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RECENT DEVELOPMENTS IN UNDERSTANDING THE CREEP OF ALUMINUM

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Abstract. This paper summarizes the recent creep research by the author on pure aluminum including classic five power-law creep, Harper-Dorn creep, ambient-temperature creep and an investigations of long-range internal stresses in creep-deformed aluminum. Many of the models and theories for these phenomena persisted for a relatively long period of time. More recent developments in these phenomena are discussed that may lead to new interpretations of creep in aluminum, as well as creep in other crystalline materials.

Keywords: creep, Harper-Dorn, five-power law creep, dislocation hardening, long-range internal stress, low-temperature creep

1. Introduction

This paper reviews recent advances in the basic understanding of creep in pure aluminum over a very large temperature range. It updates the general thinking of the creep community over the past ten to twenty years with particular attention directed toward the two years since the publication of reviews by this author [1, 2]. The topics discussed are: Harper-Dorn creep (highest temperature) followed by five-power law creep (down to about 0.6T) and low temperature creep, (less than about $0.3T_m$). Internal stresses are discussed in a separate section as they may impact creep at all temperatures.

2. Harper-Dorn Creep

Harper-Dorn creep has been described by the equation

$$\dot{\varepsilon}_{ss} = A_{HD} \left(\frac{D_{sd} G b}{kT} \right) \left(\frac{\sigma}{G} \right)^n, \tag{1}$$

where A_{HD} is the Harper-Dorn coefficient, D_{sd} the lattice self-diffusion coefficient (with Q_{sd} being the activation energy for lattice self-diffusion), G is the shear modulus, b is the Burger's vector, and σ is the stress.

Classic Harper-Dorn creep has been observed at higher temperatures, very near the melting temperature [1, 3, 8, 12]. Harper-Dorn creep has been generally suggested at high temperatures for a wide variety of crystalline materials. The generally accepted characteristics of Harper-Dorn creep include n=1, Q_c approximately equal to the activation energy for lattice self-diffusion, Q_{sd} , but many have suggested that unlike five power-law creep, the steady-state dislocation density is independent of the (modulus-compensated) stress.



Fig. 1. Steady-state creep of high-purity aluminum at high temperatures [3-9] Dark symbols are from the authors earlier work [3]. Interestingly, *both* five-power-law creep and Harper-Dorn Creep have been observed at the same low stresses

Interestingly, subgrains are generally not observed in the Harper-Dorn regime, and the Frank dislocation network would, by default, be the microstructural feature associated with the rate-controlling process for creep, as often suggested for five power-law creep. More recent [3] works suggest that Harper-Dorn may not be observed in Al at these very high temperatures, but rather five-power-law creep extends into this temperature/stress range uninterrupted by Harper-Dorn creep. Fig. 1 shows classic five-power law (n = 4.5) behavior at higher stress, but at lower stresses, such as below $\sigma/G = 10^{-6}$, either n = 1 (Harper-Dorn) or n= 3-4.5 (five-power law) behavior is observed. Recent work by the author [10] demonstrated that if the initial dislocation density is high (e.g. above) then the Frank dislocation network may frustrate at lower stresses, as suggested by Ardell and coworkers [11], and the dislocation density is constant and n = 1 is observed. It can be shown that if the dislocation density is constant, the creep rate would be expected to be proportional to the stress since the climb rate is proportional to the stress.

On the other hand, if the initial dislocation density is low, such as at values below those suggested in Fig. 2 by extrapolation of the dislocation density versus stress at low stresses into the so-called Harper-Dorn regime, then normal five-power law creep behavior may be observed. The dislocation density can increase to values expected by on the trends of Fig. 2 extended into the Harper-Dorn regime. Typical starting dislocation densities are indicated by the large vertical bracket in Fig. 2. The figure illustrates that the observed starting dislocation densities can either be below or above the "transition value" of 10^8 m/m^3 . It has been observed that initial high dislocation density values (e.g. > 10^8 m/m^3) are stable at temperatures near T_m , for periods over *one year*. Thus, dislocation frustration appears to be a genuine phenomenon. Analysis of the Orowan bowing stress (i.e $\tau = Gb/l$, where l = average network link-length) suggests that at dislocation densities of 10^8 m/m^3 , the bowing stress for

multiplication (σ/G) is about 4 x 10⁻⁶. Interesting, this is the stress at the transition point to Harper-Dorn Creep in Fig. 2. If the stress is below this value, then multiplication (e.g. Frank-Read) may not occur for this initial dislocation density since the stresses are insufficient for multiplication since the average link-length is too small for the corresponding stress. However, if the dislocation density is relatively low at 10⁶ m/m³, the stresses are sufficient within the Harper-Dorn regime to cause dislocation multiplication and yield five-power law behavior; the dislocation density can change with the applied stress.



Fig. 2. Steady-state dislocation density versus the modulus-compensated steady-state stress at an elevated temperature of 923 K (0.99 T_m) based on earlier work and the authors' previous work [1]. The data of Lin et al. [13] and that of Barrett et al. [5] suggest a lower limit of the dislocation density (ρ) with creep with decreasing stress at these very high temperatures. However, the work by Barrett et al. [5] and Kumar et al. [3] may suggest a continual decrease in the dislocation density with decreasing stress. Note that the initial dislocation densities (vertical bracket on left-hand side of the figure) are of the same order as the steady-state dislocations densities at low (e.g. Harper-Dorn) stresses. Other data in the figure are also included [8, 13-15]

In summary, Harper-Dorn may be observed when the starting dislocation density is relatively high, but (normal) five power-law creep is observed with initial dislocation densities that are relatively low and frustration does not occur.

3. Five-power-law

Diffusion (dislocation climb) control. A well-accepted equation [1] for five power-law creep is:

$$\dot{\varepsilon}_{ss} = A_1 \left(\frac{\chi}{Gb}\right)^3 \left(\frac{D_{sd}Gb}{kT}\right) \left(\frac{\sigma_{ss}}{G}\right)^5,\tag{2}$$

where χ is the stacking fault energy, A_1 is a constant, D_{sd} is the self-diffusion coefficient, and G is the shear modulus. It is fairly well established that steady-state creep in pure metals and class M alloys is controlled by dislocation climb. Some, however, have suggested that dislocation cross-slip is the rate controlling mechanism [16-19]. Recent experiments on large-strain softening in aluminum by the author add additional support for the climb contention [20,21]. The strain softening (roughly 17%) after large strain (generally >2) deformation in torsion has generally been attributed to a decrease in the average Taylor factor associated with the texture development. That is, the Schmid factor of dislocation glide decreases. However, it was recently demonstrated that the texture also predicts that softening

will occur due to an increase in the climb stress as the torsional texture develops (roughly 7%). This is an important finding as unless the climb stress increased with texture formation, leading to softening, then some question would be placed on the viability of dislocation climb as the rate-controlling mechanism for five-power-law creep. The climb stress increase may not account for all of the softening and some of the observed flow stress decrease may be attributed to slight microstructural changes as some (e.g. Nes and Pettersen, Myshlyaev et al. and Perdrix et al.) have suggested [22-24]. Interestingly, elevated-temperature compressions tests immediately following the elevated temperature torsion tests into the softened state evince an absence of softening with is perfectly consistent with the predictions of climb-control. Glide control predicts a 10% increase in stress following compression which was not observed. In summary, the softening behavior appears much more likely due to a change in the climb stress associated with texture development rather than dislocation glide control.

Rate-controlling process. The precise mechanism for creep in the five-power law regime by dislocation climb is not well-established. There are two general lines of thinking with respect to the details of the rate-controlling process: 1.) subgrain-based theories and 2.) Frank-network theories. Analysis by the author suggests that the steady-state stress in aluminum is predictable by the Taylor dislocation-hardening equation,

$$\sigma_{\rm v}|_{\dot{\sigma}_{\rm T}} = \sigma_{\rm o}' + \alpha {\rm MGb} \sqrt{\rho}$$
.

(3)

This equation very accurately predicts the elevated-temperature flow stress independent of the subgrain size. $\alpha MGb\sqrt{\rho}$ is the athermal term. The associated constant, α , in the predictive equation is within the range of values observed at lower temperature where dislocation hardening is undisputed [25-26]. One important note is that even in high purity Al, the values of σ'_o (the thermally activated term) are a significant fraction of the total stress (e.g. roughly one-third). This implies that the small amounts of impurities have a significant influence on the flow stress. Thus, the solute strengthening may complicate the analysis of dislocation hardening in that it is not completely clear how the separate strengthening variables combine to contribute to the flow stress. Here, a simple linear superposition is assumed. In summary, there is strong evidence that elevated temperature hardening is completely explainable by Frank-network hardening rather that strengthening by subgrains as commonly suggested.

4. Long Range Internal Stresses (LRIS)

Long range internal stresses (LRIS) that are 3-20 times larger than the applied stress in creep [27] are often believed to exist in creep-deformed aluminum and other crystalline materials. These high levels of LRIS have been proposed to be associated with dislocation heterogeneities such as subgrain boundaries and are associated with the rate-controlling process for creep. Convergent-beam electron diffraction (CBED) and synchrotron x-ray micro-diffraction experiments suggest that LRIS values are much lower than suggested by the early experiments and theoretical projections by others. However, one difficulty with CBED is that the regions of TEM foils used for CBED are very thin and dislocations, particularly in metals as Al where the stacking fault energy is relatively high, may escape from the foils and relax any internal stresses. The foils may also bend in these thin sections and complicate the stress analysis. Static recovery, including recrystallization, at ambient temperature is also possible [28]. Finally, the CBED analysis is performed in an unloaded specimen at ambient temperature. Of course, in-situ assessment (i.e. under load) would be preferred. Some in-situ x-ray work was performed by Blum and coworkers on a Cu alloy [29] where the details of x-ray peaks were analyzed from reflections by a large number of grains in the specimen. The x-ray peak asymmetry was related to the long-range internal stress. It was shown that on unloading, most (e.g. 2/3) of the LRIS remain at ambient temperature in the unloaded state.

This suggests some validity in assessing LRIS by us in unloaded specimens in our CBED work. The problem with pure Al is that the stresses are very low in creep and the latticeparameter change measurement (for LRIS) uncertainly with the x-ray peak asymmetry experiments is of the order of the applied stress. Thus, LRIS may not be detected. In fatigued pure single crystal Cu where the stresses are much higher than in Al, LRIS were also not observed by CBED [20]. At higher stresses in heavily deformed commercial-purity Al by equal channel angular pressing (ECAP) (impurities preclude ambient temperature recrystallization [28]) LRIS, of the order of the applied stress, by both CBED and by x-ray microbeams at a synchrotron facility [30], are observed.

In summary, there is no evidence for significant long range internal stresses in creep deformed metals within the five power-law regime as investigated by convergent beam electron diffraction. In recent cases where LRIS are confirmed by x-ray microbeams in ambient temperature severely deformed aluminum [30], the CBED consistently finds the same magnitude of long range internal stress as the more reliable x-ray microbeams (bulk samples) at a synchrotron facility. Thus, the absence of significant LRIS in creep-deformed pure Al by CBED experiments has additional validity.

5. Low Temperature Creep in Aluminum

Analysis of low-temperature experiments of creep below $0.3T_m$ reveals that the activation energy for creep is relatively low and cannot be easily explained by a dislocation-climb controlled process. The observed activation energies below $0.3T_m$ range from about 0.75 down to $0.1Q_{sd}$, the value of lattice self-diffusion activation energy [31, 32]. At low temperatures we observe primary creep at the small strains rather than steady-state creep as with the discussion in the above sections. Metallic primary-creep can usually be described by either a power-law or a logarithmic equation:

$$\varepsilon_{\rm p} = at^b \,. \tag{4}$$

$$\varepsilon_{\rm p} = \alpha {\rm lnt} + {\rm c}_2 \,. \tag{5}$$

Our analysis revealed that most of the metals and alloys deformed at low temperature under constant stress conditions exhibit logarithmic behavior. The analysis of aluminum shows that at 0.32 m the creep behavior is better described by the power law equation. Our analysis showed that, in general, logarithmic behaving metals approached power-law behavior as the temperature increased into the intermediate temperature range (i.e. $T > 0.3T_m$). At a lower temperature {77K (0.08 T_m) τ_G , the backstress, is assumed to be approximately equal to zero [33, 34]}, both behaviors were evident in Al but at lower stresses, logarithmic behavior was observed.

The mechanism for creep plasticity at $T < 0.3T_m$ is unclear. While for metals such as copper, (lower stacking fault energy), the classic Seeger rate-equation

$$\dot{\gamma} = NAb \, v_o \exp\left\{\frac{-\Delta H_o - v(\tau - \tau_G)}{kT}\right\},\tag{6}$$

where $\dot{\gamma} = \text{strain-rate}$, $N = \text{number of dislocation segments per unit volume held up at the intersection points of mean spacing, <math>\boldsymbol{l}$, v_o is an atomic frequency of the order of the Debye frequency, $\Delta H_o = \text{energy required for the intersection process}$, (i.e. the energy for jog formation $\approx \frac{Gb^2}{10}$)] describes the creep behavior and measured creep rates of our Cu data fairly well, the Seeger equation fails to properly describe the behavior of Al.

