(\frac{I_{cs1}}{\sigma_Y}\right)^n + K_{p1} \left(\frac{I_{cs2}}{\sigma_Y}\right)^m - 1 = 0, \tag{11}$$

where $I_{cs1} = \sqrt{\frac{1}{2}} \left[\left(\sigma_x - \sigma_y \right)^2 + \left(\sigma_y - \sigma_z \right)^2 + (\sigma_z - \sigma_x)^2 \right], I_{cs2} = \sqrt{\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2}, K_{p1}, n, m$ – dimensionless material constants ($K_{p1} = 1.3, n = 2.4, m = 2.4$ [12]).

Studies show that no plasticity criterion can accurately describe the behavior of a material under a complex stress state. Different criteria are more consistent with the experimental data obtained from testing various materials and conditions.

In the present work, we focused on investigating SX material behavior under complex loading and a yield criterion based on the systematization of experimental data.

2. Experimental investigation

An experimental investigation of the yield criteria was conducted by testing thin-walled tubular specimens loaded by tensile/compressive force, and torque. In addition to the yield strength, several characteristics at various stress levels were studied. The stress state was assumed to be approximately plane.



a) view of the specimen b) drawing of the specimen **Fig. 2.** Thin-walled tubular specimen for testing under the complex stress state

SX specimens were cast so that the axis of the specimen matched with the crystallographic orientation (CO) <001>[13]. A drawing and view of the specimen are shown

in Fig. 2. A secondary orientation does not affect the general deformed state of axisymmetric specimens. Nevertheless, its search makes sense because SX materials are known to have a strong anisotropy of properties. Therefore, plastic strains could be unevenly distributed around the circumference of the specimens.

The test method corresponded with the requirements of regulatory documents [13]. The tests were conducted on a certified testing machine (Fig. 3). The testing machine works with tubular thin-walled specimens and is capable of loading them with tensile or compressive forces, torque, and internal pressure. However, in this work the specimens were not loaded by internal pressure.



Fig. 3. Testing machine POZ 0909 manufactured by Schenk GmbH (Germany) with a control system BiSS (India), a maximum tensile/compressive load of 630 kN, and a maximum torque of 8 kNm

The specimen was fixed in the testing machine using special equipment, excluding its slipping both at tension and at torsion. The tests were carried out under the control of the axial load and torque at a temperature of 20°C.

Strain gauges were used to measure the strains of the specimens. When a tension, compression, or torsion test is performed, conducting strain gauging becomes intuitively clear. However, if the stress state is complex, how to choose the angles for gluing on the specimen of the strain gauges is unclear. Strain gauges (Fig. 5) can measure only tensile or compressive strains. Thus, strain gauges are glued to the specimens in the directions where there are no shear strains (i.e., in the direction of the principal strains). The feature of isotropic materials is that normal stresses do not cause shear strains and that shear stresses do not cause tensile or compressive deformations. In this case, the directions of the principal stresses and principal deformations coincide, and determining these directions can be carried out according to a known stress state. Determining the principal stresses is a well-known eigenvalue problem described by Equation (12):

$$[\sigma - \lambda E]\{l\} = 0,$$

(12)

where σ is the stress tensor, λ is one of the principal stresses, and E is the unit tensor. If

(13)

relation (13) holds, the system (12) will have a solution. $det|\sigma - \lambda E| = 0.$

The definition of the determinant leads to a cubic equation, the solution of which contains the eigenvalues or principal stresses. Then, the system of Equation (12) is solved given Equation (14):

$$l_1^2 + l_2^2 + l_3^2 = 1,$$
 (14)
where l_1, l_2, l_3 are the directing cosines.

When SX specimens (anisotropic) are tested, tensile stresses can cause shear strains and vice versa. In this case, the directions of the principal stresses may differ from the directions of the principal strains, and recalculating the stresses into the strains is necessary using the generalized Hooke's law for an anisotropic material (15) [14]. Next, calculating the principal strains and their directions is necessary in the same way as in the stresses. $\{\epsilon\} = [S]\{\sigma\},$ (15)

where $\{\varepsilon\}$ is the strain column vector, [S] is the anisotropic compliance tensor, and $\{\sigma\}$ is the stress column vector.

In the beginning, we were faced with the issue of an unknown azimuthal orientation of the SX. The annular plates were cut from the end face of the specimen blanks (Fig. 4) and marked with marks on the cut and mating parts to identify the azimuthal orientation. The specimen blanks were sent for mechanical treatment, and the annular plates were sent for etching to identify the SX texture and determine the azimuthal CO. After etching and specimen fabrication, the separated parts were combined according to the previously identified marks. Thus, the azimuthal orientation of the SX in the specimens was determined.

Fig. 4. Annular plates after etching and the SX texture

The known azimuthal orientation of the SX shows how to recalculate the elastic tensor, as it depends on the orientation of the SX in the specimen, and to calculate the strain tensor. After determining the principal strains and their directions, the gluing of the strain gauge was conducted (Fig. 5).

The experimental design and yield strength values are presented in Table 1. Seven SX specimens were tested.

As a result of the tests, all specimens were destroyed in a brittle manner. Figure 6 shows the destroyed specimens after the tensile, compression, and torsion tests.

The following types of stress state were realized: uniaxial tension ($\sigma_1 = \sigma_{Ten}, \sigma_3 = 0$), uniaxial compression ($\sigma_3 = \sigma_{Com}, \sigma_1 = 0$), pure shear ($\sigma_1 = -\sigma_3$), and the combinations of tension-torsion and compression-torsion. The stress-strain diagram was obtained under a complex stress state in the coordinates of stress intensity-strain intensity. The yield strengths were calculated based on the fact that residual strains after unloading should not exceed 0.2% (Fig. 7a, black line).





Fig. 5. Specimen with strain gauges before torsion testing (principal strains are located at an angle of 45° to the axis of the specimen)

Table 1. The	ratio	of	torque	and	tensile	load	when	SX	specimens	were	tested	and
experimental	results											

Number of	Ratio of torque	Ratio of	Yield strength	Ultimate
points on the	and tensile load	principal	$(\sigma_{\rm Y})$, MPa	strength
figure	$\left(\frac{M}{N}\right)$, $\frac{\mathrm{kN}\cdot\mathrm{mm}}{\mathrm{kN}}$	stresses $\left(\left \frac{\sigma_1}{\sigma_3} \right \right)$		($\sigma_{ m u}$), MPa
1	0	Inf.	873	960
2	7.57	3	952	1067
3	17.5	3/2	1219	1276
4	Inf.	1.0	1306	1368
5	-17.5	2/3	1415	1445
6	-7.57	1/3	1181	1235
7	-0	0	999	1029

Note: Sign «-» indicates that the specimen is under compression.



b) compression c **Fig. 6.** Brittle destruction of specimens from SX alloy

To trace the evolution of plastic strains, the proportionality limit, the stresses at which residual strains were 0.1%, and the ultimate strength were determined. To determine the proportional limit, a black dashed line was used (Fig. 7a) (the tangent between the black dashed line and the abscissa axis is 50% less compared to Young's modulus). The stress-strain

diagram was compared to various types of stress states (Fig. 7b). These curves are clearly shown to be significantly different. This is explained by the anisotropy of the material and the fact that the modulus of elasticity and modulus of shear are not dependent quantities.



a) an example of the determination of some alloy b) strain-stress curves for various types of stress characteristics states

Fig. 7. Stress-strain curves for the SX nickel-based alloy

The diagram for the dimensionless reference axis σ_1 - σ_3 was obtained (Fig. 8a). An attempt was made to describe the experimental results using the most popular plasticity criteria [4-6,10-12]: Tresca yield criterion (3), von Mises (4), Pisarenko-Lebedev (7) Hill (8,9), Schmid (10), modified Hill criterion (11) and a modified Pisarenko-Lebedev yield criterion developed by the authors in (16).

$$\chi \sqrt{\frac{{\sigma_1}^2 + \gamma {\sigma_1} {\sigma_3} + {\sigma_3}^2}{2}} + (1 - \chi) \sigma_1 = \sigma_Y, \tag{16}$$

where γ is the shear/tensile yield strength ratio. The values of constant of the proposed criterion:

 $\sigma_Y = 873 MPa$ (yield strength in <001> crystallographic direction), $\chi = 0.874, \gamma = 1.495$.

Credibility was evaluated (Table 2) using Equation (17) and (18) for various yield criteria. This value shows the accuracy of matching with the experimental data of one or another plasticity criterion.

$$K_{EC} = 1 - \frac{\sum |y_i - \hat{y}_i|}{\sum |y_i|},$$
(17)

$$R^{2} = 1 - \frac{\sum (y_{i} - \hat{y}_{i})^{2}}{\sum (y_{i} - \bar{y})^{2}},$$
(18)

where y_i is the experimental value of the yield strength, and \hat{y}_i is the predicted value of the

yield strength, \bar{y} is the average value among experimental data of yield strength.

Estimation criteria	Yield criteria								
	von Mises	Tresca	Pisarenko- Lebedev	Schmid's low	Hill	Hill (SX)	Power criterion	Modified Pisarenko- Lebedev	
K _{EC}	78%	74%	83%	92%	94%	73%	94%	96%	
<i>R</i> ²	-	-	-	-	41%	-	42%	75%	

Table 2. Evaluation of credibility of various yield criteria

Most of the widely used yield criterion was not capable of describing the behavior of a given SX alloy. Therefore, the development of a modified criterion, which allows the reliable evaluation of the behavior of the material under complex stress–inelastic state, is required.

Based on the developed modified yield criterion, an attempt was made to trace the behavior of the material along the entire strain path (Fig. 8b). Four points were selected for each deformation curve: proportionality limit, stress at which the residual strain after unloading becomes 0.1%, yield strength, and ultimate stress limit. The behavior of the material changed depending on the type of stress state. The researched values and stress range between the proportionality limit and the ultimate stress limit changed, directly affecting the tangent modulus.



 σ_{prop} $\Delta \sigma_i = 275 \text{ MPa}$ σ₀₁ (*) σ_{γ} (x) $\Delta \sigma_i = 364 \text{ MPa}$ σ_r (•) -200 $\Delta \sigma_i = 390 \text{ MPa}$ $\Delta \sigma = 363 \text{ MPa}$ -400 $\Delta \sigma_i = 306 \text{ MPa}$ б $\Delta \sigma_i = 243 \text{ MPa}$ -600 $\Delta \sigma_i = 150 \text{ MPa}$ -800 -1000 ò 200 400 600 800 1000 σ_1

a) description of the yield strength using the popular yield criteria and the modified Pisarenko-Lebedev (MPL) yield criterion



Fig. 8. Diagrams of the characteristics of the SX alloy depending on the type of stress state

The approach proposed by the authors allows to describe the behavior of the material more accurately than previously developed approaches (Table 2 and Fig. 8a). Taking into account the tension–compression asymmetry of the material is an additional advantage of the proposed approach.