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A SIMPLIFIED MODEL EXPLAINING THE FORMATION OF InAs NANOWIRES ON GaAs NANOMEMBRANES

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Abstract. Gold-free GaAs nanomembranes have proven ideal templates for further growth of in-plane III-V nanowires. Recently, it has been demonstrated that high quality InAs nanowires with a low defect density can be obtained on top of GaAs nanomembranes by molecular beam epitaxy in wafer-scale approach and provide an excellent platform for future investigations into one-dimensional transport and quantum computation. Here, we develop a model to explain why InAs NWs form spontaneously on the top ridges of GaAs nanomembranes and not elsewhere. We speculate that the driving force for this growth mechanism is the free energy minimization including the elastic and surface energy contributions.

Keywords: InAs nanowires, GaAs nanomembranes, elastic stress relaxation, growth model

1. Introduction

Highly mismatched InAs/GaAs material system (lattice mismatch $\varepsilon_0 = 0.07$) has been used for a long time for epitaxial growth of the Stranski-Krastanow quantum dots [1, 2]. This material system is also very useful for growing high quality axial [3] and radial [4] heterostructures in vertical nanowires (NWs). More recently, defect-free GaAs nanomembranes (NMs) have been used as templates for further III-V NW growth [5, 6]. Such structures have been successfully grown by metalorganic chemical vapour deposition and molecular beam epitaxy (MBE) using a gold-free selective area approach [5 – 7]. The NMs are patternable at the wafer scale and can additionally be fabricated in the form of Y-shaped structures [6, 8]. In Ref. [8], it has been shown that InAs NWs form on the top ridges of GaAs NMs with a certain shape and aspect ratio. Such structures are scalable and provide electron confinement to the top NWs which is sufficient to produce quasi-one-dimensional conduction. Here, we present a simplified model to explain the experimentally observed morphology of the NW/NM structures.

2. Model

The InAs/GaAs NW/NM structure is shown in Fig. 1 (a) [8] and is fabricated as follows. First, <11-2>-aligned GaAs NMs are grown by selective area approach as described in Ref. [5]. These NMs have a sharp top restricted by (-11-3) and (-1-31) planes, and vertical (01-1) and (0-11) sidewalls. Then, InAs is deposited by MBE for 200 s at 540°C and accumulated at the top of the NMs, forming InAs NWs along the NM vertex. The InAs NWs are restricted by two vertical (01-1) and (0-11) sidewalls, two (-11-3) and (-1-31) planes parallel to the NM ridges, and flat (111) top. Our aim is to understand and explain this shape of InAs NWs and in particular the experimentally observed aspect ratio x = h/l of about 0.6 [8].

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Fig. 1. (a) Morphology of a single GaAs/InAs NM/NW structure [8], and (b) plan view of the model geometry showing the relevant parameters

According to the data [8], the InAs NW facets are composed of vertical, horizontal and inclined facets of the (011), (111) and (113) families, respectively (see Fig. 1 (b)). We additionally assume that the inclined NW facets are replaced by the horizontal facets at the crossing point of the initial NM facets with the inclined NW facets. From geometrical considerations, we have $a = h \cot an2\theta$ and $b = l - h \cot an\theta$, with θ as the taper angle of the NM, hence

 $b + a = l - h(\cot an\theta - \cot an2\theta)$.

(1)

The (131) facet of the InAs NW of width b + a and surface energy $\gamma_{InAs}^{(131)}$ replaces the initial facet of the GaAs NM of width l and surface energy $\gamma_{GaAs}^{(131)}$. Additionally, the NW formation creates the InAs-GaAs interface of width l and interfacial energy $\gamma_{InAs-GaAs}^{(131)}$. We also create the vertical facet of height $h/\sin\theta$ having the surface energy $\gamma_{InAs}^{(011)}$, and the horizontal facet of width c and surface energy $\gamma_{InAs}^{(111)}$. From geometrical considerations,

$$c = h \frac{\sin \theta}{\sin 2\theta}.$$
 (2)

Summarizing all these surface energy terms and using $\cot a 2\theta = (1/2)(\cot a \theta - \tan \theta)$ and $\sin \theta = 2\sin \theta \cos \theta$ in Eqs. (1) and (2), respectively, the surface energy change per the length 2d (where d is the length of the initial NM) equals

$$\Delta F_{surf} = \left[\gamma_{InAs-GaAs}^{(131)} + \gamma_{InAs}^{(131)} - \gamma_{GaAs}^{(131)} \right] + \left[\frac{\gamma_{InAs}^{(011)}}{\sin \theta} - \frac{1}{2} \gamma_{InAs}^{(131)} (\tan \theta + \cot an\theta) + \frac{\gamma_{InAs}^{(111)}}{2\cos \theta} \right] h.$$
(3)

Grouping the bracket terms into C_1 and C_2 , we can write $\Delta F_{surf} = C_1 l + C_2 h$.

(4)

Clearly, the C_1 term gives the surface energy change in the (131) direction and is positive in the non-wetting and negative in the wetting cases, respectively. The C_2 term should always be positive and is associated with the InAs facets in contact with vapor.

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The surface area of half the NW cross-section s equals the area of the parallelogram lh minus the area of the upper triangle Δs . The latter is given by $h^2 / (8 \sin \theta \cos \theta)$. Therefore,

$$s = lh - \frac{h^2}{8\sin\theta\cos\theta},\tag{4}$$

where the second term is less than 10% of the first one in our geometry and can be neglected in the first approximation.

To account for the effect of the strain relaxation, we use the simplest formula [9 - 11]

$$\Delta G_{elastic} = \lambda \varepsilon^2 V \frac{1}{1 + \alpha h/l},\tag{5}$$

showing that the elastic energy (for the reduced strain ε due to dislocations) rapidly decreases ($\alpha >>1$) with increasing the aspect ratio h/l with respect to the 2D film of the same volume V. These dislocations are seen at the InAs/GaAs interface, with a density of ~ 100/µm of length, reducing the lattice mismatch to $\varepsilon \approx 0.03$ [8].

Using $V \cong 2dlh$ and dividing Eq. (5) to the facet length 2d, we arrive at the equation expressing the free energy $\Delta F = \Delta F_{surf} + \Delta F_{elastic}$ [with $\Delta F_{elastic} = \Delta G_{elastic} / (2d)$] of forming InAs NW of width *l* and height *h* on top of the GaAs NM

$$\Delta F(l,h) = C_1 l + C_2 h + \frac{C_3 l h}{1 + \alpha h / l}.$$
(6)

This free energy is defined per unit length of the structure. The C_1 term gives the surface energy change upon covering the GaAs (131) facets with InAs, and is proportional to the NW width l. The C_2 term ($C_2 > 0$) stands for the surface energy of all other InAs facets, and is proportional to the NW height h. The last term gives the elastic energy of InAs NW, proportional to the NW cross-sectional area $s \cong lh$, with C_3 being the elastic energy per unit volume for the reduced mismatch [9], and α describing the stress relaxation with the aspect ratio h/l [9 – 11]. We also assume that the term associated with the dislocation energy is roughly the same for any aspect ratio, which should be valid for large enough volumes of deposited InAs with the NW heights already well above the critical thickness for forming misfit dislocations (~1.2 nm).

3. Results and discussion

To access the preferred shape of InAs on top of GaAs, we minimize the formation energy given by Eq. (6) in h at a fixed $s \cong lh = const$, corresponding to a fixed volume of deposited InAs [12]. Using l = s/h, Eq. (6) can be re-arranged in terms of h only:

$$\Delta F(h) = C_1 \frac{s}{h} + C_2 h + \frac{C_3 s}{1 + \alpha h^2 / s}.$$
(7)

It is interesting to note that the derivative of this free energy with respect to h depends solely on the aspect ratio x = h/l. Introducing $f = \Delta F/C_2$ (C_2 is always positive), we obtain

$$\frac{df}{dh} = 1 - \frac{A}{x} - \frac{vx^{1/2}}{(1 + \alpha x)^2}.$$
(8)

Here, $A = C_1/C_2$ is the normalized surface energy change in the (131) plane, which is positive in the non-wetting and negative in the wetting case, and $v = 2\alpha(C_3/C_2)s^{1/2}$ is the strain-induced factor that increases with the amount of deposited InAs per unit area *s*. The preferred aspect ratio is now defined by the stable zero point of df/dh corresponding to the minimum free energy.

Figure 2 shows two possible cases with the preferred $x \approx 0.6$, as observed experimentally in Ref. [6]. Of course, the three-dimensional (3D) geometry will occur in the non-wetting case with A > 0 even without any lattice mismatch, because the surface energy minimization leads to a reduction of the energetically costly InAs-GaAs interface [11]. This is shown by the dashed curve in Fig. 2. We believe, however, that our GaAs/InAs system is initially wetting. Therefore, the surface energy favours two-dimensional (2D) growth of InAs on GaAs, while 3D structures emerge only after the formation of a continuous wetting layer, as in the Stranski-Krastanow growth [11]. The energetics of the system is then described by the solid line in Fig. 2. In this case, reaching a high aspect ratio on the order of 0.6, which is necessary to form the NWs on top of the NMs, can only be due to strain relaxation and requires a high value of the strain-induced coefficient v of about 140. The C_3 coefficient equals $\lambda \varepsilon^2$, with $\lambda = 1.22 \times 10^{11}$ J/m³ as the elastic modulus of InAs and ε as the reduced lattice mismatch. With the experimentally observed $\varepsilon = 0.03$, this yields v = 140 at $\alpha = 15$ (Ref. [10]) for a plausible value of $C_2 = 0.091$ J/m².



Fig. 2. Derivative of the free energy of forming InAs NW on GaAs NM with respect to the aspect ratio, obtained from Eq. (8) in the non-wetting (A > 0) and wetting (A < 0) case

The zero point at $h/l \approx 0.6$ corresponds to the minimum free energy of forming the NW, because its derivative is negative for smaller and positive for larger aspect ratios. The real curve is expected to be the one in the wetting case, where the system surpasses an energetic barrier at a small x as in the Stranski-Krastanow growth. The value of v = 140 corresponds to the parameters of InAs with the reduced mismatch $\varepsilon = 0.03$. The insert shows the geometry, the approximation $s \approx lh$ used in the calculations neglects truncation of the full parallelogram in the top NW part.

4. Conclusions

In conclusion, our model shows that formation of InAs NWs on the top ridges of GaAs NMs is driven by minimization of the formation energy including the surface and elastic contributions. In the wetting case, relevant for this material system, the existence of the optimal aspect ratio of InAs NWs ~ 0.6 can only be due to the elastic energy relaxation with the reduced strain. This energy minimum follows from the model with plausible parameters.

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We now plan to consider other material systems, including a very promising case of InSb, using similar methods. It is also interesting to study in more detail the nucleation stage [13], growth kinetics of in-plane III-V NWs on the NM templates [14], and in particular three-fold symmetrical Y-shaped structures.

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NUMERICAL ANALYSIS OF EFFECTIVE PROPERTIES OF HETEROGENEOUSLY POLARIZED POROUS PIEZOCERAMIC MATERIALS WITH LOCAL ALLOYING PORE SURFACES

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Abstract. The paper considers homogenization problems for porous piezoceramic material with partially metallized pore surfaces. It is assumed that the thickness of the metal layer at the boundaries of the pores is infinitesimally small, and the metallization effect is entirely described by setting the boundary conditions for equipotential surfaces. Following previous research of the authors, here the heterogeneity of piezoceramic polarization was taken into account. The homogenization problems were solved, using the effective moduli method, the finite element method, and the representative volumes with random closed porosity. An analysis of the effective moduli on porosity was carried out for homogeneous and inhomogeneous polarization fields.

Keywords: piezoelectricity, porous piezoceramics, microstructure, metallized micropores, nonuniform polarization, effective moduli, representative volume, finite element method

1. Introduction

Nowadays, active elements of piezoelectric transducers are often made of piezoelectric materials on the base of Lead Zirconate Titanate (PZT) or Barium Titanate. PZT-ceramic, which is the most in-demand material for hydroacoustic devices, has high electroacoustic effectiveness. However, it has relatively large acoustic impedance, and this fact require using the transition layers for better coordination of the impedance of emitting body with the impedance of acoustic medium. The results of the range of experimental and theoretical investigations have shown that porous piezoceramic can significantly increase the properties of the transducers and widen the area of piezoelectric material use ([1 - 3] and others). Porous piezoceramic has high piezoelectric sensitivity and large thickness coefficient of electromechanical coupling, but it has smaller acoustic impedance in comparison with dense piezoceramic. Meanwhile, porous piezoceramic without modifiers has relatively low mechanical strength, due to its internal structure.

For the majority of applications, porous materials with the pore size less than 100 mkm can be considered as quasi-homogeneous materials with effective moduli. The effective material properties of porous piezoelectric composites or composites with elastic inclusions of different coupling types were investigated earlier with the help of various theoretical models ([2-16] and others). For example, the Mori-Tanaka theory, popular in composite mechanics, and the differential micromechanics theory were extended in [6], in order to consider effective characteristics of piezocomposite materials. The application of these

theories is based on the solution of a 3D static problem of ellipsoidal inclusion in infinite piezoelectric medium. The solutions of such problems can be obtained using analytical approaches presented in [18 - 21]. Theoretical models for piezocomposites that include the methods of optimization and averaging were suggested in [15]. These models proved their efficiency on the example of periodic piezocomposite materials.