3. Conclusions

Test data analysis of specimens made from an SX nickel-based alloy, which were tested at various types of stress states at a temperature of 20°C, showed that the widely used yield

criteria of von Mises, Pisarenko-Lebedev, and Tresca were not able to reliably describe the behavior of the material under a complex stress state. A specialized criterion based on the systematization of experimental data was developed that could accurately describe the behavior of most materials. The type of stress state could affect the tangent modulus. In this case, the law of hardening of the material depends on the type of stress state.

This work may be further developed by conducting experimental studies on the alloy under complex stress conditions at elevated temperatures and tests under biaxial tension and their combination.

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STABILITY OF THE MICROPOLAR THIN ROUND PLATE

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Abstract. In this paper, a thin round plate of isotropic micropolar elastic material is considered, in which the elastic deflections are comparable with their thickness, and small in relation to the basic size, also both the angles of rotation of the normal elements to the middle plane before deformation and their free rotations are small. Thus, the strain tensor and tensor of bending-torsion takes into account not only linear but also the nonlinear terms in the gradients of displacement and rotation. The stability problem is solved in the case when the solid round plate is hinge supported along the contour and is under the action of radial compressive forces. After solving the obtained boundary value problem, the critical value of the external force is determined. The critical force of the micropolar problem is compared with the value of the classical solution. The important properties of micropolar material are established.

Keywords: micropolar, elastic, thin round plate, curvilinear coordinates, geometrically nonlinear, applied model, stability

1. Introduction

As structural elements, thin rods, plates, and shells are widely used, the bearing capacity of which is determined mainly by their stability. The theory of stability of thin rods, plates, and shells in the framework of the classical theory of elasticity is described in monographs [1,2,etc.]. The work [3] is devoted to the stability problem in the framework of the micropolar (momental) theory of elasticity. Review of works on the micropolar theory of thin plates and shells was carried out in work [4]. In works [5-8], on the basis of the hypothesis method (which has an asymptotic substantiation), the linear theory of micropolar elastic flexible plates and shells are constructed. In works [9,10], the theory of micropolar elastic rectangular plates is studied.

In this paper, the stability problem of micropolar elastic round solid plate in an axisymmetric formulation is studied, when on its contour uniformly distributed radial load is applied. To obtain stability equations, disturbance is given to the initial state of the plate, equations of micropolar flexible plates are used, performing linearization. The boundary-value problem of stability of micropolar elastic round plate is solved exactly using Bessel functions; as a result, the critical value of the load is determined. After comparison with the classical case, effective manifestations of the micropolarity of the material are established.

2. Geometrically nonlinear mathematical model of micropolar elastic thin plates in curvilinear coordinates with independent fields of displacements and rotations

We consider a plate of constant thickness 2h as a three-dimensional elastic isotropic body. We assign the plate to the curvilinear coordinate system α_1, α_2, z . The coordinate plane α_1, α_2 will be combined with the median plane of the plate. The axis Oz is directed along the normal to the median plane.

The basic equations and the natural boundary conditions of micropolar elastic geometrically nonlinear thin plates with independent fields of displacements and rotations in curvilinear coordinates have the form [10]:

$$\begin{split} \text{Balance Equations} \\ &\frac{1}{A}\frac{\partial T_{ij}}{\partial \alpha_i} + \frac{1}{A_A}\frac{\partial A_j}{\partial \alpha_i}(T_{ii} - T_{ji}) + \frac{1}{A_j}\frac{\partial S_{ji}}{\partial \alpha_j} + \frac{1}{A_AA_j}\frac{\partial A_j}{\partial \alpha_j}(S_{ji} + S_{ij}) = -(p_i^+ - p_i^-), \\ &\frac{1}{A_i}\frac{\partial M_{ii}}{\partial \alpha_i} + \frac{1}{A_AA_j}\frac{\partial A_j}{\partial \alpha_i}(M_{ii} - M_{ji}) + \frac{1}{A_j}\frac{\partial M_{ji}}{\partial \alpha_j} + \frac{1}{A_iA_j}\frac{\partial A_j}{\partial \alpha_j}(M_{ji} + M_{ij}) - N_{3i} = -h(p_i^+ + p_i^-), \\ &\frac{1}{A_iA_2}\left\{ \left[\frac{\partial (A_2N_{13})}{\partial \alpha_1} + \frac{\partial (A_iN_{23})}{\partial \alpha_2} \right] + \frac{A_2}{\partial \alpha_i}\frac{\partial^2 w}{\partial \alpha_i^2}T_{1i} + \frac{A_i}{A_j}\frac{\partial^2 w}{\partial \alpha_i^2}T_{22} + \frac{\partial^2 w}{\partial \alpha_i \partial \alpha_2}(S_{12} + S_{21}) + \\ &+ \frac{\partial w}{\partial \alpha_i} \left[\frac{A_i}{A_i}\frac{\partial T_{1i}}{\partial \alpha_1} - \frac{A_i}{A_i}\frac{\partial A_i}{\partial \alpha_i}T_{1i} + \frac{1}{A_i}\frac{\partial A_2}{\partial \alpha_i}T_{1i} + \frac{1}{2}\frac{\partial (S_{12} + S_{21})}{\partial \alpha_2} \right] + \\ &+ \frac{\partial w}{\partial \alpha_2} \left[\frac{A_i}{A_2}\frac{\partial T_{22}}{\partial \alpha_2} - \frac{A_i}{A_2^2}\frac{\partial A_2}{\partial \alpha_2}T_{22} + \frac{1}{2}\frac{\partial (A_i}{\partial \alpha_i}T_{22} + \frac{1}{2}\frac{\partial (S_{12} + S_{21})}{\partial \alpha_i} \right] \right] = -(p_3^+ - p_3^-), \\ &\frac{1}{A}\frac{\partial L_{ii}}{\partial \alpha_i} + \frac{1}{A_Aj}\frac{\partial A_i}{\partial \alpha_i}(L_{ij} - L_{ji}) + \frac{1}{A_j}\frac{\partial L_{ji}}{\partial \alpha_j}T_{22} + \frac{1}{2}\frac{\partial (A_i}{\partial \alpha_i}(L_{ji} + L_{ij}) + \\ &+ (-1)^i(N_{i3} - N_{3i}) = -(m_i^+ - m_i^-), \\ &\frac{1}{A_i} \left[\frac{\partial (A_2L_{13})}{\partial \alpha_1} + \frac{\partial (A_iL_{23})}{\partial \alpha_2} \right] - (M_{12} - M_{21}) = h(m_3^+ + m_3^-). \\ & & \text{Elasticity Relations} \\ &T_{ii} = \frac{2Eh}{1 - v^2} [T_{ii} + vT_{jj}], \quad S_{ij} = 2h[(\mu + \alpha)T_{ij} + (\mu - \alpha)T_{jj}], \\ &N_{i3} = 2h[(\mu + \alpha)T_{i3} + (\mu - \alpha)T_{3i}], \quad N_{3i} = 2h[(\mu + \alpha)T_{3i} + (\mu - \alpha)T_{i3}], \\ &L_{ii} = 2h[(\beta + 2\gamma)\kappa_{ii} + \beta(\kappa_{ji} + i)], \\ &L_{3i} = 2h[(\beta + 2\gamma)i + \beta(\kappa_{ji} + i)], \\ &L_{3i} = 2h[(\beta + 2\gamma)i + \beta(\kappa_{ji} + i)], \\ &L_{3i} = 2h[(\beta + 2\gamma)i + \beta(\kappa_{ji} + i)], \\ &L_{3i} = 2h[(\beta + 2\gamma)i + \beta(\kappa_{1i} + \kappa_{2j})], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa_{ji}], \\ &L_{ij} = 2h[(\gamma + \varepsilon)\kappa_{ij} + (\gamma - \varepsilon)\kappa$$

$$\Gamma_{ij} = \frac{1}{A_i} \frac{\partial u_j}{\partial \alpha_i} - \frac{1}{A_i A_j} \frac{\partial A_i}{\partial \alpha_j} u_i - (-1)^j \Omega_3 + \frac{1}{2} \frac{1}{A_1 A_2} \frac{\partial w}{\partial \alpha_1} \frac{\partial w}{\partial \alpha_2}, \ \Gamma_{3i} = \psi_i - (-1)^j \Omega_j,$$

Stability of the micropolar thin round plate

$$K_{ii} = \frac{1}{A_i} \frac{\partial \psi_i}{\partial \alpha_i} + \frac{1}{A_i A_j} \frac{\partial A_i}{\partial \alpha_j} \psi_j, \quad K_{ij} = \frac{1}{A_i} \frac{\partial \psi_j}{\partial \alpha_i} - \frac{1}{A_i A_j} \frac{\partial A_i}{\partial \alpha_j} \psi_i - (-1)^j \iota,$$

$$\kappa_{ii} = \frac{1}{A_i} \frac{\partial \Omega_i}{\partial \alpha_i} + \frac{1}{A_i A_j} \frac{\partial A_i}{\partial \alpha_j} \Omega_j, \quad \kappa_{33} = \iota, \quad \kappa_{ij} = \frac{1}{A_i} \frac{\partial \Omega_j}{\partial \alpha_i} - \frac{1}{A_i A_j} \frac{\partial A_i}{\partial \alpha_j} \Omega_i,$$

$$\kappa_{i3} = \frac{1}{A_i} \frac{\partial \Omega_3}{\partial \alpha_i}, \quad l_{i3} = \frac{1}{A_i} \frac{\partial \iota}{\partial \alpha_i}.$$
(3)

Boundary conditions

$$T_{11} = T_{11}^{0}, \ S_{12} = S_{12}^{0}, \ M_{11} = M_{11}^{0}, \\ M_{12} = M_{12}^{0}, \\ T_{11} \frac{1}{A_1} \frac{\partial w}{\partial \alpha_1} + \frac{S_{12} + S_{21}}{2} \frac{1}{A_2} \frac{\partial w}{\partial \alpha_2} + N_{13} = N_{13}^{0}, \\ L_{11} = L_{11}^{0}, \ L_{12} = L_{12}^{0}, \ \Lambda_{13} = \Lambda_{13}^{0}.$$
(4)

Here u_1, u_2 – are displacements of the points of the median plane of the plate around the axes α_1, α_2 ; w – is displacement of the points of the median plane of the plate in the direction of the axis z; ψ_1, ψ_2 – are complete rotation angles; $\Omega_1, \Omega_2, \Omega_3$ – are certain free rotations of the initially normal elements around the axes α_1, α_2, z ; t – is intensity of the free rotation ω_3 around the axis z; Γ_{ii} – are elongation deformations in the directions α_1, α_2 ; $\Gamma_{ii}, \Gamma_{ij}, \Gamma_{i3}, \Gamma_{3i}$ – are shears in the corresponding planes; K_{ii} – are flexures of the plate median plane caused by the stresses; K_{ij} – are torsions of the plate median plane caused by the stresses; κ_{ii}, κ_{33} – are flexures of the plate median plane caused by the couple stresses; κ_{ij} – are torsions of the plate median plane caused by the couple stresses; κ_{ij} – are torsions of the plate median plane caused by the couple stresses; $L_{ii}, L_{ij}, L_{i3}, L_{33}$ – are averaged moments from the stresses; M_{ii}, H_{ij} – are averaged moments from the stresses; $L_{ii}, L_{ij}, L_{i3}, L_{33}$ – are external forces and moments on the planes $z = \pm h$; A_i – are Lame coefficients [8].

Let us note that from this model we can obtain the corresponding geometrically linear model by discarding nonlinear terms [8]. We also can get a geometrically nonlinear classical Timoshenko-type model, if to put $\alpha = 0$.

3. Geometrically nonlinear applied model of micropolar elastic thin round plates

In the case of round plates in Equations (1) - (4) we will accept $A_1 = 1$, $A_2 = r$ and use the polar coordinates r, θ . As a result, we get:

Balance Equations

$$\frac{\partial T_{11}}{\partial r} + \frac{1}{r}(T_{11} - T_{22}) + \frac{1}{r}\frac{\partial S_{21}}{\partial \theta} = -(p_1^+ - p_1^-), \quad \frac{1}{r}\frac{\partial T_{22}}{\partial \theta} + \frac{\partial S_{ji}}{\partial r} + \frac{1}{r}(S_{12} + S_{21}) = -(p_2^+ - p_2^-),$$

$$\frac{\partial L_{13}}{\partial r} + \frac{1}{r}L_{13} + \frac{1}{r}\frac{\partial L_{23}}{\partial \theta} + (S_{12} - S_{21}) = -(m_3^+ - m_3^-),$$

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$$\begin{split} \frac{\partial N_{13}}{\partial r} &+ \frac{1}{r} N_{13} + \frac{1}{r} \frac{\partial N_{23}}{\partial r} + \frac{\partial^2 w}{\partial r^2} T_{11} + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} T_{22} + \frac{1}{r} \frac{\partial^2 w}{\partial r \partial \theta} \left[S_{12} + S_{21} \right] + \\ &+ \frac{\partial w}{\partial r} \left[\frac{\partial T_{11}}{\partial r} + \frac{1}{r} T_{11} + \frac{1}{2r} \frac{\partial (S_{12} + S_{21})}{\partial \theta} \right] + \frac{\partial w}{\partial \theta} \left[\frac{1}{r^2} \frac{\partial T_{22}}{\partial \theta} + \frac{1}{r} T_{11} + \frac{1}{2r} \frac{\partial (S_{12} + S_{21})}{\partial r} \right] = -(p_3^* - p_3^*), \\ \frac{\partial L_{11}}{\partial r} + \frac{1}{r} (L_{11} - L_{22}) + \frac{1}{r} \frac{\partial L_{21}}{\partial \theta} + N_{32} - N_{12} = -(m_1^* - m_1^*), \\ \frac{\partial L_{12}}{\partial r} + \frac{1}{r} \frac{\partial L_{22}}{\partial \theta} + \frac{1}{r} (L_{12} + L_{21}) + N_{31} - N_{13} = -(m_2^* - m_2^*), \\ N_{31} - \left(\frac{\partial M_{11}}{\partial r} + \frac{1}{r} (M_{11} - M_{22}) + \frac{1}{r} \frac{\partial M_{21}}{\partial \theta} \right) = h(p_1^* + p_1^-), \\ N_{32} - \left(\frac{1}{r} \frac{\partial M_{22}}{\partial \theta} + \frac{\partial M_{22}}{\partial r} + \frac{1}{r} (M_{12} + M_{21}) \right) = h(m_3^* + m_3^*). \\ N_{32} - \left(\frac{1}{r} \frac{\partial M_{22}}{\partial \theta} + \frac{\partial M_{22}}{\partial r} + \frac{1}{r} (M_{12} + M_{21}) \right) = h(m_3^* + m_3^-). \\ N_{32} - \left(\frac{1}{r} \frac{\partial M_{22}}{\partial \theta} + \frac{\partial M_{22}}{\partial r} + \frac{1}{r} (M_{12} - M_{21}) \right) = h(m_3^* + m_3^-). \\ N_{33} - \frac{\partial \Lambda_{13}}{\partial r} - \frac{1}{r} \Lambda_{13} - \frac{1}{r} \frac{\partial \Lambda_{23}}{\partial \theta} - (M_{12} - M_{21}) \right) = h(m_3^* + m_3^-). \\ (5) \\ Physical-Geometrically Relations \\ T_{11} &= \frac{2Eh}{1 - v^2} \left[\frac{1}{r} \frac{\partial u_2}{\partial \theta} + \frac{1}{r} u_1 + \frac{1}{2} \frac{1}{r^2} \left(\frac{\partial w}{\partial \theta} \right)^2 + v \left(\frac{\partial u_1}{\partial r} + \frac{1}{r} (\frac{1}{r^2} \frac{\partial w}{\partial \theta} \right)^2 \right] \right], \\ S_{21} &= 2h \left[(\mu + \alpha) \left(\frac{1}{r} \frac{\partial u_1}{\partial \theta} - \frac{1}{r} u_2 \right) + (\mu - \alpha) \left(\frac{\partial u_2}{\partial r} + \frac{1}{r} \frac{\partial w}{\partial \theta} \right) \right], \\ N_{13} &= 2h \left[(\mu + \alpha) \left(\frac{1}{r} \frac{\partial u_1}{\partial \theta} - \frac{1}{r} u_2 \right) + (\mu - \alpha) \left(\frac{\partial u_2}{\partial r} + 2\alpha \Omega_3 + \mu \frac{1}{r} \frac{\partial w}{\partial \theta} \frac{\partial w}{\partial \theta} \right) \right], \\ N_{31} &= 2h \left[(\mu + \alpha) \frac{\partial w}{\partial r} + (\mu - \alpha) \frac{\partial w}{\partial r} - 2\alpha \Omega_2 \right], \\ N_{32} &= 2h \left[(\mu + \alpha) \frac{1}{r} \frac{\partial w}{\partial r} + (\mu - \alpha) \left(\frac{1}{r} \frac{\partial w_2}{\partial \theta} + \frac{1}{r} w_1 \right) \right], \\ M_{12} &= \frac{2Eh^3}{3} \left[(\mu + \alpha) \frac{1}{2r} \frac{\partial w_2}{\partial r} + (\mu - \alpha) \left(\frac{1}{r} \frac{\partial w_1}{\partial \theta} - \frac{1}{r} w_2 \right) - 2\alpha 1 \right], \\ M_{11} &= \frac{2Eh^3}{3} \left[(\mu + \alpha) \left(\frac{1}{r} \frac{\partial w_1}{\partial r} + \frac{1}{r} w_2 \right) + (\mu - \alpha) \left(\frac{\partial$$

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$$L_{12} = 2h \left[(\gamma + \varepsilon) \frac{\partial \Omega_2}{\partial r} + (\gamma - \varepsilon) \left(\frac{1}{r} \frac{\partial \Omega_1}{\partial \theta} - \frac{1}{r} \Omega_2 \right) \right], \ \Lambda_{13} = \frac{2h^3}{3} \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{\partial \iota}{\partial r},$$

$$L_{21} = 2h \left[(\gamma + \varepsilon) \left(\frac{1}{r} \frac{\partial \Omega_1}{\partial \theta} - \frac{1}{r} \Omega_2 \right) + (\gamma - \varepsilon) \frac{\partial \Omega_2}{\partial r} \right], \ \Lambda_{23} = \frac{2h^3}{3} \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{1}{r} \frac{\partial \iota}{\partial \theta},$$

$$L_{33} = 2h \left[(\beta + 2\gamma)\iota + \beta \left(\frac{\partial \Omega_1}{\partial r} + \frac{1}{r} \frac{\partial \Omega_2}{\partial \theta} + \frac{1}{r} \Omega_1 \right) \right].$$
(6)

Now we consider the axisymmetric problem, in this case, we will have: Balance Equations

$$\frac{dT_{11}}{dr} + \frac{1}{r} \left(T_{11} - T_{22} \right) = -\left(p_1^+ - p_1^- \right), \frac{dS_{12}}{dr} + \frac{1}{r} \left(S_{12} + S_{21} \right) = -\left(p_2^+ - p_2^- \right), \\
\frac{dL_{13}}{dr} + \frac{1}{r} L_{13} + \left(S_{12} - S_{21} \right) = -\left(m_3^+ - m_3^- \right), \\
\frac{dN_{13}}{dr} + \frac{1}{r} N_{13} + \frac{1}{r} \frac{d}{dr} \left(rT_{11} \frac{dw}{dr} \right) = -\left(p_3^+ - p_3^- \right), \\
\frac{dL_{11}}{dr} + \frac{1}{r} \left(L_{11} - L_{22} \right) + N_{23} - N_{32} = -\left(m_1^+ - m_1^- \right), \\
\frac{dL_{12}}{dr} + \frac{1}{r} \left(L_{12} + L_{21} \right) + N_{31} - N_{13} = -\left(m_2^+ - m_2^- \right), \\
N_{31} - \left(\frac{dM_{11}}{dr} + \frac{1}{r} \left(M_{11} - M_{22} \right) \right) = h \left(p_1^+ + p_1^- \right), \\
N_{32} - \left(\frac{dM_{12}}{dr} + \frac{1}{r} \left(M_{12} + M_{21} \right) \right) = h \left(p_2^+ + p_2^- \right), \\
L_{33} - \frac{d\Lambda_{13}}{dr} - \left(M_{12} - M_{21} \right) = h \left(m_3^+ + m_3^- \right).$$
(7)