This work continues investigations of microporous piezocomposites [22 - 25] that have metal microparticles precipitated on the boundaries between the pores and the piezoceramic skeleton. Such composites can be produced by transporting the particles of special substances into piezoceramic materials [26]. The effective properties of these microporous piezoceramic materials can be determined by a complex approach including the effective moduli method, the representative volume simulation and the finite element solution of a set of static problems of piezoelectricity with special boundary conditions. The methodology of numerical investigation of the effective properties of microporous piezoceramic materials with fully electrodized pore boundaries was presented in [23], where the pore surface metallization was taken into account by the boundary conditions of free electrodes, and in [24] with more general approach, where the mechanical properties of the metallized pore boundaries were also taken into account by using shell elements. Meanwhile, the models with partial pore surface metallization are more close to real world. Such case of the composite was considered in [25] and in this paper. As it was done in [25], here the pore surface metallization was simulated only by the conditions of free electrodes, and the technique of the effective properties calculation was implemented in ANSYS finite element package. It should be also noted that our previous papers [22 - 25] considered only homogeneously polarized pizoceramic, despite the presence of pores and metallized surfaces. In this work, similarly to [12], we investigate the influence of the inhomogeneous polarization on the effective moduli.

2. Mathematical models and the effective moduli method

In this section, we present the model of inhomogeneously polarized porous piezoelectric composite with the pore boundaries partially covered by a thin layer of metal. We will consider a porous composite as a two-phase composite in which the first phase (the skeleton) is a piezoceramic material with inhomogeneous polarization, and the second phase forms a set of pores that do not contact each other.

Let us denote a representative volume of the composite as Ω , $\Gamma = \partial \Omega$ is the external normal of the volume. We consider that there are N_p nontouching pores Ω_{pi} with the boundaries $\Gamma_{pi} = \partial \Omega_{pi}$, $i = 1, 2, ..., N_p$. We also introduce the following notations: $\Omega_p = \bigcup_i \Omega_{pi}$ is the set of pore volumes occupied by the second phase; $\Omega_m = \Omega \setminus \Omega_p$ is the domain, occupied by the material of the first phase, which is assumed to be a coupled phase; **n** is the unit normal vector to the boundary $\Gamma_m = \partial \Omega_m$, external to the volume of the main material; **x** is the radius-vector of the point in the Cartesian coordinate system. It is also assumed that the boundary Γ_{pi} of each pore is divided into the metallized parts Γ_{pij}^e , $j = 1, 2, ..., J_i^e$, and nonmetallized parts Γ_{pij}^u , $j = 1, 2, ..., J_i^u$. Thus, $\Gamma_{pi} = (\bigcup_j \Gamma_{pij}^e) \cup (\bigcup_j \Gamma_{pij}^u)$. In the elasticity theory, the metallized surfaces of ceramics are often called electrodized, and nonmetallized surfaces are called nonelectrodized, or the parts free from electrodes.

In order to determine the effective moduli of the considered material, we will consider the following boundary-value homogenization problems [22]:

$$\mathbf{L}^{*}(\nabla) \cdot \mathbf{T} = 0, \ \nabla \cdot \mathbf{D} = 0, \ \mathbf{T} = \mathbf{c}^{E} \cdot \mathbf{S} - \mathbf{e}^{*} \cdot \mathbf{E}, \ \mathbf{D} = \mathbf{e} \cdot \mathbf{S} + \mathbf{\epsilon}^{S} \cdot \mathbf{E},$$
(1)

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$$\mathbf{S} = \mathbf{L}(\nabla) \cdot \mathbf{u}, \ \mathbf{E} = -\nabla \varphi, \ \mathbf{L}^*(\nabla) = \begin{bmatrix} \partial_1 & 0 & 0 & 0 & \partial_3 & \partial_2 \\ 0 & \partial_2 & 0 & \partial_3 & 0 & \partial_1 \\ 0 & 0 & \partial_3 & \partial_2 & \partial_1 & 0 \end{bmatrix}, \ \nabla = \begin{cases} \partial_1 \\ \partial_2 \\ \partial_3 \end{cases},$$
(2)

$$\mathbf{u} = \mathbf{L}^{*}(\mathbf{x}) \cdot \mathbf{S}_{0}, \quad \varphi = -\mathbf{x} \cdot \mathbf{E}_{0}, \quad \mathbf{x} \in \Gamma,$$
(3)
where
$$\mathbf{T} = \{\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}\}, \quad \mathbf{S} = \{\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}, 2\varepsilon_{12}\}, \quad \sigma_{ii}, \quad \varepsilon_{ii} \quad \text{are the}$$

where $\mathbf{I} = \{O_{11}, O_{22}, O_{33}, O_{23}, O_{13}, O_{12}\}$, $\mathbf{S} = \{E_{11}, E_{22}, E_{33}, 2E_{23}, 2E_{13}, 2E_{12}\}$, σ_{ij} , E_{ij} are the components of the stress and strain tensors; **D**, **E** are the electric flux density vector and the electric field vector, respectively; **u** is the vector-function of mechanical displacement; φ is the function of electric potential; \mathbf{c}^{E} is the 6×6 matrix of elastic stiffness moduli; **e** is the 3×6 matrix of piezoelectric moduli; $\mathbf{\varepsilon}^{S}$ is the 3×3 matrix of dielectric permittivity moduli; $\mathbf{S}_{0} = \{S_{01}, S_{02}, S_{03}, S_{04}, S_{05}, S_{06}\}$; $S_{0\beta}$ are some constant values that do not depend on **x**; \mathbf{E}_{0} is some constant vector; (...)^{*} is the transpose operation; and (...)·(...) is the scalar product operation.

We note that problem (1)–(3) should be solved in an inhomogeneous volume Ω , where $\mathbf{c}^{E} = \mathbf{c}^{E(r)}$, $\mathbf{e} = \mathbf{e}^{(r)}$, $\mathbf{\varepsilon}^{S} = \mathbf{\varepsilon}^{S(r)}$ for $\mathbf{x} \in \Omega_{r}$, r = m, p. We consider that the pores are filled with piezoelectric material with negligibly small elastic stiffness, piezomoduli and dielectric permittivities equal to the dielectric permittivity of the vacuum $\varepsilon_{0} = 8.85 \cdot 10^{-12}$ (F/m).

In the absence of metal layer on the pore boundaries, the following conditions should be satisfied:

$$\mathbf{L}^{*}(\mathbf{n}) \cdot \mathbf{T} = 0, \ \mathbf{n} \cdot \mathbf{D} = 0, \ \mathbf{x} \in \Gamma_{pi}, \ i = 1, 2, ..., N_{p}.$$
(4)

These conditions also hold with high precision when the pores are filled with the piezoelectric material with small moduli, as taken in the models of representative volumes.

Meanwhile, if we assume that the pore boundaries are partially covered by a metal layer of negligibly small thickness, then conditions (4) should be kept at these parts Γ_{pij}^{u} , but on the parts Γ_{pij}^{e} it is necessary to adopt the boundary conditions of free electrodes ($i = 1, 2, ..., N_{p}$). As a result, instead of (4) we will have the following boundary conditions:

$$\mathbf{L}^{*}(\mathbf{n}) \cdot \mathbf{T} = 0, \ \mathbf{n} \cdot \mathbf{D} = 0, \ \mathbf{x} \in \Gamma_{pij}^{u}, \ j = 1, 2, ..., J_{i}^{u},$$
(5)

$$\mathbf{L}^{*}(\mathbf{n}) \cdot \mathbf{T} = 0, \ \varphi = \Phi_{ij}, \ \mathbf{x} \in \Gamma_{pij}^{e}, \ \int_{\Gamma_{pij}^{e}} \mathbf{n} \cdot \mathbf{D} \, d\Gamma = 0 \quad j = 1, 2, ..., J_{i}^{e},$$
(6)

where Φ_{ij} are constant unknown electric potentials Γ_{pij}^{e} .

In the case of porous piezoceramic of 6mm class, in order to determine its ten independent effective moduli ($c_{11}^{E\,\text{eff}}$, $c_{12}^{E\,\text{eff}}$, $c_{33}^{E\,\text{eff}}$, $c_{33}^{E\,\text{eff}}$, $e_{31}^{e\,\text{eff}}$, $e_{33}^{e\,\text{eff}}$, $e_{31}^{e\,\text{eff}}$, $e_{33}^{e\,\text{eff}}$, $e_{$

I.
$$S_{0\beta} = S_0 \delta_{1\beta}, \ \mathbf{E}_0 = 0 \implies c_{1k}^{E \text{ eff}} = \langle \sigma_{kk} \rangle / S_0; \ k = 1, 2, 3; \ e_{31}^{\text{eff}} = \langle D_3 \rangle / S_0,$$
 (7)

II.
$$S_{0\beta} = S_0 \delta_{3\beta}, \ \mathbf{E}_0 = 0 \implies c_{k3}^{E \text{ eff}} = \langle \sigma_{kk} \rangle / S_0; \ k = 1, 2, 3; \ e_{33}^{\text{eff}} = \langle D_3 \rangle / S_0,$$
 (8)

III.
$$S_{0\beta} = S_0 \delta_{4\beta}$$
, $\mathbf{E}_0 = 0 \implies c_{44}^{\text{Leff}} = \langle \sigma_{23} \rangle / S_0$; $e_{15}^{\text{eff}} = \langle D_2 \rangle / S_0$, (9)

IV.
$$\mathbf{S}_0 = 0, \ E_{0l} = E_0 \delta_{1l} \implies e_{15}^{\text{eff}} = -\langle \sigma_{13} \rangle / E_0; \ \varepsilon_{11}^{S \text{ eff}} = \langle D_1 \rangle / E_0,$$
 (10)

V.
$$\mathbf{S}_{0} = 0, \ E_{0l} = E_{0}\delta_{3l} \implies e_{3k}^{\text{eff}} = -\langle \sigma_{kk} \rangle / E_{0}; \ k = 1, 2, 3; \ \varepsilon_{33}^{\text{S eff}} = \langle D_{3} \rangle / E_{0},$$
 (11)

where δ_{ij} is the Kronecker symbol; and the angle brackets denote the averaged by the volume Ω values: $\langle (...) \rangle = (1/|\Omega|) \int_{\Omega} (...) d\Omega$.

These problems will be solved in a representative volume numerically by the finite element method.

3. Models of representative volumes

Finite element simulation of the representative volume Ω of the porous composite with closed porosity is based on the basic cubic cell Ω_c with the edge l_c . Along each edge the cell Ω_c is divided into three segments with the lengths a_p , l_p , a_p , where $l_c = l_p + 2a_p$, $l_p = k_p l_c$, $k_p < 1$. Thus, a basic cell is divided into 27 hexahedrals, which we initially assume to be dielectric finite elements. The center of the basic cell is the main (central) cubic finite element with the edge l_p . Then we translate the basic cell Ω_c n_c times by three coordinate axes and obtain an array of finite elements Ω by the size $L \times L \times L$ ($L = n_c l_c$), consisting of n_c^3 basic cells.

We assume that central finite elements inside basic cells can have material properties of pores. These "porous" finite elements are selected according to the following algorithm. We set a desired porosity p_s as a ratio of the desired volume of the pores to the total volume. Then the number N_p of central finite elements that can be pores will be determined according to the formula: $N_p = [p_s(n_c/k_p)^3]$, where [...] is the integer part of the number. We select these N_p central finite elements using a random number generator and then modify their material properties to the properties of pores. As a result, real porosity $p = N_p(k_p/n_c)^3$ will slightly differ from p_s . For example, with $n_c = 10$, $k_p = 0.8$ when p_s changes from 0.1 to 0.5 with the step 0.1 we have: $|p_s - p| \le 0.022$.

In order to simulate a partial metallization, we will assume that among six faces of "porous" finite element, two opposite faces, which are located perpendicular to one of the axial direction x_k , are electrodized. This direction x_k is chosen randomly for each "porous" element among the directions of three coordinate axes x_1 , x_2 and x_3 . Thus, in the representative volume Ω there will be N_p "porous" elements, which have $2N_p$ electrodized faces, where these paired faces are oriented randomly along the coordinate axes.

One of the cases of the volume Ω , built according to the described algorithm when $n_c = 10$, $k_p = 0.8$, $p_s = 0.1$, is given in Fig. 1. We note that the elements Ω_{pi} $(i = 1, 2, ..., N_p)$ are randomly chosen among central elements of the cells, and therefore the next run of the algorithm changes their location (Fig. 1b). The choice of metallized surfaces (Fig. 1c) is not deterministic as well. Thus, the next run of the algorithm will also change the location of the generated surfaces Γ_{pi} , even in the case when the porous elements are the same.

In the result, we will obtain a representative volume of porous material with closed 3-0 porosity of partially stochastic structure. In this volume, there will be N_p elements-pores Ω_{pi} , all faces of which are in full contact with the boundaries of the neighboring elements of the composite material skeleton. Moreover, in each pore two opposite faces are assumed to be metallized.