Physical-Geometrically Relations

$$\begin{split} T_{11} &= \frac{2Eh}{1-v^2} \Bigg[\frac{du_1}{dr} + \frac{1}{2} \bigg(\frac{dw}{dr} \bigg)^2 + v \frac{1}{r} u_1 \Bigg], S_{12} &= 2h \Bigg[(\mu + \alpha) \frac{du_2}{dr} - (\mu - \alpha) \frac{1}{r} u_2 - 2\alpha \Omega_3 \Bigg], \\ T_{22} &= \frac{2Eh}{1-v^2} \Bigg[\frac{1}{r} u_1 + v \bigg(\frac{du_1}{dr} + \frac{1}{2} \bigg(\frac{dw}{dr} \bigg)^2 \bigg) \Bigg], S_{21} &= 2h \Bigg[-(\mu + \alpha) \frac{1}{r} u_2 + (\mu - \alpha) \frac{du_2}{dr} + 2\alpha \Omega_3 \Bigg], \\ N_{13} &= 2h \Bigg[(\mu + \alpha) \frac{dw}{dr} + (\mu - \alpha) \psi_1 + 2\alpha \Omega_2 \Bigg], N_{23} &= 2h [(\mu - \alpha) \psi_2 - 2\alpha \Omega_1], \\ N_{31} &= 2h \Bigg[(\mu + \alpha) \psi_1 + (\mu - \alpha) \frac{dw}{dr} - 2\alpha \Omega_2 \Bigg], N_{32} &= 2h [(\mu + \alpha) \psi_2 + 2\alpha \Omega_1], \\ M_{12} &= \frac{2h^3}{3} \Bigg[(\mu + \alpha) \frac{d\psi_2}{dr} - (\mu - \alpha) \frac{1}{r} \psi_2 - 2\alpha i \Bigg], M_{11} &= \frac{2Eh^3}{3(1-v^2)} \Bigg[\frac{d\psi_1}{dr} + v \frac{1}{r} \psi_1 \Bigg], \\ M_{21} &= \frac{2h^3}{3} \Bigg[-(\mu + \alpha) \frac{1}{r} \psi_2 + (\mu - \alpha) \frac{d\psi_2}{dr} + 2\alpha i \Bigg], M_{22} &= \frac{2Eh^3}{3(1-v^2)} \Bigg[\frac{1}{r} \psi_1 + v \frac{d\psi_1}{dr} \Bigg], \\ L_{11} &= 2h \Bigg[(\beta + 2\gamma) \frac{d\Omega_1}{dr} + \beta \frac{1}{r} \Omega_1 + \beta i \Bigg], L_{22} &= 2h \Bigg[(\beta + 2\gamma) \frac{1}{r} \Omega_1 + \beta \frac{d\Omega_1}{dr} - \beta i \Bigg], \end{split}$$

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$$L_{12} = 2h \left[(\gamma + \varepsilon) \frac{d\Omega_2}{dr} - (\gamma - \varepsilon) \frac{1}{r} \Omega_2 \right], \ L_{21} = 2h \left[-(\gamma + \varepsilon) \frac{1}{r} \Omega_2 + (\gamma - \varepsilon) \frac{d\Omega_2}{dr} \right],$$
$$L_{33} = 2h \left[(\beta + 2\gamma)\iota + \beta \left(\frac{d\Omega_1}{dr} + \frac{1}{r} \Omega_1 \right) \right], \ \Lambda_{13} = \frac{2h^3}{3} \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{d\iota}{dr}, \ L_{13} = \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{d\Omega_3}{dr}.$$
(8)

To the Equations (5), (6), or (7), (8) need to join the corresponding boundary conditions (4). From systems (5), (6), and (7), (8) we can obtain the basic equations regarding the displacements and rotations.

4. The linearized equations of stability of micropolar elastic round plates. The critical force of compressed round micropolar plate

Let us consider micropolar elastic round solid plate under the action of radial compression P, which is uniformly distributed along the contour. The flat stress-strain state (SSS) has been implemented, we will call it the main subcritical state, and it is the solution to the following linear system of equations of the generalized plane stress state of micropolar elastic thin round plate (as in the case of the classical theory [2]):

Balance Equations

$$\frac{dT_{11}^{0}}{dr} + \frac{1}{r} \left(T_{11}^{0} - T_{22}^{0} \right) = 0, \ \frac{dS_{12}^{0}}{dr} + \frac{1}{r} \left(S_{12}^{0} + S_{21}^{0} \right) = 0, \ \frac{dL_{13}^{0}}{dr} + \frac{1}{r} L_{13}^{0} + \left(S_{12}^{0} - S_{21}^{0} \right) = 0.$$
(9)
Physical-Geometrically Relations

$$T_{11}^{0} = \frac{2Eh}{1 - v^{2}} \left[\frac{du_{1}^{0}}{dr} + v \frac{1}{r} u_{1}^{0} \right], \ T_{22}^{0} = \frac{2Eh}{1 - v^{2}} \left[\frac{1}{r} u_{1}^{0} + v \frac{du_{1}^{0}}{dr} \right],$$

$$S_{12}^{0} = 2h \left[(\mu + \alpha) \frac{du_{2}^{0}}{dr} - (\mu - \alpha) \frac{1}{r} u_{2}^{0} - 2\alpha \Omega_{3}^{0} \right],$$

$$S_{21}^{0} = 2h \left[-(\mu + \alpha) \frac{1}{r} u_{2}^{0} + (\mu - \alpha) \frac{du_{2}^{0}}{dr} + 2\alpha \Omega_{3}^{0} \right], \ L_{13}^{0} = \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{d\Omega_{3}^{0}}{dr}.$$
(10)

The following boundary conditions must be satisfied on the contour of round solid plate (Fig. 1):

$$T_{11}^0 = -P$$
, $u_2^0 = 0$, $L_{13}^0 = 0$, at $r = R$, where $p = const$. (11)



Fig. 1. Middle surface of the round plate

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The components of displacements, deformations, force, and moment stresses corresponding to this SSS are marked with superscripts zero. In case of loss of stability, subcritical SSS will receive some disturbances. The values characterizing the SSS caused by these disturbances, we will imagine that they are marked with the asterisk at the top. The perturbed SSS in the plate is characterized by the values of the corresponding sums with indices of zero and asterisk.

Perturbations (i.e. the values with asterisks at the top) are small and during the transformations, we will neglect their powers higher than the first.

It is easy to notice that the solution of the subcritical boundary value problem (9) - (11)has the form (which satisfy the indicated equations and boundary conditions):

$${\stackrel{0}{T}}_{11} = const = -P, \quad {\stackrel{0}{T}}_{22} = const = -P, \quad {\stackrel{0}{u}}_2 \equiv 0, \quad {\stackrel{0}{S}}_{12} = {\stackrel{0}{S}}_{21} \equiv 0, \quad {\stackrel{0}{L}}_{13} = {\stackrel{0}{L}}_{31} \equiv 0, \quad {\stackrel{0}{\Omega}}_3 \equiv 0 \text{ (12)}$$

The displacement u_1^0 is determined on the basis of the expressions for T_{11}^0 and T_{22}^0 from (10).

We investigate the stability of a round solid plate of radius R, with the hinge supported contour and under the action of radial compressive forces P uniformly distributed along the contour of the plate. We assume that the curved surface is axisymmetric [2].

We substitute the noted total relations into the system of equations of the geometrically nonlinear theory of micropolar plates (7), (8), then we obtain the equations of the perturbed stress state in the form:

Balance Equations

...

$$\frac{dT_{11}}{dr} + \frac{1}{r} \left(T_{11} - T_{22} \right) = 0, \quad \frac{dS_{12}}{dr} + \frac{1}{r} \left(S_{12} + S_{21} \right) = 0, \\
N_{32} - \left(\frac{dM_{12}}{dr} + \frac{1}{r} \left(M_{12} + M_{21} \right) \right) = 0, \quad \frac{dL_{13}}{dr} + \frac{1}{r} L_{13} + \left(S_{12} - S_{21} \right) = 0, \\
\frac{dL_{11}}{dr} + \frac{1}{r} \left(L_{11} - L_{22} \right) + N_{23} - N_{32} = 0, \quad L_{33} - \frac{d\Lambda_{13}}{dr} - \left(M_{12} - M_{21} \right) = 0, \\
\frac{dN_{13}}{dr} + \frac{1}{r} N_{13} + \frac{1}{r} \frac{d}{dr} \left(rP \frac{dw}{dr} \right) = 0, \\
N_{31} - \left(\frac{dM_{11}}{dr} + \frac{1}{r} \left(M_{11} - M_{22} \right) \right) = 0, \\
\frac{dL_{12}}{dr} + \frac{1}{r} \left(L_{12} + L_{21} \right) + N_{31} - N_{13} = 0.$$
(13)

Physical-Geometrically Relations

$$\begin{split} T_{11} &= \frac{2Eh}{1-\nu^2} \left[\frac{du_1}{dr} + \nu \frac{1}{r} u_1 \right], \ S_{12} &= 2h \left[(\mu + \alpha) \frac{du_2}{dr} - (\mu - \alpha) \frac{1}{r} u_2 - 2\alpha \Omega_3 \right], \\ T_{22} &= \frac{2Eh}{1-\nu^2} \left[\frac{1}{r} u_1 + \nu \frac{du_1}{dr} \right], \ S_{21} &= 2h \left[-(\mu + \alpha) \frac{1}{r} u_2 + (\mu - \alpha) \frac{du_2}{dr} + 2\alpha \Omega_3 \right], \\ M_{12} &= \frac{2h^3}{3} \left[(\mu + \alpha) \frac{d\psi_2}{dr} - (\mu - \alpha) \frac{1}{r} \psi_2 - 2\alpha \iota \right], \ N_{23} &= 2h \left[(\mu - \alpha) \psi_2 - 2\alpha \Omega_1 \right], \\ M_{21} &= \frac{2h^3}{3} \left[-(\mu + \alpha) \frac{1}{r} \psi_2 + (\mu - \alpha) \frac{d\psi_2}{dr} + 2\alpha \iota \right], \ N_{32} &= 2h \left[(\mu + \alpha) \psi_2 + 2\alpha \Omega_1 \right], \\ L_{11} &= 2h \left[(\beta + 2\gamma) \frac{d\Omega_1}{dr} + \beta \frac{1}{r} \Omega_1 + \beta \iota \right], \ L_{22} &= 2h \left[(\beta + 2\gamma) \frac{1}{r} \Omega_1 + \beta \frac{d\Omega_1}{dr} - \beta \iota \right], \\ L_{33} &= 2h \left[(\beta + 2\gamma) \iota + \beta \left(\frac{d\Omega_1}{dr} + \frac{1}{r} \Omega_1 \right) \right], \ \Lambda_{13} &= \frac{2h^3}{3} \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{d\iota}{dr}, \ L_{13} &= \frac{4\gamma\varepsilon}{\gamma + \varepsilon} \frac{d\Omega_3}{dr}, \end{split}$$
(15)

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$$M_{11} = \frac{2Eh^{3}}{3(1-v^{2})} \left[\frac{d\psi_{1}}{dr} + v\frac{1}{r}\psi_{1} \right], N_{13} = 2h \left[(\mu + \alpha)\frac{dw}{dr} + (\mu - \alpha)\psi_{1} + 2\alpha\Omega_{2} \right],$$

$$M_{22} = \frac{2Eh^{3}}{3(1-v^{2})} \left[\frac{1}{r}\psi_{1} + v\frac{d\psi_{1}}{dr} \right], N_{31} = 2h \left[(\mu + \alpha)\psi_{1} + (\mu - \alpha)\frac{dw}{dr} - 2\alpha\Omega_{2} \right],$$

$$L_{12} = 2h \left[(\gamma + \varepsilon)\frac{d\Omega_{2}}{2} - (\gamma - \varepsilon)\frac{1}{2}\Omega_{2} \right], L_{21} = 2h \left[-(\gamma + \varepsilon)\frac{1}{2}\Omega_{2} + (\gamma - \varepsilon)\frac{d\Omega_{2}}{2} \right]$$
(16)

$$L_{12} = 2h \left[(\gamma + \varepsilon) \frac{d\Omega_2}{dr} - (\gamma - \varepsilon) \frac{1}{r} \Omega_2 \right], \quad L_{21} = 2h \left[-(\gamma + \varepsilon) \frac{1}{r} \Omega_2 + (\gamma - \varepsilon) \frac{d\Omega_2}{dr} \right]$$
(16)
Hinge supported boundary conditions:

$$\Omega_1 = 0, \quad \psi_2 = 0, \quad \Lambda_{13} = 0, \text{ at } r = R,$$
(17)

$$w = 0, \quad M_{11} = 0, \quad L_{12} = 0, \text{ at } r = R.$$
 (18)

Problem (13), (15), (17) has a trivial solution, and problem (14), (16), (18) can be reduced to the following form with respect to displacement w and rotations ψ_1 and Ω_2 :

$$\left(\frac{d}{dr} + \frac{1}{r}\right)\left(\left((\mu + \alpha) - \frac{P}{2h}\right)\frac{dw}{dr} + (\mu - \alpha)\psi_1 + 2\alpha\Omega_2\right) = 0,$$
(19)

$$(\mu - \alpha)\frac{dw}{dr} - 2\alpha\Omega_2 + (\mu + \alpha)\psi_1 - \frac{Eh^2}{3(1 - v^2)}\Delta\psi_1 = 0, \qquad (20)$$

$$(\gamma + \varepsilon)\Delta\Omega_2 - 4\alpha\Omega_2 + 2\alpha \left(\psi_1 - \frac{dw}{dr}\right) = 0, \qquad (21)$$

$$w = 0, \quad \frac{\partial \psi_1}{\partial r} + \frac{v}{r} \psi_1 = 0, \quad (\gamma + \varepsilon) \frac{\partial \Omega_2}{\partial r} - (\gamma - \varepsilon) \frac{1}{r} \Omega_2 = 0, \text{ at } r = R.$$
(22)

Here we note

$$\Delta = \frac{d}{dr} \left(\frac{d}{dr} + \frac{1}{r} \right). \tag{23}$$

By integrating equation (19) we can obtain:

$$\left((\mu+\alpha)-\frac{P}{2h}\right)\frac{dw}{dr}+(\mu-\alpha)\psi_1+2\alpha\Omega_2=\frac{C_1}{r}.$$
(24)

In the case of the solid plate we have $C_1 = 0$.

Then we can obtain a differential equation along the ψ_1 :

$$B_1 \Delta \Delta \psi_1 + B_2 \Delta \psi_1 + B_3 = 0, \qquad (25)$$

where

$$B_{1} = -\frac{(\gamma + \varepsilon)}{2\alpha} \left[(\mu + \alpha) - \frac{P}{2h} \right] \frac{1}{2\mu - \frac{P}{2h}} \frac{Eh^{2}}{3(1 - v^{2})}, \quad B_{3} = \frac{P}{2h} \frac{2\mu}{2\mu - \frac{P}{2h}},$$

$$B_{2} = \frac{(\gamma + \varepsilon)}{2\alpha} \left[(\mu + \alpha) - \frac{P}{2h} \right] \frac{2\mu}{2\mu - \frac{P}{2h}} - \frac{(\gamma + \varepsilon)}{2\alpha} (\mu - \alpha) + \left(2\mu - \frac{P}{h} \right) \frac{1}{2\mu - \frac{P}{2h}} \frac{Eh^{2}}{3(1 - v^{2})}.$$
(26)

If we have a solution of differential equation (25), then w and Ω_2 are defined as follows:

$$\Omega_2 = \frac{1}{2\alpha} \left((\mu + \alpha) - \frac{P}{2h} \right) \frac{dw}{dr} + \frac{(\mu - \alpha)}{2\alpha} \psi_1,$$
(27)

$$\frac{dw}{dr} = -\frac{2\mu}{2\mu - \frac{P}{2h}}\psi_1 + \frac{1}{2\mu - \frac{P}{2h}}\frac{Eh^2}{3(1 - v^2)}\frac{d}{dr}\left(\frac{d}{dr} + \frac{1}{r}\right)\psi_1.$$
(28)

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Differential equation (25) can be represented as:

$$(\Delta - \lambda_1)(\Delta - \lambda_2)\psi_1 = 0$$
, (29)

where λ_1, λ_2 are the roots of the next second-degree equation: $B_1\lambda^3 + B_2\lambda^2 + B_3 = 0,$ (30)

or

$$\lambda_{1,2} = \frac{-B_2 \pm \sqrt{(B_2)^2 - 4B_1 B_3}}{2B_1} \,. \tag{31}$$

The solution of differential equation (29) for a solid plate has the form:

$$\psi_1(r) = C_1^1 J_1 \left(-i\sqrt{\lambda_1} r \right) + C_2^1 J_1 \left(-i\sqrt{\lambda_2} r \right).$$
(32)

Substituting (32) into (17) and (28) and integrating the result, we obtain:

$$w(r) = C_1^2 J_0 \left(-i\sqrt{\lambda_1} r \right) + C_2^2 J_0 \left(-i\sqrt{\lambda_2} r \right) + C_3^2,$$

$$\tilde{\Omega}_2(r) = C_1^3 J_1 \left(-i\sqrt{\lambda_1} r \right) + C_2^3 J_1 \left(-i\sqrt{\lambda_2} r \right),$$
(33)
(34)

$$D_{2}(r) = C_{1}^{3} J_{1}(-i\sqrt{\lambda_{1}}r) + C_{2}^{3} J_{1}(-i\sqrt{\lambda_{2}}r),$$
(34)

where $J_0(x)$, $J_1(x)$ are the Bessel functions of the valid argument of the zero and first orders.

$$C_n^2 = \frac{\left(\frac{Eh^2}{3\left(1-\nu^2\right)}\lambda_n + 2\mu\right)}{\left(\frac{P}{2h} - 2\mu\right)}C_n^1,$$
(35)

$$C_{n}^{3} = -\frac{\frac{Eh^{2}}{3(1-\nu^{2})}\frac{\mu+\alpha}{2\alpha}\lambda_{n} + 2\mu + \frac{P}{2h}\left(\frac{\mu+\alpha}{2\alpha} - \frac{Eh^{2}}{3(1-\nu^{2})}\lambda_{n}\right)}{\frac{P}{2h} - 2\mu}C_{n}^{1}.$$
(36)

To satisfy the boundary conditions (22), we obtain homogeneous algebraic equations along to the C_1^1, C_2^1, C_3^2 . Further, demanding a nonzero solution, as a result, we obtain the transcendental equation with respect to P, which we can represent in compact form: $Det |a_n^m| = 0, \quad n, m = 1, 2, 3,$ (37)

where

$$a_{i}^{1} = \frac{i2h(Eh^{2}\lambda_{i} - 6\mu(1 - v^{2}))(-1 + I_{0}(R\sqrt{\lambda_{i}}))}{3\sqrt{\lambda_{i}}(P - 4h\mu)(1 - v^{2})}, a_{3}^{1} = 1,$$

$$a_{i}^{2} = \left(\sqrt{\lambda_{i}}I_{0}(R\sqrt{\lambda_{i}}) - \frac{(1 - v)I_{1}(R\sqrt{\lambda_{i}})}{R}\right), a_{3}^{2} = a_{3}^{3} = 0,$$

$$a_{i}^{3} = \left(R(\gamma + \varepsilon)\sqrt{\lambda_{i}}\left(P(Kh^{2}\lambda_{i} - 3(\mu + \alpha)(1 - v^{2})) - 2h(Kh^{2}\lambda_{i}(\mu + \alpha) - 12\mu\alpha(1 - v^{2}))\right)\right) \times \times I_{0}(R\sqrt{\lambda_{i}}) + 2\gamma\left(2Kh^{3}\lambda_{i}(\mu + \alpha) - 24h\mu\alpha(1 - v^{2}) - P(Kh^{2}\lambda_{i} - 3(\mu + \alpha)(1 - v^{2}))\right)I_{1}(R\sqrt{\lambda_{i}}).$$
(38)

Here $I_0(x), I_1(x)$ – Bessel functions of purely imaginary argument of the zero and the first orders.



Fig. 2. Dependence of the dimensionless quantity $P_{mic.}/P_{class.}$ on the dimensionless physical parameter α/μ

We consider a specific numerical example for hypothetic material: R = 0.07 m, $h = \frac{a}{40}$, $\mu = 2 MPa$, $\lambda = 3 MPa$, $\gamma = \varepsilon = 150$ H. On Fig. 2 the dependence of the dimensionless quantity $P_{mic.}/P_{class.}$ on the dimensionless physical parameter, α/μ is presented, $P_{mic.}$ is the critical value of the external force for micropolar theory, $P_{class.}$ is the same quantity for classical theory. As we note we can get a geometrically nonlinear classical Timoshenko-type model from the micropolar model if to put $\alpha = 0$. For more large values of α , we obtain more large values for the $P_{mic.}$ compared to the value $P_{class.}$. So it is easy to verify that with increasing α/μ , the value $P_{mic.}/P_{class.}$ increases, which means that in the case of micropolar material the round plate is more stable.

5. Conclusion

In the work, the stability problem of micropolar elastic round plates is studied. During the study of the problem, the stability equations are obtained using the linearization procedure in the geometrically nonlinear equations.

The concrete stability problem of round micropolar plate was studied, and it was shown that, with other parameters being equal, the round micropolar plate is more stable than the round plate with the classical material.

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ANALYTICAL DESCRIPTION OF QUANTUM EFFECTS AT CURRENT FILAMENTATION IN CHALCOGENIDE GLASSES

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Abstract. Quantum effects occurring during current filamentation in a chalcogenide glass are considered. Under the conditions considered, the current filament appears as a set of concentric tubes with different temperatures. In every tube, the electron has a specific wave function and a specific energy level. The radii of the tubes appear to be proportional to natural numbers n. The dependence of maximal temperature on the electrical field is obtained. The Schroedinger equation is reduced to the first order differential equation. The type of energy of an electron at the tube is close to exciton energy dependence. The potential energy of an electron is described with the first order polynom of temperature. The temperature distribution in the filament is shown as an interference of the electron.