Fig. 1. Example of a representative volume: (*a*) whole volume, (*b*) porous elements, (*c*) metallized pore surfaces

4. Simulation of inhomogeneous polarization and finite element solution

A piezoceramic is a transversally isotropic material of 6mm class. Usually it is assumed to be homogeneously polarized in one direction (for example, along Ox_3 -axis). For the polarization of a piezoceramic sample, it necessary to have process electrodes through which a strong electric field exceeding the coercive field can be applied. Thus, the polarization is defined not only by the material itself, but by geometry of the device as well. At microlevel, a porous piezoceramic is an inhomogeneous material Therefore, the polarization field around the pores can be inhomogeneous. Despite the fact that usually the effective properties of porous piezoceramic are defined in assumption of homogeneous polarization, some papers [23, 24] also investigated the influence of inhomogeneous polarization. As it has been shown in these papers, for small and average porosity this influence is rather small.

Obviously, for a porous piezoceramic with metallized pore surfaces, taking into account the inhomogeneity of the polarization field is more important. Indeed, the metallization of the pores is obtained by piezoceramic sintering, which is followed by the material polarization. It is clear that then the presence of conductive surfaces inside the material will additionally affect the distribution of the polarization field. In connection to this, in order to take into account inhomogeneous polarization of a porous piezoceramic around the pores, at the initial stage of the simulation we can model the process of polarization along Ox_3 -axis. In order to do this, we solve a finite element problem of quasielectrostatic for a porous dielectric in a representative volume Ω , generated by the method described in the previous section.

Then, for the inhomogeneous cube Ω with the side *L* in Cartesian coordinate system $Ox_1x_2x_3$, we have the following boundary-value problem:

$$\nabla \cdot \mathbf{D} = 0, \ \mathbf{D} = \boldsymbol{\varepsilon} \cdot \mathbf{E}, \ \mathbf{E} = -\nabla \varphi, \ \mathbf{x} \in \Omega$$
(12)

$$\varphi = V_j, \quad \mathbf{x} \in \Gamma_{\varphi_j}, \quad j = 1,2; \quad \mathbf{n} \cdot \mathbf{D} = 0, \quad \mathbf{x} \in \Gamma_{\varphi_j}, \tag{13}$$

where $\Gamma = \bigcup_{j} \Gamma_{\varphi j} \bigcup \Gamma_{q}$; $\Gamma_{\varphi j}$ are the electrodes $x_3 = 0$ and $x_3 = L$; $\varepsilon = \varepsilon(\mathbf{x})$ is the matrix of dielectric permittivities of a nonpolarized ceramic with pores.

Problem (12), (13) should be supplemented by electric boundary conditions for pores from (5), (6). After solving the formulated problem, we can find the values of the polarization vectors $\mathbf{P}^{ek} = \mathbf{D}^{ek} - \varepsilon_0 \mathbf{E}^{ek}$ in a central point of each finite element with the number k, which is not a pore. With these elements we associated their element coordinate systems $Ox_1^{ek}x_2^{ek}x_3^{ek}$,

for which the axes Ox_3^{ek} were chosen such that their directions coincided with the directions of the polarization vectors \mathbf{P}^{ek} .

At the second stage, the finite elements of electrostatics were modified into the elements with possibilities of piezoelectric analysis. New elements were given material properties of two types, namely, the property of polarized piezoceramic for the elements of the material skeleton, and the negligibly small moduli for the pores. The finite elements of the skeleton were related to the element coordinate systems $Ox_1^{ek}x_2^{ek}x_3^{ek}$, defined by the polarization vectors \mathbf{P}^{ek} . Then, in order to determine the effective moduli, we solved the problems of electroelasticity (1)–(4) or (1)–(3), (5), (6) by the cases (7)–(11). We emphasize that with accounting for inhomogeneous polarization the problem of electroelasticity is solved for an inhomogeneous structure, where each finite element of the polarized piezoceramic has its own moduli \mathbf{c}^{Eek} , \mathbf{e}^{ek} , $\mathbf{\varepsilon}^{Sek}$, obtained by known formulas for recalculation of tensor components at the transfer from crystallographic Cartesian coordinate system $Ox_1x_2x_3$ to the element coordinate systems $Ox_1^{ek}x_2^{ek}x_3^{ek}$.

If we do not take inhomogeneous polarization into account, then problem (12), (13) is not used and in problem (1)–(4) or (1)–(3), (5), (6) all elements have either the properties of a piezoceramic material of 6mm class polarized along Ox_3 -axis, or the properties of pores.

5. Numerical examples

The homogenization problems were solved by the finite element method in ANSYS finite element package using the technique described above and in [23-25]. Special programs in ANSYS APDL were written for the representative volume generation, solution of the electrostatics problem (12), (13) and subsequent solution of five homogenization problems (1)–(4) or (1)–(3), (5), (6) with different boundary conditions (7)–(11). After solving the problems, the averaged characteristics were automatically calculated in ANSYS and thus the full set of the effective moduli was obtained. For the calculations, we used an eight-node finite element SOLID5 with the displacements and the electric potential as degrees of freedom in each node. For the problem of electrostatics, the option of only electric potential as degree of freedom was chosen. Numerical experiments were performed in ANSYS 11.0. However, the developed programs in ANSYS APDL will work in other versions of ANSYS that support piezoelectric analysis and finite element SOLID5.

To provide an example, we consider a porous pizoceramic PZT-4. For the dense piezoceramic PZT-4 we take the following values of material constants [27]: $c_{11}^E = 13.9 \cdot 10^{10}$, $c_{12}^E = 7.78 \cdot 10^{10}$, $c_{13}^E = 7.74 \cdot 10^{10}$, $c_{33}^E = 11.5 \cdot 10^{10}$, $c_{44}^E = 2.56 \cdot 10^{10}$ (N/m²); $e_{33} = 15.1$, $e_{31} = -5.2$, $e_{15} = 12.7$ (C/m²); $\varepsilon_{11}^S = 730\varepsilon_0$, $\varepsilon_{33}^S = 635\varepsilon_0$. For the pores, we set negligibly small elastic moduli $c_{\alpha\beta}^{E_p} = \kappa c_{\alpha\beta}^{E}$, $\kappa = 10^{-10}$, piezomoduli $e_{i\alpha}^p = \kappa$ (x1 C/m²) and $\varepsilon_{ii}^{S_p} = \varepsilon_0$. We consider a nonpolarized ceramic to be an isotropic material with the dielectric permittivity $\varepsilon = \varepsilon_{11}^S$. (a specific value of ε in the problem of electrostatics is not important, as the aim of this problem consists only in the determination of the polarization vector direction inside the composite material.) For the representative volume, we take the following geometric parameters: L = 500 (µm), $n_c = 10$, $k_p = 0.8$. In this case, the pores have the edges $l_p = k_p L/n_c = 40$ (µm).

We note that specific size L of the representative volume is not significant here, because we solve linear problem. On the contrary, the parameter n_c , which denotes the number of basic cells along coordinates axes, has great impact. It was verified that the chosen

value $n_c = 10$ ensures the stability of the solution results under random generation of porosity for different launches of the program. The homogenized material has the same anisotropy class 6mm, as the initial material of piezoceramic PZT-4.

We will compare two model cases of the porous piezoceramics. In Case 1, we take into account the pore metallization by using the boundary conditions of free electrodes (5), (6). In Case 2, we consider ordinary porous piezoceramic, when only conditions (4) are held on the pore boundaries, and no equipotentiality conditions are satisfied on these boundaries. In addition, for each case we will consider the case of homogeneously polarized piezoceramic and the case of homogeneously polarized piezoceramic.

We are going to analyze the relative effective moduli. For example, $r(c_{\alpha\beta}^{E}) = c_{\alpha\beta}^{Eeff} / c_{\alpha\beta}^{E}$ are the values of the effective moduli $c_{\alpha\beta}^{Eeff}$, related to the corresponding values of the moduli $c_{\alpha\beta}^{E}$ for the dense piezoceramic, and so on. Also, we will use the index l = 1, 2 in more precise notation $r(c_{\alpha\beta}^{E})_{l} = (c_{\alpha\beta}^{Eeff})_{l} / c_{\alpha\beta}^{E}$ to denote the number of Case l, for which the moduli calculation was performed.



Fig. 2. Dependencies of the effective elastic stiffness (*a*) and dielectric permittivity (*b*) on porosity

Typical behavior of the effective elastic stiffness moduli and the dielectric permittivity moduli are shown in Fig. 2 for the examples of the moduli $(c_{33}^{Eeff})_l$ and $(\varepsilon_{33}^{Seff})_l$, l = 1,2. Here and after the black curves correspond to the case of inhomogeneously polarized piezoceramic and the magenta curves correspond to the case of the piezoceramic with homogenous polarization.

As it can be seen in Fig. 2a, the stiffness moduli decrease with the porosity growth in both cases, and the account for inhomogeneous polarization field has a weak effect on the stiffness moduli. Meanwhile (see Fig. 2b), the effective moduli of the dielectric permittivities decrease with the porosity growth (curves 2). However, the effective moduli of the dielectric permittivities for the porous piezoceramic with metallized pores increase when the porosity grows till p = 0.3 (curves 1), and this increase is stronger for the case of inhomogeneously polarized piezoceramic skeleton of the composite.

The piezomoduli behavior (Figs. 3, 4) is of more interest. For example, the piezomoduli $(e_{33}^{\text{eff}})_2$ and $(e_{31}^{\text{eff}})_2$ for ordinary porous piezoceramic decrease with the porosity growth. Meanwhile, for the piezoceramic with metallized pore surfaces the

piezomodulus $(e_{33}^{\text{eff}})_1$ also decreases with the growth of p, and its decrease is faster than that of $(e_{33}^{\text{eff}})_2$. On the contrary, the piezomodulus $(e_{31}^{\text{eff}})_1$ grows when the porosity increases till p = 0.3, and then it gets stabilized or slightly decreases. Taking into account the inhomogeneous polarization does not influence the behavior of the piezomodulus e_{33}^{eff} , and for the piezomodulus e_{31}^{eff} it results in slightly greater decrease for the ordinary porous piezoceramic, and slightly greater increase for the porous piezoceramic with partial pore surface metallization.



Fig. 3. Dependecies of the effective piezomoduli $r(e_{33})_l$ (a) and $r(e_{31})_l$ (b) on porosity



Fig. 4. Dependecies of the effective piezomoduli $r(d_{33})_1$ (a) μ $r(d_{31})_1$ (b) on porosity

For the piezomodulus $(d_{33}^{\text{eff}})_2$ of ordinary porous piezoceramic, its unusual property of a weak dependence on porosity is well known, however, the values of piezomodulus $(|d_{31}^{\text{eff}}|)_2$ decrease with the growth of p. As it can be seen from the curves 2 and 4, these properties are weakly dependent on the inhomogeneity of the polarization, whether it is taken into account or not.

For porous piezoceramic with metallized pore surfaces, as it can be seen in Fig. 4, the values of the piezomodulus $(|d_{31}^{\text{eff}}|)_1$ increase with the growth of p, and taking into account

the inhomogeneity of polarization results in slightly less growth of the piezomodulus $(|d_{31}^{eff}|)_1$ in its absolute value. The piezomodulus $(d_{33}^{eff})_1$, with taking the inhomogeneous polarization into account, almost does not change with the porosity growth, i. e. it behaves in the same manner as for ordinary porous piezoceramic. If we consider the piezoceramic material of the composite to be homogeneously polarized, then the piezomodulus $(d_{33}^{eff})_1$ will also increase with the growth of porosity. Thus, we can conclude, that taking into account the inhomogeneity of polarization for the piezoceramic material with partially metallized pore surfaces has a significant influence on the values of the piezomoduli d_{3i}^{eff} .

6. Conclusions

In the present work, the properties of the inhomogeneously polarized porous piezoceramic with partially metallized pore surfaces have been investigated with the help of the methods of the composite mechanics and mathematical modelling. The pore surface metallization has been taken into account only by the electric boundary conditions of equipotentiality. The results of the numerical experiments have shown that microporous piezoceramic with metallized pore surfaces has a range of unusual properties, which are perspective for practical applications [28]. The comparison of the obtained results with similar results provided in [23, 24] for the case of full pore surface metallization has shown that partial metallization slightly eliminates unusual properties of the effective moduli [25]. The computation results showed that taking into account the inhomogeneity of the polarization field of the composite material was more significant for the determination the effective values of piezomoduli and dielectric permittivities, and less important for the determination of the effective elastic stiffness moduli.

We would like to note, that the developed model of the representative volume has only partially random porosity structure, as there are domains with the thickness $2a_p$ or a_p , which go through the whole volume and do not contain pores. In connection to this, the patterns of the inhomogeneous polarization field influence can be different for other internal structures of the representative volumes. Also, the values of the effective moduli are influenced by the extent of the pore surface metallization and the thickness of the metallized covering, which was noted in [24] for the case of homogeneously polarized piezoceramic.

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MODELING THE INTERPLY SLIP DURING FORMING OF THERMOPLASTIC LAMINATES

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Abstract. Interply slip plays an important role in composite forming processes, the resulting product geometry, final fiber orientations and fiber stresses. This interply slip will depend on fiber/resin properties, the fibers distribution, the reinforcement architecture and the process conditions. In this paper, a new model, based on Reynolds equation for thin film lubrication, was developed to predict the frictional behavior of these materials. This approach should be validated by means of experiments.

Keywords: thermoforming, interply slip, thermoplastic, wrinkles

1. Introduction

Continuous fiber thermoplastic composites have been introduced as structural materials for aerospace and automotive applications [1 - 4]. Forming complex shapes from sheets of these composites, in their melt state, may be considered as a difficult process when compared to metal or plastic forming.

Recently, a large number of manufacturing processes have been developed while existing ones were modified in order to obtain a high quality process. The thermoforming technology (stamping), seems to be an attractive alternative due to low cycle times and the possibility to more or less automate the manufacturing process. Forming tools for thermoforming processes are very expensive and it is very time consuming until the optimal part quality is obtained. Therefore, simulating the process can be an effective tool to help producing parts with good quality in an efficient way.

Software's used to simulate the forming of thin parts should be able to predict the final orientation of the fibers which will determine the mechanical properties of the final part. It should also predicts wrinkling, the final thickness and the final quality of the product.

In fact, during forming, a number of different deformation mechanisms can be identified [5] in composite sheet forming. There are mainly four forming mechanisms for fabric reinforced thermoplastics: intraply shearing, interply slip, resin percolation and transverse squeeze flow [6]. Interply slip is an important phenomenon that can dominate the resulting product geometry after forming.

In this work, a model was developed that predicts the friction between subsequent plies. The model is based on the Reynolds' equation for thin film lubrication and assumes hydrodynamic lubrication at a meso-mechanical level.

2. Ply/ply and Ply/tool slip

Previous Work. During forming of a pre-consolidated laminate, the individual plies slide over each other to avoid wrinkling [7 - 13].

The constraints imposed by friction between subsequent plies and between the laminate and the tools are major factor in the laminate deformations generated during composite forming.

Friction depends on the forming process parameters like the pressure, the mold temperature, the part temperature and the sliding velocity.

Murtagh et al. [7], observed a resin rich layer existed between different plies and showed that the viscosity dominate the slip behavior at elevated temperature.

Later, Murtagh et al. [8] worked on an interply slip tests carried out under varying conditions of temperature and pressure, results has allowed the development of a power law model which predicts shear stresses in the interlayer between plies as a function of applied strain in the plies and interply shearing velocity.

The first model of friction for the tool/ply interface [14] assumes fully hydrodynamic lubrication by means of a resin layer of thickness h between the laminate and the tool.

In 2002, Chow [15] proposed an analytical model for friction behavior of a woven fabric between the binder ring and the die from his test results for a commingled glass–polypropylene four-harness satin-weave fabric. His analytical model incorporated weighted effects of Coulomb and hydrodynamic friction models to predict the effective friction coefficient for different testing parameter values that could be used in numerical simulations. He first theorized that the transition between these two friction mechanisms for various combinations of the testing parameters resulted in a relationship similar to the Stribeck curve (Fig. 1), which plots the coefficient of friction versus the Hersey number H in the transition region between elasto-hydrodynamic lubrication and hydrodynamic lubrication.





The Hersey number *H*:

$$H = \frac{\eta \cdot V}{P},\tag{1}$$

where η is the resin viscosity, V is the fabric velocity and P the normal pressure.

Chow [15] proposed that this relationship was applicable to the thermoforming of a commingled glass–polypropylene four-harness satin-weave fabric after conducting a set of experiments using a specific setup.

The tests parameters used by chow are shown in table below.

Point	Tool temperature	Initial specimen	Velocity	Norma Force			
Number	(°C)	temperature (°C)	(mm/s)	(N)			
1	85	200	16.67	4000			
2	85	200	16.67	3000			
3	85	200	8.33	1500			
4	85	200	16.67	1500			
5	85	180	16.67	1500			
6	85	200	41.67	4000			

Table 1. Specific parameters used by [15]

He noted that his data followed the trend indicated by the Stribeck-curve (Fig. 2).

On the other hand, this reasoning remains week. It should be noted that we can obtain the same number H for various values of the normal pressure and the velocity.

However, according to the Stribeck theory, each number H corresponds to a single coefficient of friction. A thorough study of this work must therefore be carried out to validate the Chow model.



Fig. 1. Stribeck curve obtained by [15]

As an alternative, Gorzcyca [10] started from a Stribeck curve (Fig. 1), plotting the coefficient of friction as a function of Hersey number H.

A second-generation apparatus and associated procedure was designed and used to develop the current friction model for a larger range of processing parameters (Fig. 3).

It was determined that velocity, tool temperature and normal force had the greatest effects on the friction coefficient μ . Temperature is included via the viscosity term.

However, the temperature used to calculate the viscosity was the initial fabric temperature through the use of appropriate Power-Law parameters. As the tool temperature is lower than the melting point of the polypropylene, it cannot be directly considered with the viscosity calculation.



Fig. 2. Schematic representation of the pull-out experiment, to characterize ply-ply or tool-ply friction

The resulting master curve for one specific type of Twintex was presented for hydrodynamic lubrication region as: (2)

$$\mu = 6.1191 \times H + 0.2718.$$

Based on the work of Gorzcyca, Konstantine [16] confirmed that, velocity, normal force and tool temperature influence the friction coefficient. This coefficient vary with velocity and normal pressure similarly at both the fabric/tool and the fabric/fabric interfaces, and show a relation to the hydrodynamic region of stribeck curve.

Akkerman and al. developed a model that predicts friction between thermoplastic laminates and a rigid tool by assuming hydrodynamic lubrication at a meso-mechanical level [12]. The pressure in the matrix material starts to build up as it squeezed in the wedgeshaped cavities between the weave and the tool surface [17]. The film thickness was derived iteratively from the Reynolds' equation for thin film lubrication. The fabric geometry and the matrix materials were used as the input parameters.

Reynolds equation resolution. In this section, it is assumed that the equation governing the flow between subsequent plies is the incompressible, stationary Reynolds equation. A matrix film separates the two surfaces and the process could be considered like a flow between two surfaces for which only the top one can moves. The higher surface is defined by the equation z = h(x, y) (Fig. 4).

In this case, the process is governed by the Reynolds' equation which for the two dimensional state reads:

$$div \left[\frac{\left(h_1^3 - h_2^3 - 3h_1^2 h_2 + 3h_2^2 h_1\right)}{12\eta} g \overrightarrow{rad} P - \frac{\left(h_1 + h_2\right)}{2} \vec{V} \right] = 0,$$
(3)

where P is the pressure, $(h_1 - h_2)$ the local film thickness, η the viscosity and V is the slip velocity.

The resolution of equation (3) is usually made using a finite element method. In our case and considering a periodic profile for $h_1(x, y)$ and $h_2(x, y)$, a pseudo spectral method could be used. One boundary condition is needed.

$$P(0,0) = 0. (4)$$

The inner surface velocity is written: $\vec{V} = u\vec{i} + v\vec{j}$. (5)



Fig. 3. Schematic representation of two subsequent plies

In pseudospectral Fourier approximation, the problem involves periodic boundary conditions. Thus, all functions appearing in the problem are periodic. Let P(x, y) be smoothly differentiable function with period T_x in x direction and T_y in the y direction. First, we approximate P(x, y) by a trigonometric polynomial function that interpolates it at one of the following sets of points:

$$\begin{cases} x_i = \frac{T_x i}{2N} \\ y_j = \frac{T_y j}{2N} \end{cases}$$
(6)

$$P(x, y) = \sum_{i} \sum_{j} a_{ij} F_i(x) F_j(y),$$
(7)

where, a_{ij} is the unknown matrix to be determined.

When the collocation points given by equation (6) are used, the Reynolds equation has the form:

$$A(x_{k}, y_{l})\sum_{i}\sum_{j}a_{ij}F_{i}'(x_{k})\cdot F_{j}(y_{l}) + A(x_{k}, y_{l})\sum_{i}\sum_{j}a_{ij}F_{i}(x_{k})\cdot F_{j}''(y_{l}) + B(x_{k}, y_{l})\sum_{i}\sum_{j}a_{ij}F_{i}'(x_{k})\cdot F_{j}(y_{l}) + C(x_{k}, y_{l})\sum_{i}\sum_{j}a_{ij}F_{i}(x_{k})\cdot F_{j}'(y_{l}) - R(x_{k}, y_{l}) = 0,$$
(8)

where:

$$A(x,y) = \frac{1}{4\eta} \left(\frac{5}{3} h_1^3 + \frac{5}{3} h_2^3 + h_1 h_2^2 + h_2 h_1^2 \right), \tag{9}$$

$$B(x, y) = \frac{1}{4\eta} \left(5h_1^2 + h_2^2 + 2h_1h_2 \right) \cdot \frac{\partial h_1}{\partial x} + \frac{1}{4\eta} \left(5h_2^2 + h_1^2 + 2h_1h_2 \right) \cdot \frac{\partial h_2}{\partial x},$$
(10)

$$C(x, y) = \frac{1}{4\eta} \left(5h_1^2 + h_2^2 + 2h_1h_2 \right) \cdot \frac{\partial h_1}{\partial y} + \frac{1}{4\eta} \left(5h_2^2 + h_1^2 + 2h_1h_2 \right) \cdot \frac{\partial h_2}{\partial y},$$
(11)

$$R(x, y) = -\frac{3}{2}u\left(\frac{\partial h_1}{\partial x} - \frac{\partial h_2}{\partial x}\right) - \frac{3}{2}v\left(\frac{\partial h_1}{\partial y} - \frac{\partial h_2}{\partial y}\right).$$
(12)

And, $F_j(y_l) = \delta_{jl}$ and $F_i(x_k) = \delta_{ik}$, $F_i(x)$ and $F_j(y)$ are polynomial in the functions $\sin x$, $\cos x$ of degree at most N.

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Explicitly,

$$(F')_{jn} = \begin{cases} \frac{1}{2} (-1)^{j+n} \cot \frac{x_j - x_n}{2}, \ j \neq n \\ 0, \ j = n \end{cases} \& (F'')_{jn} = \begin{cases} \frac{1}{2} (-1)^{j+n+1} \frac{1}{\sin^2((x_j - x_n)/2)}, \ j \neq n \\ -\frac{2N^2 + 1}{6}, \ j = n \end{cases}$$
(1)

Modeling the interply slip. It's important to notice through the writing of the Reynolds equation between two surfaces that the pressure depends linearly on velocity. For this reason, we will try first, and using method described in previous section to solve the Reynolds equation for two different cases where in the first one, the moved plan slips in the *x* direction, whereas in second case this plan slips in the *y* direction. The respective solutions will be called $P_1(x, y)$ and $P_2(x, y)$.

The linear solution could be written like

$$\vec{P} = \eta \cdot (V_x \cdot \vec{P_1}(x, y) + V_y \cdot \vec{P_2}(x, y)), \qquad (2)$$

where, $V = (V_x, V_y)$ is the velocity vector.

The pressure gradient is calculated:

$$\overrightarrow{grad}P = \eta \cdot V_x \, \overrightarrow{grad}P_1 + \eta \cdot V_y \, \overrightarrow{grad}P_2 = \eta \cdot \left[\overrightarrow{grad}P_1 \otimes \overrightarrow{e_x} + \overrightarrow{grad}P_2 \otimes \overrightarrow{e_y}\right] \cdot \overrightarrow{V} = \eta \cdot \overline{\overrightarrow{M}} \cdot \overrightarrow{V}, \quad (15)$$
where $\overline{\overrightarrow{M}} = \overrightarrow{grad}P_1 \otimes \overrightarrow{e_x} + \overrightarrow{grad}P_2 \otimes \overrightarrow{e_y}.$

Integrating the shear stress over the sliding surface allows calculating the friction force:

$$\vec{F} = \iint_{xy} \tau(x, y) dx dy = \iint_{xy} -\frac{(h_1 + h_2)}{2} \overrightarrow{grad} P + \eta \frac{V}{h_1 - h_2} dx dy =$$
$$= \iint_{xy} \left[-\frac{(h_1 + h_2)}{2} \overrightarrow{\overline{M}} + \frac{\eta}{h_1 - h_2} \overrightarrow{\overline{I}} \right] dx dy \cdot \overline{V} = \overrightarrow{\overline{C_f}} \cdot \overline{V}.$$
(16)

This model predicts the friction force F_f as a function of the friction matrix C_f and velocity V. The friction matrix C_f depends on both plies geometries, described by h_1 and h_2 , and on the pressure gradient.

3. Model Analyses

The previous model shows that the coefficient of friction is not scalar according to the velocity (Fig. 5).

After calculating Eigen values λ_1 , λ_2 and their corresponding Eigen vectors u_1 and u_2 , of matrix C_f , we deduced that friction force is only collinear to velocity when this one is collinear to u_1 or u_2 vectors.

$$\overline{F_1} = \lambda_1 \cdot \left(\beta \cdot \overline{u_1}\right), \tag{17}$$

$$\overline{F_2} = \lambda_2 \cdot \left(\beta \cdot \overline{u_2}\right)$$
(18)

 λ_1 , λ_2 , u_1 and u_2 depend on the film thickness, distribution and regularity.