Keywords: chalcogenide glasses; current filament; quantization

1. Introduction

Formation of current filaments (current filamentation, or crowding) is a phenomenon that often occurs in chalcogenide glasses, which are considered to be the material of choice for the next-generation phase-change memory (PCM) devices [1,2]. This effect consists of a significantly higher current density in a certain coordinate region [3,4]. When the radius of the current filament decreases down to tens of nanometers, one can expect the appearance of quantum effects consisting in the fact that the diameter of the filament would take only certain, albeit close to each other, values. Taking into account that quantization of current and conductance were observed in, e.g., superconductors [5], carbon nanotubes [6], and metallic nanowires [7], this hypothesis is worth verification in application to chalcogenide glasses, too.

In this paper, the formation of a current filament is analyzed with allowance for quantum effects, and a simple analytical formula describing the quantization phenomena is presented. Additionally, a description of the filament is proposed as an object in which the energy of an electron has a form similar to the energy of an exciton in a solid or an electron in a hydrogen atom.

2. The model

In general, quantization can take place in all three coordinates. In the case of the current filament, however, only the radius will take certain values, since we assume that the length of the filament is $L \sim 10^{-6}$ m, which is too large a value for the manifestation of quantum effects. Assuming in the first approximation that the electrons do not interact with each other, we suggest that it is possible to describe the quantum scale of the resulting filament with the formula:

 $\int_0^{r_c} \sqrt{2mkT(r)} \, dr = nh.$

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Analytical description of quantum effects at current filamentation in chalcogenide glasses

Here T is the temperature, k is Boltzmann's constant, m is the electron mass. Expression (1) is an integral of work in time, and when it becomes of the same order of magnitude as Planck's constant h, quantum effects should appear. Here, we integrate from zero to the radius of the filament r_c the momentum of an electron moving along the radial coordinate r in a medium with a certain temperature distribution. As a result, a value is obtained that has the same dimension as that of the angular momentum, yet is not exactly the momentum, as the angular momentum of an electron moving along the radius is equal to zero. The temperature in the stationary case is represented by the formula:

$$T(x) = T_0 + (T_m - T_0)exp\left(\frac{-ax^2}{4}\right).$$
Here
(2)

$$x = \frac{r}{r_0}, \qquad a = \frac{F^2}{F_s^2} exp\left(\frac{-1}{t_m}\right) \frac{1}{t_m^2} - 1; F_s^2 = \frac{2\lambda\Delta E}{\sigma_0 L k},$$

where *F* is the electric field, $F_0=10^6$ V/m, λ is the heat sink coefficient, ΔE is the energy of activation of conductivity, T_m is a filament temperature of radius $x_c(n)$, T_0 is the room temperature, σ_0 is the initial conductivity, r_0 is a constant of the order of 1 µm, $t_m = \frac{kT_m}{\Delta E}$. In this consideration, the conductivity of the glass was taken in the form that summarizes its temperature and electric field dependences [3],[8],[9]:

$$\sigma = \sigma_0 \exp(-\frac{\Delta E}{\mathrm{kT}} + \frac{F}{F_0})$$

Expression (2) describes the temperature in the filament as satisfactory; therefore, r_c can be taken as the radius of the filament, since outside the radius of the filament as the coordinate increases, the sample temperature is not described by a simple analytical formula. Taking into account that the action takes place on a small scale, formula (2) can be expanded in Taylor's series up to the second term and substituted in (1). As a result, we get an equation of the third degree:

$$p_m x - p_m \frac{T_m - T_0}{T_m} \frac{ax^3}{24} = n \frac{h}{r_0},$$
(3)
where $n_n = \sqrt{2km} \frac{T}{T_n}$ Equation (3) is then reduced to the canonical form:

where
$$p_m = \sqrt{2km_e T_m}$$
. Equation (3) is then reduced to the canonical form:
 $x^3 - \frac{24T_m}{a(T_m - T_0)}x + \frac{24nhT_m}{r_0 p_m a(T_m - T_0)} = x^3 + px + q = 0.$
(4)

The roots of a given polynomial can be found using Cardano's formulas. Omitting the consideration of the choice of the legible roots, which will be presented in details elsewhere, we come straight to the expression for the current filament radius with a number n:

$$x_{c}(n) = \frac{3nh}{2r_{0}p_{m}}; p_{m} = \sqrt{2kmT_{m}}.$$
(5)

The quantized radius was defined as Bohr radius or quantized resistance by using the Heisenberg principle. The current filament is formed gradually. First, a filament with a large radius is formed, then a filament of a smaller radius is formed inside the first filament, and in a few nanoseconds, a structure consisting of a number of concentric tubes is obtained.

The authors attempted to describe a behavior of an electron in every ring considering a thermal potential:

U(x) = C - kT(x).

Here C is a constant with its value laying in the range from 1 to 4 eV; it describes total energy of an electron and cannot exceed the value of work function, otherwise, the electron will leave the filament and the material. The subtrahend in this equation is the kinetic energy of the electron.

The first order Schroedinger equation of this potential:

$$y' + y^2 + \frac{y}{x} - \frac{2mr_0^2}{\hbar^2} U(x) + \frac{2mr_0^2}{\hbar^2} E = 0,$$

$$y(x) = (f'(x)), \psi(x) = Aexp(f(x)), \psi(x) \text{ is a Schroedinger function.}$$
(6)

The thermal electron energy depends on the quantum filament radius. The dependence is similar to that of the exciton energy.

$$E_n = U(x(n)) - \frac{\hbar^2}{8mr_0^2 x_n^2}$$
(7)

If $n \to \infty$, $E_n \to C - kT_0$. This result does not contradict physical meaning. E_n is the absolute value of energy for the electron in the conduction band.

The probability of the appearance of the filament with zero radius is zero because of $\psi^2(x)x = 0$ when n=0. Indeed, from the classical theory of the current filament [2], it follows that a filament with zero radius should be formed at an infinitely high electric field. The energy of an electron in a filament of zero radius is infinite and negative. This can be interpreted as if the electron is placed in an infinite field and at the same time is located in a quantum well. When $T_0 \rightarrow 0$, T_m decreases for a given n. On the contrary, the difference between the adjacent radii $x_c(n)$ increases. All this leads to a more pronounced manifestation of quantum effects.

In addition to the analytical solution, values of E_n were calculated numerically by solving the Schroedinger equation using Matlab software. The results are presented in Table 1. A good agreement between the analytically and numerically calculated values is observed. The subtrahend $\frac{\hbar^2}{8mr_0^2 x_n^2} \ll C - kT$, which, in fact, means, that the quantization effects are rather weak. The most interesting is the first (more precisely, zero) energy level. As can be seen in Table 1, this energy very much differs in value from the subsequent values lying in the interval kT_m . The change of the sign of the potential energy did not affect the position of the energy level E_0 . The wave functions were calculated and the behavior of an electron seems similar to the interference of light. For the electron, the probabilities to be found exist in a certain area of the sample appear to be periodical with different magnitudes (Fig. 1). The ringlike (or, rather, tube-like) areas with different temperatures are separated from each other. The temperature distribution is continuous in the case of large areas where quantum effects disappear. Thus, we assume that this energy near zero coordinates corresponds to the colder region of the glass and that the filament has the shape of empty tubes with similar temperature distributions with a cold area existing at the center of the current filament.

n, quantum number	E_n , eV (numerical)	E_n , eV (analytical)		
0	1.6092	-		
1	1.9482	1.9512		
2	1.9594	1.9591		
3	1.9670	1.9665		
4	1.9717	1.9711		

Table 1. Calculated values of electron energy

Also, the formula for calculation of the temperature T_m in each ring was derived:

$$\frac{9n^2h^2}{r_0^2} = F'(t_m), F'(t_m) = \frac{2m\Delta E t_m^4}{\left(\beta exp\left(\frac{-1}{t_m}\right) - t_m^2\right)(t_m - t_0)}$$
(8)
Here, $\theta_m E^2/E^2$, $t_m = \frac{kT_m}{t_m}$, $t_m = t_m$,

Here $\beta = F^2/F_s^2$, $t_m = \frac{\kappa_{1m}}{\Delta E}$ is the maximum temperature of heating for each ring, $t_0 = \frac{\kappa_{10}}{\Delta E}$. The value of t_m cannot possibly be smaller than t_0 and $n \to \infty$ if $t_m \to t_0$. It means that filaments do not form at low currents. The width of every filament is of the order of 10 nm.



Fig. 1. The wave functions of the electron at the potential U(x) = C - kT(x), $T_0 = 300K$, $T_m = 1000K$, $F = 4 \cdot 10^6 V/m$

Figure 2 shows the relation between the maximum temperature and the electric field. In the case presented in Fig. 2, the quantum number *n* (in this case, n = 2 and $\frac{9n^2h^2}{r_0^2} = 5.49 \cdot 10^{-5}$, which is shown as a solid blue horizontal line) intersects the graph of the function *F*. The maximum temperature t_m is searched at the points of the intersection of the two lines. The most probable t_m is the maximal root of equation (8).



Fig. 2. The relation between the maximum temperature and the electric field. In the case considered, n = 2 and $\frac{9n^2h^2}{r_0^2} = 5.49 \cdot 10^{-5}$ (shown as a horizontal line)

3. Conclusion

In this work, an attempt was made to develop a quantum approach to the formation of a current filament in a cylindrical sample of chalcogenide glass with a conductivity that exponentially depends on the inverse temperature taken with a negative sign. It is shown that quantum effects can manifest themselves in current filaments on scales of tens of nanometers at high fields and a glass sample thickness of the order of a micrometer. The radius of the

filament has been refined; the formed filament has a certain radius and a certain maximum temperature in the center. A law has been established according to which the maximum temperature depends on the electric field. Every filament represents a set of concentric tubes, each up to ten nanometers wide, with a specific temperature that drops sharply from maximum to room temperature. An exception is the central region of the filament; the authors believe that a cold "spot" is formed in the very center of such a filament. The second-degree differential equation describing the probability of an electron to be in a certain quantum of the filament has been replaced by an equation of the first degree, which simplified the approach.

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ОЦЕНКА СКОРОСТИ РОСТА РАССЛОЕНИЙ В КВАЗИИЗОТРОПНЫХ КОМПОЗИТАХ С ИСПОЛЬЗОВАНИЕМ МОДЕЛИ ДЕГРАДАЦИИ ЖЕСТКОСТИ

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Аннотация. Рассмотрены основные особенности физического моделирования роста расслоений при циклическом растяжении квазиизотропных композиционных материалов с использованием модели снижения начальной жесткости. Отмечено, что эти особенности имеют значительные отличия от положений классической механики межслойного разрушения композиционных материалов. В качестве определенного развития этого направления на основе использования модели деградации жесткости предложен ряд новых соотношений, позволяющих более точно, чем существующие модели, выполнять расчетные оценки скорости роста расслоений. Проведена верификация предложенных соотношений на примере расчетных оценок скорости роста расслоений в квазиизотропном ламинате углепластика XAS/914 [45/90/-45/0]_s.