Fig. 4. Schematic representation of friction force when velocity is collinear with u_1 or u_2 vectors

4. Numerical results and discussion

In this section, three examples will be treated to show the validity and usability of our model.

Example 1. First, we will study the interply slip between a unidirectional ply with an arbitrary geometry and a fixed plan ply. The thickness of resin film separating the two surfaces must be obtained experimentally but in our case, we represent it by the following equation:

$$Z(x, y) = h_1(x, y) = h_0 \times \left(1 - \varepsilon_1 \sin\left(\frac{2\pi x}{T_x}\right) - \varepsilon_2 \sin\left(\frac{2\pi y}{T_y}\right)\right).$$
(19)

The parameters of the problem are represented in the following table.

Tuolo 2. Spoolilo parallotolis of enalipio 1					
Parameter	Value	Unit			
\mathcal{E}_1	0.1				
ε_2	0.1, 0.3, 0.5, 0.7				
T_x, T_y	0.06	m			
Н	100	Pa·s			
h_0	6×10 ⁻⁶	m			
N (number of collocation points)	15				

Table 2. Specific parameters of example 1

We represent in Fig. 6 the profiles of both surfaces when varying the parameter ε_2 . This variation causes a change in minimum and maximum resin film thicknesses.

For each case, the pressure $P_1(x, y)$ and $P_2(x, y)$ and their respective gradients can be deduced by solving the Reynold's equation and similarly, we can calculate using equation (16), the friction matrix C_f .



Fig. 5. Profiles schematization when: (a) $\varepsilon_2 = 0.1$; (b) $\varepsilon_2 = 0.3$; (c) $\varepsilon_2 = 0.5$; (d) $\varepsilon_2 = 0.7$

To study the influence of the resin thickness on the friction matrix C_f we did, and in each case, the calculation of the eigen values and the eigen vectors of this matrix (Table 3).

Parameter	Value			
\mathcal{E}_1	0.1	0.1	0.1	0.1
\mathcal{E}_2	0.1	0.3	0.5	0.7
$e_{\min}(\mu m)$	5.3	4	3	2
$e_{\max}(\mu m)$	6.3	7.5	9	10
λ_1	630.49	682.83	803.21	1124.47
U_1	$0.709\dot{i} - 0.705\dot{j}$	$0.325\dot{i} - 0.945\dot{j}$	$0.224\dot{i} - 0.974\dot{j}$	$0.19\dot{6i} - 0.98\dot{j}$
λ_2	613.013	618.38	640.7	633.32
U_2	$0.709\dot{i} - 0.705\dot{j}$	$0.325\dot{i} - 0.945\ddot{j}$	$0.224\dot{i} - 0.974\dot{j}$	$0.19\dot{6i} - 0.98\dot{j}$

Table 3. Obtained result for example 1

Figure 7 shows that the two Eigen values of the matrix C_f increase when the minimum thickness of the resin film is well below the maximum thickness of that film. The anisotropy factor λ_2/λ_1 is then dependent on a certain factor e_{\min}/e_{\max} (Fig. 8).



Fig. 6. Eigen values and Eigen vectors of C_f for different (e_{\min}/e_{\max})



Fig. 7. Variation of anisotropy factor with film irregularity

Example 2. In this example, the previously presented model in equation 16 will be used to calculate the friction parameters between two 3×3 Twill plies as shown in (Fig. 9).



Fig. 8. Inter-ply slip between two 3x3 Twill plies
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The geometric equations of both plies are given by:

$$h_1(x, y) = h_1^* \left[1 + \varepsilon_1 \cos\left(\frac{2\pi x}{T_x}\right) \cdot \cos\left(\frac{2\pi y}{T_y}\right) \right], \tag{20}$$

$$h_2(x, y) = h_2^* \left[1 - \varepsilon_2 \cos\left(\frac{2\pi x}{T_x}\right) \cdot \cos\left(\frac{2\pi y}{T_y}\right) \right].$$
(21)

The maximum and the minimum film thicknesses are equal to:

$$e_{\max} = h_1^* (1 + \varepsilon_1) - h_2^* (1 - \varepsilon_2),$$

$$e_{\min} = h_1^* (1 - \varepsilon_1) + h_2^* (1 + \varepsilon_2).$$
(22)

As h_1^* , h_2^* , ε_1 , ε_2 , T_x , T_y and N, the number of collocation points, are the imposed values (Table 3), $P_1(x, y)$, $P_2(x, y)$ and their respective gradients could now be calculated using the pseudo-spectral Fourier method (Fig. 10).

Parameter	Value	Unit
h_1^*	12.10 ⁻⁶	m
h_2^*	6.10 ⁻⁶	m
\mathcal{E}_1	0.2	
\mathcal{E}_2	0.2	
T_x	0.06	m
T_y	0.06	m
Н	100	Pa·s
N	15	

Table 3. Specific parameters of example 2

As demonstrated before, the friction matrix C_f , which characterize the relation between friction force and velocity, is dependent from both plies geometries h_1 and h_2 . Or in other terms, the thickness of resin film layer formed between both plies will play an important role in the variation of the components of C_f .

To evaluate this influence, we calculated C_f for different (e_{\min}/e_{\max}) values. Figure 11 shows that changing film thickness did not affect the Eigen vectors. In our case, when the velocity vector is deflected by a ±45° angle with x-axis, friction force is collinear to this vector whatever the film thickness variation is.

On the other hand, the irregularity of film thickness has a significant effect on λ_1 and λ_2 . With the increase of (e_{\min}/e_{\max}) , the values of λ_1 and λ_2 will finish by being equal (Fig. 12).

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Fig. 9. Different pressure and gradient of pressure profiles



Fig. 10. Influence of film thickness on the friction matrix C_f

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Fig. 11. Variation of anisotropy factor with film irregularity

Example 3. In this example, and using the same geometries as in example 2, we studied the influence of displacing the upper ply on the anisotropy of the matrix C_f and the effect of this variation on the the friction force.

First, we assumed that the upper ply slips with a known velocity vector which component along x axis is equal to 15mm/ s and the one in y direction is equal to zero.

The friction matrix C_f was calculated in five positions, where each one represents the state of the plies at instant:

t= 0: initial position

t=1 s: the upper ply is displaced by 15 mm from his initial position

t=2 s: the upper ply is displaced by 30 mm from his initial position

t=3 s: the upper ply is displaced by 45 mm from his initial position

t=4 s: the upper ply is displaced by one period from his initial position

Knowing that both plies are periodic in the *x* and *y* directions, the profiles corresponding to each displacement are represented in the figure below (Fig. 13).

The friction matrix is calculated as usual by solving Reynold's equation in each case. Then and using model described by (eq. 16), we can deduce the friction force in each state of displacement.

The obtained results (Table 5) show that in each position, friction matrix components do change and as well the anisotropy factor λ_2/λ_1 is variable with the displacement (Fig. 14, Fig. 15).

Time	0	1	2	3
$e_{\min}(\mu m)$	2	4.14	7.2	4.14
$e_{\max}(\mu m)$	16	13.8	10.8	13.8
λ_1	525	434.33	422.47	456.13
U_1	$0.699\dot{i} - 0.699\dot{j}$	$-0.99\dot{i}-0.626\dot{j}$	$-0.71\dot{i}-0.71\dot{j}$	$0.99\dot{i} - 0.95\dot{j}$
λ_2	475.9	445.12	405.35	446.33
U_2	$-0.71\dot{i}-0.71\ddot{j}$	$0.0075\dot{i} - 0.779\dot{j}$	$0.7\dot{i} + 0.7\dot{j}$	$-0.017\dot{i}+0.28\dot{j}$

Table 5. Obtained result for example 3



Fig. 12. Profiles description at: (a) t=0 s and t=4 s; (b) t=1 s; (c) t=2 s; t=3 s



Fig. 13. Variation of friction matrix components at each state of displacement

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Fig. 14. Variation of anisotropy factor with the displacement

These results show that during forming, the upper ply will rotate depending on his position because of, and in all cases, the non-linearity between the imposed velocity vector and the friction force one.

5. Conclusions

The proposed model consider that a thin film of resin builds up between the layers and plays an important role in forming processes of thermoplastic laminates. In this model, we supposed that a hydrodynamic lubrication exists between the layers in contact.

The pressure and its gradient generated in the fluid are obtained by the resolution of the equation of Reynolds.

As a result the relation between the friction force and the velocity is not scalar knowing that this model requires only the knowledge of the layers geometry and the viscosity of the used resin.

The friction force vector is equal to the product of a matrix C_{f} by the vector velocity.

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TWO-DIMENSIONAL MODEL FOR HYDRAULIC FRACTURING WITH FOAMS

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Abstract. A simple and accurate model of foam hydraulic fracturing is developed with both compressibility and rheology being taken into account. The governing equations for a compressible power-law fracturing fluid are derived for the classical PKN fracture geometry. Numerical simulations reveal an influence of compressibility and rheology on the temporal evolution of the fracture opening.

Keywords: hydraulic fracturing, compressibility, rheology, foam, numerical solution

1. Introduction

Foam fracturing modern technique of the hydraulic fracturing looks promising due to several advantages: foam minimizes usage of liquid, limits fluid retention in the formation and has better proppant transport properties due to its high viscosity. However, a modeling of foam faces serious difficulties. Apart from the foam saturation and stability, it is necessary to take into account compressibility and non-Newtonian character of the foam viscosity. Moreover, foam contains both liquid and gas parts. Taking into account all these factors is a difficult task. The compressibility of foam is usually introduced through its quality or the importance of the gas part [1 - 4]. Modeling of viscosity is simpler for incompressible fluids [4 - 9], and for compressible foam experimental data is usually used to fit power-law model [10, 11].

Existing models of foam fracturing could be divided into two groups. The first group uses simpler considerations and models foam as a single-phase fluid with effective properties depending on the foam quality and pressure. Gu's and Mohanty's model [12] is neglecting changing density of the foam and models its properties by relations for the power-law parameters depending on the fluid pressure in the fracture and given constant quality of the foam. For the two-dimensional model, it results in a difference in geometries of the fracture with the same fracturing conditions but different chosen foam qualities, while the total volume of the fracture remains constant. Another model, Park's approach [13], accounts for compressibility of foam by adding formation volume factor to the time-depended term in the continuity equation. Wang's et al. model [3] allows investigating influence of compressibility of fracturing fluid using linear density-pressure relation.

The second group of models is considering foam as a multi-phase fluid under different assumptions (e.g. dimensions, pressure, temperature, solubility etc.) [10, 11, 14]. The systems of governing equations for these models became more accurate, but at the same time they became noticeably more complex, requiring more setting parameters and increasing time of calculations, especially for three-dimensional cases.

Our goal is to develop quite simple and fast but accurate model of foam fracturing, which takes into account fluid compressibility and non-Newtonian character of its viscosity by introducing both density-quality and rheology-quality relations. The governing equations are derived for the classical PKN [15] fracture geometry in order to develop two-dimensional model and qualitatively investigate it using numerical simulation.

2. Governing equations

We consider a problem of a hydraulic fracture propagation driven by injection of compressible non-Newtonian fluid in an infinite homogenous linear elastic medium. The geometry of the problem presented in Fig. 1:



Fig. 1. PKN fracture geometry

This is a classical PKN [15] fracture geometry approach: the length of the fracture L is much greater than its constant height H, and height is much greater than fracture opening w. Then the approximate plane strain condition can be assumed in every plane orthogonal to the direction of propagation. Assuming that net pressure is independent of *y*-axis leads to elliptical fracture cross section. The fracture width along *z*-axis is then given by [15]:

$$w(z, x, t) = p_{net}(x, t) \frac{1}{E} \sqrt{H^2 - 4z^2},$$
(1)
where E' is defined as
$$z' = \frac{G}{2}$$

$$E' = \frac{G}{1-\nu}$$

 $p_{net} = p - \sigma_{\min}$, p is fluid pressure, σ_{\min} is minimum horizontal stress, v is Poisson's ratio, G is the shear modulus.

It is assumed that density and pressure of foam are constant in the each fracture cross section: $\rho = \rho(x,t)$, p = p(x,t). Under these assumptions and according to the fracture geometry the continuity equation is given by:

$$\frac{\pi H}{4} \frac{\partial}{\partial t} (\rho w_{max}) + \frac{\partial}{\partial x} (\rho q) = 0,$$
(2)
where q is the volumetric flow rate, $w_{max} = w(0, x, t).$

Two-dimensional model for hydraulic fracturing with foams

Equations of motions for single-phase fluid with one-dimensional flow in an elliptical fracture are reduced to the simple relation between volumetric flow rate and pressure gradient, neglecting inertial terms for Newtonian fluid:

$$q = -\frac{\pi w_{max}{}^{3}H}{}\frac{\partial p}{\partial x},\tag{3}$$

where μ is Newtonian viscosity. However, most investigations [16 – 19] are showing that foams rheology is well approximated by power-law models. That is why it can also be used another known relation for power law fluid motion in an elliptical fracture [20]:

$$q = -\frac{\varphi(n)H(\pi w_{max})^{2n+1/n}}{(2K)^{1/n}} \left(\frac{\partial p}{\partial x}\right)^{1/n} \operatorname{sign}\left(\frac{\partial p}{\partial x}\right),\tag{4}$$

where sign(x) is a signum function, K is flow consistency index and n is flow behavior index. Term $\varphi(n)$ depends on the fracture's cross section geometry and is derived as follows:

$$\varphi(n) = \frac{n}{2(2n+1)H} \int_{-H/2}^{H/2} \left(\frac{w}{w_{max}}\right)^{\frac{2n+1}{n}} dy.$$
(5)

For the elliptic cross section, the solution is known as [21]:

$$\varphi(n) = \frac{n}{2(2n+1)} \frac{\Gamma\left(\frac{4n+1}{2n}\right)}{\Gamma\left(\frac{5n+1}{2n}\right)} \left(\frac{2}{\sqrt{\pi}}\right)^{\frac{3n+2}{n}},\tag{6}$$

where $\Gamma(x)$ is gamma-function.

3. Foam compressibility model

The quality of the foam Γ is introduced as [1, 2]

$$\Gamma = \frac{V_g}{V_g + V_l},\tag{7}$$

where V_g , V_l are the volumes of the gas and liquid phases of the foam respectively. The presence of a gas phase makes foams highly compressible. Indeed, for isothermal processes the Boyle's law is

$$p_0 V_{0g} = p V_g , \qquad (8)$$

where p_0 is the injection pressure in our case, V_{0g} is initial volume of gas phase. It follows from Eqs. (7), (8) that

$$\frac{p}{p_0} = \frac{\Gamma_0 (1 - \Gamma) V_{0l}}{(1 - \Gamma_0) \Gamma V_l},\tag{9}$$

where Γ_0 is the foam injection quality, V_{0l} is initial volume of liquid phase. The density of the foam ρ is defined as

$$\rho = \frac{\rho_l v_l + \rho_g v_g}{v_l + v_g} = (1 - \Gamma)\rho_l + \Gamma \rho_g.$$
⁽¹⁰⁾

Equation (9) allows us to express quality through the pressure p. Substitution of the resulting expression into Eq. (10) gives rise to the connection between density and pressure,

$$\rho = \frac{\Gamma_0 p_0}{\Gamma_0 p_0 + (1 - \Gamma_0) p} \rho_g + \frac{(1 - \Gamma_0) p}{\Gamma_0 p_0 + (1 - \Gamma_0) p} \rho_l.$$
(11)

The second term in Eq. (11) is negligibly small for low quality foams due to $\frac{\mu_g}{\rho_l} \ll 1$.

Then the compressibility relationship is

$$\rho = \frac{(1 - \Gamma_0)p}{\Gamma_0 p_0 + (1 - \Gamma_0)p} \rho_l.$$
(12)

However, for the high quality foam the density of gas becomes comparable with the density of the liquid phase, so at least an estimation for ρ_g is needed. We assume that the value of ρ_g can be simply estimated as the density of an ideal gas at the defined values of pressure and temperature *T*:

$$\rho_g = \frac{Mp}{RT},\tag{13}$$

where M = 28 g/mol for N_2 and M = 44 g/mol for CO_2 , R is ideal gas constant. As we consider isothermal case, the averaged temperature of the reservoir is assumed to be known and used in Eq. (13).

4. Foam rheology model

We consider foams as non-Newtonian fluids by using known models that predict power law parameters of the foam as functions of quality. In presented work we are using known empirical correlations [22] for $K(\Gamma)$ and $n(\Gamma)$.

The correlation for 20-lbm/Mgal foam is:

$$n = n_0(1 - 2.1006\Gamma^{7.3003}), \ K = K_0 \exp(-1.9913\Gamma + 8.9722\Gamma^2)$$
(14)
orrelation for 30-lbm/Mgal form is:

$$n = n_0(1 - 0.1535\Gamma^{6.5152}), K = K_0 \exp(-2.3761\Gamma + 8.8830\Gamma^2)$$
(15)
The correlation for 40-lbm/Mgal foam is:

$$n = n_0(1 - 0.6633\Gamma^{5.1680}), \ K = K_0 \exp(-0.4891\Gamma + 5.6203\Gamma^2)$$
(16)

 K_0 and n_0 are constant power law parameters of the base fluid which are assumed to be known. It should be noted that any other known correlations (e.g., Ref. [16 – 19]) for $K(\Gamma)$, $n(\Gamma)$ may be used instead of Eqs. (14), (15) and (16). It is also possible to use Newtonian $\mu(\Gamma)$ correlations (e.g., Ref. [5, 23]) with Eq. (3) in order to simplify the model.

5. Numerical simulation

Equations (1), (2), (4), (6), (11), (13) and relations (14), (15) or (16) together form a closed system of equations and can be modified to a single pressure or a fracture width equation. It can be solved implicitly using FDM with inner iterations. The boundary conditions are:

 $w_{max}(x,t)|_{x=L}=0,$ $\rho q|_{x=0} = Q_{in},$ where Q_{in} is an inlet mass flow rate. Fracture length L(t) is evaluated as follows: $L(t) = \min(x|_{w_{max}(x)=0}).$ The initial condition is a closed fracture:

 $w_{max}(x,0) = 0.$

Following hydraulic fracturing parameters are chosen to be fixed during the numerical simulations in order to investigate the dependence of the initial foam quality and its rheology on the fracture geometry:

$$Q_{in} = 1.5 \text{ kg/s}, P_0 = 1 \text{ MPa},$$

 $\rho_l = 1000 \text{ kg/m}^3, K_0 = 0.01 \text{ Pa} \cdot \text{s}, n_0 = 1,$
 $E = 25 \text{ GPa}, H = 20 \text{ m}, \sigma = 1 \text{ MPa}$

Firstly, we are studying the influence of rheology relations defined by Eqs. (14), (15) and (16) for the different initial foam qualities by comparing obtained numerical results with the constant viscosity case $(K(\Gamma) = K_0 = \text{const}, n(\Gamma) = n_0 = \text{const})$. The fracture width distributions along L at t = 1000 s are shown for $\Gamma_0 = 0.25$, $\Gamma_0 = 0.5$ and $\Gamma_0 = 0.75$ in Fig. 2, Fig. 3, Fig. 4 respectively. For this set of initial parameters non-Newtonian character of the foam viscosity starts to influence fracture geometry at $\Gamma_0 = 0.5$, and its influence become essential for the case $\Gamma_0 = 0.75$: fracture width is increasing while the fracture length decreases. In addition, it is shown that for different foams (20, 30 and 40lbm/Mgal) fracture geometry is changing not significantly.

(17)



Fig. 2. Fracture width distribution for initial foam quality 0.25



Fig. 3. Fracture width distribution for initial foam quality 0.5



Fig. 4. Fracture width distribution for initial foam quality 0.75

Secondly, we investigate the compressibility factor influence on the fracture geometry. Considering constant viscosity $K(\Gamma) = K_0 = \text{const}$, $n(\Gamma) = n_0 = \text{const}$ for all the simulations we compare fracture propagation process for incompressible fluid (Fig. 5), compressible CO_2 -foam with $\Gamma_0 = 0.25$ (Fig. 6), $\Gamma_0 = 0.5$ (Fig. 7) and $\Gamma_0 = 0.75$ (Fig. 8) at 50*K*-temperature cases. The numerical results show that increasing of initial foam quality leads to an increase in the final volume of the fracture for similar mass flow rate. For $\Gamma_0 = 0.25$ overall calculated mass fraction of pumped gas in foam is equal to ~ 0.54\%, for $\Gamma_0 = 0.5$ this value reaches ~ 1.54\%, and for $\Gamma_0 = 0.75$ is ~ 4.69%.



Fig. 5. Fracture growth for incompressible fluid

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Fig. 6. Fracture growth for 0.25-quality foam (no rheology)



Fig. 7. Fracture growth for 0.5-quality foam (no rheology)



Fig. 8. Fracture growth for 0.75-quality foam (no rheology)

Also it should be noted that assuming $\Gamma_0 = 0$ and $n(\Gamma) = 1$ (the case corresponding to Fig. 5) the model reduces to classical PKN model for an incompressible fracturing fluid without leak-off.

Finally we present the numerical results (Fig. 9) for 0.75-quality 30-lbm/Mgal foam (rheology is defined by Eq. 15). Comparing to the no-rheology case (Fig. 8) the modeling results show that the length of the fracture is decreasing while the fracture width increases.



Fig. 9. Fracture growth for 0.75-quality 30-lbm/Mgal foam

6. Conclusion

The two-dimensional model of foam fracturing is presented. It takes into account fluid compressibility and non-Newtonian character of its viscosity by introducing density-quality relation based on the Boyle's law and rheology-quality correlations. This model allows to calculate fracture geometry for the foams with different quality at given pressure. Both rheology and compressibility properties have been studied independently and together. The developed model shows that for higher quality foam it is expected to produce a fracture with higher opening value and lower length due to rheology properties, and with greater volume for the same mass of pumped foam due to compressibility. Due to the simplicity of the introduced system of equations, it is expected that one may develop fast and accurate pseudo3D foam fracturing model based on the presented model.

However, the presented model does not take into account very important aspects of hydraulic fracturing, such as leak-off and proppant transport. Future generalization of the problem implies not only conversion to pseudo3D-geometry, but also consideration of proppant transport, its influence on the foam rheology and adding multi-phase leak-off terms to the governing equations.

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"WANDERING" NATURAL FREQUENCIES OF AN ELASTIC CUSPIDAL PLATE WITH THE CLAMPED PEAK

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Abstract. Cuspidal irregularities of solids have been recognized as Vibrating Black Holes for elastic and acoustic waves. The corresponding absorption phenomenon is caused, in particular, by the appearance of the continuous spectrum $[\kappa_{+}, +\infty)$ of the Lame system in a two-dimensional plate with the sharp cusp that provokes for wave processes in a finite volume. However, if the plate is clamped in the small *h*-neighborhood of the cusp top, the spectrum becomes discrete and consists of isolated natural frequencies κ_j^h of finite multiplicity. The asymptotics of κ_j^h as $h \to +0$ is constructed that describes the effect of the "wandering" of the natural frequencies above the threshold $\kappa_{+} > 0$, namely the asymptotic formula $\kappa_j^h = K_j(\ln h) + O(h^{\delta})$ with $\delta > 0$ is valid where K_j is a periodic function. In other words, some of frequencies flounce in the semi-axis ($\kappa_{+}, +\infty$) at a quite high rate $O(h^{-1})$. At the same time, natural frequencies below the threshold get the sustainable behaviour $\kappa_p^h = \kappa_p^0 + O(h^{\delta})$, $\delta > 0$, as $h \to +0$.

Keywords: vibrating black holes, cuspidal plate, continuous spectrum, clamped peak, wandering eigenvalues, asymptotics

1. Formulation of the elasticity problems in a cuspidal solid

Let Ω be a two-dimensional isotropic and homogeneous elastic plate and let its edge $\Gamma = \partial \Omega$ be smooth everywhere with exception of the point \mathcal{O} , the origin of the Cartesian coordinate system $x = (x_1, x_2)$. In a neighborhood of \mathcal{O} , the domain gets the cuspidal shape, i.e., $\{x \in \Omega: x_1 \leq d\} = \Pi_d$, where $\Pi_d = \{x \in \mathbb{R}^2: x_1 \in (0, d], |x_2| < Hx_1^2\}, \qquad d > 0, H > 0.$ (1)

First of all, we assume that the plate edge Γ is traction-free. Then the longitudinal oscillations of the plate Ω are described by the spectral boundary-value problem

$$-\partial_1 \sigma_{j1}(u;x) - \partial_2 \sigma_{j2}(u;x) = \rho \kappa^2 u(x), \quad x \in \Omega, \quad j = 1,2,$$

$$(2)$$

$$\sigma_{j}^{(n)}(u;x) \coloneqq n_{1}(x) \,\sigma_{j1}(u;x) - n_{2}(x) \,\sigma_{j2}(u;x) = 0 \,, \ x \in \Gamma \backslash \mathcal{O}, \ j = 1,2.$$
(3)

Here $\partial_j = \partial/\partial x_j$, $u = (u_1, u_2)$ is the displacement vector, $\sigma^{(n)} = (\sigma_1^{(n)}, \sigma_1^{(n)})$ is the normal vector of stresses, and the Cartesian components of the stress tensor $\sigma(u)$ are given by $\sigma_{jk}(u) = \mu (\partial_j u_k + \partial_k u_j) + \lambda \, \delta_{j,k} (\partial_1 u_1 + \partial_2 u_2)$, j, k = 1, 2. (4)

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(6)

Moreover, $\lambda \ge 0$, $\mu > 0$ and $\rho > 0$ are the Lame constants and the density of the elastic material, respectively. Finally, $n = (n_1, n_2)$ is the unit vector of the outward normal, $\delta_{j,k}$ is the Kronecker symbol, and $\kappa \ge 0$ is the frequency of harmonic-in-time oscillations. We reduce the characteristic size of the domain Ω to unity and make dimensionless the coordinates x_1, x_2 and all geometric parameters.