Ключевые слова: квазиизотропные композиционные материалы, расслоение, циклическое растяжение, деградация жесткости, скорость роста расслоения

1. Введение

Известно, что расслоение является одним из наиболее опасных и трудно контролируемых повреждений слоистых полимерных композиционных материалов (ПКМ). Именно поэтому исследованию возникновения и роста расслоений в ПКМ посвящены работы многих авторов.

Исследования по определению доминирующей моды разрушения при начале и росте расслоения сфокусированы на механике межслойного разрушения, в рамках которой требуется определить, прежде всего, изменение энергии деформации за единицу площади приращения расслоения [1]. Этот параметр называется интенсивностью высвобождения упругой энергии в вершину трещины G. С целью определения, будет ли расслоение расти, вычисленные значения G сравниваются с критическими значениями G_c и делается вывод о разрушении при статическом нагружении. Как правило, рассматриваются три моды разрушения: мода I (от напряжений отрыва); мода II (от напряжений поперечного сдвига) и мода III (от напряжений продольного сдвига). Моды I и II считаются наиболее критичными и поэтому им уделяют наибольшее внимание при разработке методов испытаний и в расчетных исследованиях [2-3]. Подобный подход требует как компьютерного моделирования, так и определения целого ряда экспериментальных характеристик.

Второй подход заключается в оценке роста расслоений при циклическом (усталостном) нагружении. В работах [2-7] представлен ряд уравнений для оценки скорости роста расслоений при различных модах разрушения. В работе [3] http://dx.doi.org/10.18149/MPM.4612020 20

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представлено, например, следующее уравнение для оценки скорости роста расслоения для смешанной моды разрушения (I+II):

$$\frac{dL}{dn} = m_1 \left(\frac{G_I}{G_{Ic}}\right)^{n_1} + m_2 \left(\frac{G_{II}}{G_{IIc}}\right)^{n_2},\tag{1}$$

где:

- $\frac{dL}{dn}$ рост расслоения за один цикл усталостного нагружения;
- *G_I* действующее значение интенсивности высвобождения упругой энергии по моде I при рассматриваемом цикле нагружения;
- *G_{II}* действующее значение интенсивности высвобождения упругой энергии по моде II при рассматриваемом цикле нагружения;
- *G*_{*lc*} критическое значение интенсивности высвобождения упругой энергии по моде I характеристика трещиностойкости (определяется экспериментально, как правило, меньше значения *G*_{*lc*} при статическом разрушении);
- *G*_{*IIc} критическое значение интенсивности высвобождения упругой энергии по моде II характеристика трещиностойкости (определяется экспериментально, как правило, меньше значения <i>G*_{*IIc*} при статическом разрушении);</sub>
- m_1, m_2, n_1, n_2 константы материала.

Анализируя уравнение (1) можно заключить, что оно является достаточно сложным и предполагает значительный объем предварительных экспериментальных исследований, что ставит под сомнение перспективы широкого использования этого уравнения для инженерных оценок начала и длительности расслоения в конкретных слоистых материалах.

Следует также отметить, что представленное уравнение практически непригодно для инженерных оценок роста расслоений в слоистых ПКМ *при циклическом растяжении*. Вместе с тем известно, что подобный расчетный случай и подобная мода повреждения являются достаточно распространенными и поэтому заслуживают отдельного рассмотрения и анализа.

2. Физическая модель роста расслоений при циклическом растяжении квазиизотропных композитов

В работах [8-10] представлены основные положения физической модели роста повреждений при циклическом нагружении слоистых ПКМ, которые имеют значительные отличия от методов линейной механики межслойного разрушения.

В работе [11] в качестве одного из частных случаев этой модели представлены основы физического моделирования роста расслоений в слоистых ПКМ при циклическом растяжении. Иллюстрация моды "расслоение" при подобном нагружении представлена на Рис. 1.

К основным особенностям физического моделирования роста расслоений в слоистых ПКМ при циклическом растяжении по данным работы [11] можно отнести следующие.

Введено понятие параметра расслоения D как нормализованное расслоение площади A/A_0 , где A – фактическая (измеренная) площадь расслоения, а A_0 – общая площадь, доступная для расслоения.


Рис. 1. Иллюстрация моды "расслоение" при растяжении слоистых ПКМ: а) ламинат без расслоения; b) полное расслоение; c) частичное расслоение

Предполагается, что существует соотношение между параметром *D* и модулем упругости Юнга для рассматриваемого слоистого композита, которое можно записать как:

(2)

$$E = E_0 \cdot g(D),$$

где E – текущее значение модуля упругости; E_0 – начальное значение модуля упругости для неповрежденного материала; g(D) – некая функция.

Предложена простая модель для оценки снижения значения модуля упругости при росте расслоений:

$$E = E_0 + (E^* - E_0) \frac{A}{A_0},$$

где E^* – значение модуля упругости, соответствующее полному расслоению композита. На основании обработки известных экспериментальных данных в работе [12] сделан вывод, что когда $A/A_0 = 1$, $E/E_0 = 0.65$.

Функция g(D) в выражении (2) в виде

 $g(D) = a + b \cdot D$

может быть построена по двум точкам: $D_1 = 0$; g(D) = 1; $D_2 = 1$; g(D) = 0.65.

Таким образом, функцию g(D) в выражении (2) можно записать как

g(D) = 1 - 0.35D.

Из этого следует, что:

$$E = E_0(1 - 0.35D);$$
 $D = 2.857 \left(1 - \frac{E}{E_0}\right);$

И

$$\frac{dD}{dn} = -2.857 \left(\frac{1}{E_0} \frac{dE}{dn} \right).$$
(3)

На Рис. 2 представлены экспериментальные данные зависимости

$$\frac{dD}{dn} = -2.857 \left(\frac{1}{E_0} \frac{dE}{dn} \right) = f \left(\frac{\Delta \sigma}{\sigma_{UTS}} \right)$$
(3,a)

для квазиизотропного ламината углепластика XAS/914 [45/90/-45/0]_s при циклическом растяжении с R=0.1, где σ_{UTS} =550 МПа - предел прочности рассматриваемого ламината на растяжение (данные работы [12]). Там же приведен пример аппроксимации рассмотренных экспериментальных данных, выполненный в работе [12] с использованием уравнения, сходного по форме с известным уравнением Пэриса:

В.Е. Стрижиус





По результатам анализа данных, представленных на Рис. 2, можно сделать вывод, что аппроксимация экспериментальных данных зависимостью (4) в области малых и больших значений параметра $\Delta \sigma / \sigma_{UTS}$ не может быть признана достаточно успешной, так как в этих областях можно отметить значительное расхождение между расчетными и экспериментальными данными.

Следует также отметить следующее. Соотношение (3) содержит достаточно важный параметр – dE/dn, который отсутствует в соотношении (4). Таким образом, соотношение (4) практически не учитывает влияние на скорость роста расслоения изменения жесткости слоистого композита в процессе накопления усталости, что с физической точки зрения является очевидным недостатком этого соотношения. Ввиду этого соотношение (4) можно считать достаточно приближенным, при использовании этого соотношения отсутствует возможность исследования изменения скорости роста расслоения в процессе накопления усталости, что, безусловно, представляет значительный научный интерес.

3. Оценка скорости и длительности роста расслоений при циклическом растяжении квазиизотропных композитов с использованием модели деградации жесткости

Известно, что в процессе накопления усталости происходит снижение (деградация) начальной жесткости слоистых композитов. Этой проблеме посвящено достаточно большое количество зарубежных исследований, среди которых, прежде всего, можно отметить работы [13-18]. В этих работах сформированы основные положения модели

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деградации жесткости слоистых композитов, причем эти положения, как правило, не связаны с расслоением композита, как с конкретной модой разрушения.

По результатам обзора и анализа данных, представленных в этих работах, можно сделать следующие выводы.

- 1. Остаточная жесткость композиционного материала, также как и остаточная прочность, является функцией уровня и числа циклов приложенных напряжений.
- 2. Модели деградации жесткости интересны многим исследователям, так как остаточная жесткость может быть использована как «неразрушающая» мера оценки повреждения ПКМ.
- 3. Для представления остаточной жесткости как функции уровня и числа циклов в работе [18] для однонаправленного ламината при одноосном циклическом нагружении с постоянной амплитудой приведено следующее уравнение:

$$E(n) = (E_0 - \frac{\sigma}{\varepsilon_f}) \times \left(1 - \left(\frac{\lg(n) - \lg(0.25)}{\lg(N) - \lg(0.25)}\right)^{\lambda}\right)^{\frac{1}{\gamma}} + \frac{\sigma}{\varepsilon_f},\tag{5}$$

где:

- E(n) остаточная жесткость;
- E_0 начальная (статическая) жесткость;
- *σ* величина прикладываемых напряжений;
- *ε_f* средняя деформация при статическом разрушении;
- *n* число приложенных циклов;
- N усталостная долговечность (число циклов до разрушения) при уровне напряжений σ, определятся, как правило, с использованием S-N кривой усталости слоистого ПКМ (кривой Веллера);

 $1-\gamma$

• λ и γ – экспериментальные параметры.

Предполагается, что уравнение (5) может быть использовано для решения рассматриваемой задачи – оценки скорости и длительности роста расслоения при циклическом растяжении квазиизотропных композитов.

Действительно, производная функции *E*(*n*) равна:

$$E'(n) = \frac{dE}{dn} = -(E_0 - \frac{\sigma}{\varepsilon_f}) \times \frac{1}{\gamma} \times \left(1 - \left(\frac{\lg(n) - \lg(0.25)}{\lg(N) - \lg(0.25)}\right)^{\lambda}\right)^{\frac{1}{\gamma}} \times \frac{1}{\lg(N) - \lg(0.25)} \times \frac{1}{\log(N) - \lg(0.25)} \times \frac{1}{n \cdot \ln 10}.$$
(6)

Подставляя соотношение (6) в соотношение (3), может быть определена скорость роста расслоения в процессе накопления усталости при растяжении квазиизотропного композита:

$$\frac{dD}{dn} = -2.857 \left(\frac{E'(n)}{E_0}\right) = f_1(\sigma, R, n/N).$$
(7)

Анализируя соотношение (7), можно сделать вывод, что с использованием этого соотношения возможна оценка скорости роста расслоения не только в зависимости от уровня действующих напряжений, но и от уровня накопленной усталости, которая характеризуется величиной n/N. В этом плане можно утверждать, что соотношение (7) описывает изменение скорости расслоения более "физично", чем соотношение (4).

Уравнение (5) можно переписать в следующем виде:

$$\frac{E(n)}{E_0} = (1 - \frac{\sigma}{\varepsilon_f \cdot E_0}) \times \left(1 - \left(\frac{\lg(n) - \lg(0.25)}{\lg(N) - \lg(0.25)}\right)^{\lambda}\right)^{\frac{1}{\gamma}} + \frac{\sigma}{\varepsilon_f \cdot E_0}.$$
(8)

Очевидно, что с использованием соотношения (8) могут быть построены графические зависимости

$$\frac{E(n)}{E_0} = f_2(\sigma, R, n, N), \qquad (9)$$

с помощью которых можно продемонстрировать процесс накопления меры расслоения в рассматриваемом ламинате.

Расчетная оценка «разрушающей» меры расслоения выполняется при n = N.

4. Верификация предложенных соотношений

Верификация предложенного соотношения (7) проведена на примере расчетных оценок скорости роста расслоения в рассмотренном выше квазиизотропном ламинате углепластика XAS/914 [45/90/-45/0]_s при циклическом растяжении с R=0.1 при максимальных напряжениях цикла $\sigma_{max} = 300, 360, 420, 515$ МПа.

При выполнении расчетных оценок использованы следующие уравнения и значения:

- σ_{UTS} =550 МПа предел прочности рассматриваемого ламината на растяжение (данные работы [12]).
- Уравнение S-N кривой усталости уравнение Менделла [19] для ламината из углепластика XAS/914 [45/90/-45/0]_s при циклическом растяжении с R=0.1, получено по результатам обработки данных работы [12]: σ_{max} = 801.664 – 71.666 · lg N – для σ_{max} = 300 ÷ 515 МПа.
- *ε_f* =0.0136 − средняя деформация при статическом разрушении значение принято на основании данных работы [20].
- 4. $E_0 = \sigma_{UTS} / \varepsilon_f = 40441 \,\text{M}\Pi a$ начальная (статическая) жесткость.
- 5. $\lambda = 14.57$ и $\gamma = 0.3024$ значения параметров λ и γ приняты на основании данных работы [20].

На Рис. 3-4 представлены зависимости (7), построенные для рассматриваемого ламината при рассматриваемых уровнях нагружения.

На Рис. 5 приведены результаты расчетных оценок *максимальных* скоростей роста расслоений, выполненных с использованием соотношения (7), и сравнение этих результатов с экспериментальными данными и расчетными данными, полученными с использованием соотношения (4).

На Рис. 5 представлены также результаты *аппроксимации* расчетных оценок *максимальных* скоростей роста расслоений, выполненной с использованием экспоненциальной зависимости (10):

$$\frac{dD}{dn} = 2 \times 10^{-9} \times e^{11.236\Delta\overline{\sigma}},\tag{10}$$

где $\Delta \overline{\sigma} = \Delta \sigma / \sigma_{UTS}$.

Верификация соотношений (8)-(9) проведена на примере расчетных оценок «разрушающей» меры расслоения $E(n)/E_0$ в рассмотренном ламинате при максимальных напряжениях цикла σ_{\max} =360, 420, 500 МПа.



Рис. 3. Зависимости (7) для ламината углепластика XAS/914 [45/90/-45/0]_s при максимальных напряжениях циклического растяжения σ_{max} =300 и 360 МПа



Рис. 4. Зависимости (7) для ламината углепластика XAS/914 [45/90/-45/0]_s при максимальных напряжениях циклического растяжения σ_{max} =420 и 515 МПа



Рис. 5. Результаты расчетных оценок *максимальных* скоростей роста расслоений и сравнение этих результатов с экспериментальными данными для ламината углепластика XAS/914 [45/90/-45/0]_s



Рис. 6. Графические зависимости (9) для ламината углепластика XAS/914 [45/90/-45/0]_s

Оценка скорости роста расслоений в квазиизотропных композитах с использованием модели деградации...

На Рис. 6 для рассматриваемого ламината при рассматриваемых уровнях напряжения представлены графические зависимости (9), с использованием которых могут быть выполнены оценки «разрушающей» меры расслоения при достижении наработки n = N.

В Таблице 1 представлено сравнение выполненных таким образом расчетных оценок «разрушающей» меры расслоения $E(n)/E_0$ с экспериментальными данными, приведенными в работе [12].

Таблица 1. Сравнение расчетных оценок «разрушающей» меры расслоения $E(n)/E_0$ в ламинате углепластика XAS/914 [45/90/-45/0]_s с экспериментальными данными работы [12]

		$E(n)/E_0$,	$E(n)/E_0$,
$\sigma_{\scriptscriptstyle m max}$, MПa	N, циклы	расчет (9)	эксперимент
360	1 455 000	0.65	0.67
420	212 000	0.76	0.78
500	16 190	0.91	0.94

5. Обсуждение результатов

Анализ представленных на Рис. 3-4 зависимостей (7) для квазиизотропного ламината углепластика XAS/914 [45/90/-45/0]_s при циклическом растяжении с *R*=0.1 позволяет сделать следующие выводы.

- 1. Расчетные скорости роста расслоения в рассматриваемом ламинате находятся в очевидной зависимости от уровня накопленной усталости, которая характеризуется величиной n/N. Можно предположить, что с точки зрения исследования закономерностей изменения скоростей роста расслоения от накопленной усталости использование зависимостей (7) будет представлять значительный интерес.
- 2. Расчетные скорости роста расслоения в рассматриваемом ламинате ожидаемо зависят от уровня действующих напряжений.

Анализ представленных на Рис. 5 зависимостей позволяет сделать следующие выводы.

- 1. Результаты расчетных оценок *максимальных* скоростей роста расслоений, выполненные с использованием соотношения (7), хорошо согласуются с экспериментальными данными. Очевидно, что в рассмотренном примере расчета с использованием соотношения (7) были получены более точные результаты расчетных оценок, чем с использованием соотношения (4).
- Результаты аппроксимации расчетных оценок максимальных скоростей роста расслоений, выполненной с использованием экспоненциальной зависимости (10), показали достаточно хорошее совпадение зависимости (10) с экспериментальными данными. Величина достоверности собственно аппроксимации составила R²=0.9848.
- 3. Очевидно, что зависимость (10) более точно, чем соотношение (4), описывает изменение скоростей роста расслоений в рассматриваемом ламинате в зависимости от параметра $\Delta \overline{\sigma} = \Delta \sigma / \sigma_{UTS}$.

На основании анализа данных, представленных на Рис. 6 и в Таблице 1, можно заключить следующее.

1. Графические зависимости (9), представленные на Рис. 6, достаточно наглядно демонстрируют накопление «разрушающей» меры расслоения в рассматриваемом ламинате.

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2. Расчетные оценки «разрушающей» меры расслоения, выполненные с использованием зависимостей (9), достаточно хорошо согласуются с экспериментальными данными, приведенными в работе [12].

Как отмечалось выше, базовые соотношения (5)-(7) для оценки скоростей роста расслоения справедливы для квазиизотропных композитов и не могут быть применимы для многослойных композитов с анизотропией слоев. Тем не менее, следует отметить следующее.

По данным работ [21-24] для многослойных композитов может быть использовано следующее соотношение:

$$E(n) = E_1 \times \left(1 - k_1 \times \left(\frac{\sigma_a}{E_0} \right)^{k_2} \times n \right), \tag{11}$$

где:

- E(n) остаточная жесткость;
- *Е*₀ начальная статическая жесткость;
- E_1 начальная циклическая жесткость;
- *σ_a* амплитуда циклических напряжений;
- *n* число приложенных циклов;
- k_1 и k_2 постоянные для рассматриваемого материала, получаемые по результатам обработки экспериментальных данных.

В этом случае производная функции *E*(*n*) равна:

$$E'(n) = \frac{dE}{dn} = -E_1 \times k_1 \times \left(\frac{\sigma_a}{E_0}\right)^{k_2}.$$
(12)

Подставляя соотношение (12) в соотношение (3), может быть определена скорость роста расслоения в процессе накопления усталости при растяжении многослойного анизотропного композита:

$$\frac{dD}{dn} = -2.857 \left(\frac{E'(n)}{E_0}\right) = f_2(\sigma_a).$$
(13)

Очевидно, что при наличии экспериментальных данных достаточного объема могут быть определены значения всех необходимых параметров соотношений (11-13) и может быть выполнена оценка скоростей роста расслоения в многослойных композитах с анизотропией слоев.

К сожалению, подобные экспериментальные данные в открытых публикациях практически не представлены и поэтому верификация соотношений (11)-(13) вызывает в настоящее время определенные затруднения.

6. Заключение

Представлены основные особенности физического моделирования роста расслоений в слоистых ПКМ при циклическом растяжении, изложенные в работе [11]. Отмечено, что эти особенности имеют значительные отличия от положений классической механики межслойного разрушения ПКМ.

С использованием известной модели снижения (деградации) начальной жесткости квазиизотропных композитов в процессе накопления усталости предложены новые соотношения (7) и (10), позволяющие более точно, чем существующие модели, выполнять расчетные оценки скорости роста расслоений при циклическом растяжении рассматриваемых ПКМ.

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Проведена верификация предложенных соотношений на примере расчетных оценок скорости роста расслоений в квазиизотропном ламинате углепластика XAS/914 $[45/90/-45/0]_{s}$ при циклическом растяжении с R=0.1. Показана приемлемая точность расчетных оценок.

Отмечено, что при наличии экспериментальных данных достаточного объема могут быть определены значения необходимых параметров соотношений (11-13) и в этом случае будет возможна оценка скоростей роста расслоения в многослойных композитах с анизотропией слоев.

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ESTIMATION OF DELAMINATION GROWTH RATE IN QUASI-ISOTROPIC COMPOSITES USING THE STIFFNESS DEGRADATION MODEL

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Abstract. The main features of physical modeling of the growth of delaminations under cyclic tension of quasi-isotropic composite materials are considered using the model of decreasing the initial stiffness. It is noted that these features are significantly different from the provisions of the classical mechanics of interlayer fracture of composite materials. As a definite development of this direction, based on the use of the stiffness degradation model, a number of new relationships have been proposed, which make it possible to more accurately than the existing models to carry out calculated estimates of the growth rate of delamination. Verification of the proposed relations is carried out on the example of calculated estimates of the growth rate of delaminations in a quasi-isotropic CFRP laminate XAS/914 [45/90/-45/0]_s. **Keywords:** quasi-isotropic composite materials, delamination, cyclic tension, degradation of stiffness, growth rate of delamination

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