It is known, see e.g. [1, 2], that the spectrum \wp of the problem (2), (3) has the continuous component $\wp_{co} = [\kappa_{\dagger}, +\infty)$ with the positive cutoff value

$$\kappa_{\dagger} = \frac{5}{2} H \sqrt{3\frac{\rho}{M}},\tag{5}$$

where *H* and ρ are taken from the relations (1) and (2), respectively, and $M = \frac{\mu(\lambda + \mu)}{\lambda + 2\mu}$.

The primitive formula $\wp_{co} \neq \emptyset$ follows from the fact observed in [3; Sect. 3.1], namely the traditional Korn inequality, cf., the review paper [4],

$$||u; H^{1}(\Omega)||^{2} \leq c_{\Omega}(\mathcal{E}(u; \Omega) + ||u; L^{2}(\Omega)||^{2})$$
(7)

does not hold true in the cuspidal domain (1). In (7), $L^2(\Omega)$ and $H^1(\Omega)$, respectively, are the Lebesgue and Sobolev spaces with the standard norms $||u; L^2(\Omega)|| = \left(\int_{\Omega} |u(x)|^2 dx\right)^{1/2}$ and $||u; H^1(\Omega)|| = \left(\int_{\Omega} (|\nabla u(x)|^2 + |u(x)|^2) dx\right)^{1/2}$, while $\mathcal{E}(u; \Omega)$ is the energy functional,

$$\mathcal{E}(u;\Omega) = \int_{\Omega} \left(|u_{1}(x)|^{2} + |u_{2}(x)|^{2} \right) dx + \frac{1}{2\mu} \int_{\Omega} \left(\sum_{j,k=1,2} \left| \sigma_{jk}(u;x) \right|^{2} - \frac{\lambda}{2(\lambda+\mu)} \left| \sigma_{11}(u;x) + \sigma_{22}(u;x) \right|^{2} \right) dx$$
(8)

Furthermore, the energy space $E(\Omega)$ obtained by completion of the linear set $C_c^{\infty}(\overline{\Omega} \setminus \mathcal{O})$ (infinitely differentiable vector functions vanishing near the point \mathcal{O}) with respect to the norm $||u; E(\Omega)||^2 = \mathcal{E}(u; \Omega)^{1/2}$, (9)

is much bigger that the Sobolev space $H^1(\Omega)$ and the embedding $E(\Omega) \subset L^2(\Omega)$ is not compact.

The latter assures that indeed the continuous spectrum \wp_{co} of the operator of the problem (2), (3) is not empty according to general results in the operator theory, see, e.g., the monograph [5; Ch. 9, 10].

The continuous spectrum provokes for wave processes inside the cusp (1) which are known as Vibrating Black Holes, see the papers [6-8] where concrete engineering devices based on the effect under discussion, are described as well. We mention especially the pioneering paper [6] where, for the first time, the cutoff value (5) was computed on the basis of the Kirchhoff theory of thin elastic beams with variable thickness.

Let us assume now that the peak of the cusp (1) is clamped along the short arcs

$$\gamma_h^{\pm} = \{x: x_1 \in (0, h), |x_2| = \pm H x_1^2\};$$

here $h \ll 1$ is a small parameter. Then, for a vector field $u \in H^1(\Omega)$ satisfying the Dirichlet boundary conditions

$$u_j(x) = 0, \ x \in \gamma_h = \gamma_h^+ \cup \gamma_h^-, \ j = 1,2,$$
 (10)

the Korn inequality (9) becomes valid. Indeed, one may extend by zero the vector function u from Π_h on the rectangle $Q_h = \{x: x_1 \in (0, h), |x_2| < Hh^2\}$ and apply the standard Korn

inequality, see e.g. [4], in the two domains $\Omega \setminus \Pi_h$ and Q_h with Lipschitz boundaries. Thus, the spectrum \mathcal{P}^h of the Lame system (2) with the boundary conditions (10) and

$$\sigma_j^{(n)}(u;x) = 0, \quad x \in \Gamma \setminus \overline{\gamma_h}, \quad j = 1,2, \tag{11}$$

is fully discrete due to the compact embedding $H^1(\Omega) \subset L^2(\Omega)$. By [5; Theorems 10.1.5, 10.2.2], this spectrum composes the monotone unbounded eigenvalue sequence

$$0 < \kappa_1^h \le \kappa_2^h \le \kappa_3^h \le \dots \le \kappa_p^h \le \dots \to +\infty,$$
(12)
where multiplicity is counted in

where multiplicity is counted in.

Our objective is to examine the asymptotic behavior of the eigenvalues κ_p^h as $h \to +0$. It is remarkable that asymptotic formulas become quite different below and above the threshold (5) and, for $\kappa_j^h > \kappa_{\dagger}$, they exhibit the new effect of "wandering" described in Section 5. For $\kappa_p^h < \kappa_{\dagger}$, we conclude with rather standard asymptotic expansions.

2. Waves inside the cusp

Since width $2Hx_1^2$ of the cusp (1) is much smaller than the distance $x_1 > 0$ to its top \mathcal{O} , the dimension reduction procedure, see e.g. [3; Ch. 4], can be applied in the same way as in the paper [1] in order to derive the asymptotic expansion of a solution u(x) to the problem (2), (3) when $x_1 \rightarrow +0$. Thus, we accept the standard asymptotic ansatz

$$u(x) = U^{-2}(x) + U^{-1}(x) + U^{0}(x) + U^{1}(x) + U^{2}(x) + \cdots$$
(13)

with the first terms computed, for example, in the book [3; Sections 1.3 and 4.1] and the paper [1, Section 3],

$$U^{-2}(x) = e_{(2)} w(x_1), \qquad U^{-1}(x) = -x_2 e_{(1)} \frac{dw}{dx_1}(x_1),$$

$$U^{0}(x) = e_{(2)} \frac{\lambda}{\lambda + 2\mu} \frac{x_2^2}{2} \frac{d^2 w}{dx_1^2}(x_1), \qquad U^{1}(x) = e_{(1)} \frac{3\lambda + 4\mu}{\lambda + 2\mu} \frac{x_2^3}{6} \frac{d^3 w}{dx_1^3}(x_1) -$$

$$-2e_{(1)} \frac{\lambda + \mu}{\lambda + 2\mu} H^2 x_1^4 x_2 \frac{d^3 w}{dx_1^3}(x_1) - 8e_{(1)} \frac{\lambda + \mu}{\lambda + 2\mu} H^2 x_1^3 x_2 \frac{d^2 w}{dx_1^2}(x_1),$$
(14)

where $e_{(j)}$ stands for the unit vector of the x_j -axis. To construct the next term $U^2(x)$ in (13), we have to subject the unknown scalar function w of the longitudinal variable x_1 to the ordinary differential equation for the averaged bend of beams with variable thickness, cf., the original paper [6],

$$\frac{4}{3}MH^3 \frac{d^2}{dx_1^2} x_1^6 \frac{d^2 w}{dx_1^2}(x_1) = 2H x_1^2 \rho \kappa^2 w(x_1), \quad x_1 > 0.$$
(15)

The coefficients H, ρ, κ and M are taken from the formulas (1), (2) and (6), respectively. Clearly, the equation (15) with $\kappa = 0$ has the particular solution

$$w(x_1) = C_0 + C_1 x_1. (16)$$

According to (14), the linear function (16) gives rise to the displacement field (13) which is nothing but a rigid motion. Solutions to the ordinary differential equation (15) of Euler type with $\kappa > 0$ have the form

$$w(x_1) = c x_1^{\tau - 3/2},\tag{17}$$

where the exponent τ is a root of the bi-quadratic equation

$$\left(\tau^{2} - \frac{9}{4}\right)\left(\tau^{2} - \frac{25}{4}\right) = \frac{3}{4} \frac{\rho \kappa^{2}}{MH^{2}}.$$
(18)
In the case

III the v

 $\kappa \leq \kappa_{\dagger}$,

(19)

(28)

i.e., below the threshold (5), the bi-quadratic equation (18) has four real rots but, for $\kappa > \kappa_{+}$,

i.e., above the threshold, the equation gets two real and two pure imaginary roots $\tau_{\pm}^{re} = \pm t_{\pm}$ and $\tau_{\pm}^{im} = \pm it_{\pm}$ (20) where

$$t_{\pm}^2 = T \pm \frac{17}{4} > 0, \qquad T = \frac{1}{2} \sqrt{16 + 3\frac{\rho\kappa^2}{MH^2}}.$$
 (21)

The displacement field $u_{(\pm)}^{im}(x)$ constructed through the formulas (13), (14) and (20), (21) from the oscillatory solutions, see (17) and (20),

$$w_{(\pm)}^{im}(x_1) = c_{(\pm)}^{im} x_1^{\pm it_- -3/2}$$
(22)

are interpreted as one-dimensional bending elastic waves propagating along the cusp Π_h to its top \mathcal{O} (minus) and from the point \mathcal{O} (plus), see [6] and [1, 2]. The direction of propagation is found out by means of the Umov-Mandelstam (energy) radiation principle, see the monograph [9; Ch. 1] and, e.g., the paper [10] among many other publications.

Computing components of the stress tensor $\sigma(u^0)$ according to the relations (4) and (13), (14), we obtain

$$\sigma_{11}(u^0; x) = -4Mx_2 \frac{d^2 w}{dx_1^2}(x_1) + \cdots, \qquad \sigma_{22}(u^0; x) = \cdots$$
(23)

$$\sigma_{12}(u^0; x) = 4M \left(\frac{x_2^2}{2} - \frac{H^2}{2} x_1^4\right) \frac{d^3 w}{dx_1^3}(x_1) - 8M H^2 x_1^3 \frac{d^2 w}{dx_1^2}(x_1) + \cdots,$$
(24)

where dots stand for lower-order terms, namely for $O(x_1^{-1/2})$ in (23) and $O(x_1^{+1/2})$ in (24). In view of (14), (21) and (20) integrands on the right-hand side of (8) get order x_1^{-3} so that the integrals over the cusp (1) diverge at the rate $O(|\ln x_1|)$. The latter observation, in particular, indicates transportation of energy along the cusp.

The displacement fields $u_{(+)}^{re}(x)$ constructed from the solutions

$$w_{(\pm)}^{re}(x_1) = c_{(\pm)}^{re} x_1^{\pm t_+ - 3/2}$$
 (25)
with the real exponents in (20) possess quite different properties. Indeed, by the

definitions (25), (21) and (14), (23), (24), the vector function $u_{(+)}^{re}$ gives rise to the finite energy functional $\mathcal{E}(u_{(+)}^{re};\Pi_h)$. At the same time, the integrals on the right-hand side of (8) with $u = u_{(-)}^{re}$ diverge at the power rate $O(x_1^{-2t_+})$.

In what follows we will deal with elastic fields involving the following linear combination of the constructed special displacement vectors:

$$u^{0}(x) = c_{(+)}^{im} u_{(+)}^{im}(x) + c_{(-)}^{im} u_{(-)}^{im}(x) + c_{(+)}^{re} u_{(+)}^{re}(x) + c_{(-)}^{re} u_{(-)}^{re}(x).$$
⁽²⁶⁾

Notice that imposing various relationships between the coefficients $c_{(\pm)}^{lm}$ and $c_{(\pm)}^{re}$ yields different operators of the problem (2), (3) with very distinct properties, cf., Section 5.

In the paper [2] it is proved that any solution of the problem (2), (3) verifying the estimate

$$|u(x)| \le c x_1^{-\theta - \frac{3}{2}}, \quad x \in \Omega,$$
(27)
with an exponent $\theta > t$, admits the asymptotic form

with an exponent $\theta > t_+$, admits the asymptotic form $u(x) = \chi(x_1)u^0(x) + \tilde{u}(x),$ where u^0 is a linear combination (26) with coefficients depending on the solution u, χ is a smooth cut-off function,

$$\chi(x_1) = 1 \text{ for } x_1 < \frac{d}{2} \text{ and } \chi(x_1) = 0 \text{ for } x_1 > d,$$

and the remainder \tilde{u} enjoys the estimate
 $|\tilde{u}(x)| \le c x_1^{\theta - \frac{3}{2}}, \quad x \in \Omega.$ (29)

We emphasize that the displacement fields $u_{(\pm)}^{re}$ and $u_{(\pm)}^{im}$ do not satisfy the relation (29) so that detaching a linear combination (26) is necessary to achieve the appropriate decay of the remainder $\tilde{u}(x)$ as $x \to O$.

3. The boundary layer phenomenon

In order to take into account the boundary conditions (10) we introduce the stretched coordinates

 $\xi = (\xi_1, \xi_2) = (h^{-2}(x_1 - h), h^{-2}x_2).$ (30) The coordinate dilation $x_1 + \xi_2$ and formal softing h = 0 turn the own Π into the

The coordinate dilation $x \mapsto \xi$ and formal setting h = 0 turn the cusp Π_h into the infinite strip

 $\mathcal{S} = \{ \xi \in \mathbb{R}^2 \colon \xi_1 \in \mathbb{R}, |\xi_2| < H \}$

of width 2*H*. Since the endpoints $x = (h, \pm Hh^2)$ of the arcs γ_h^{\pm} are mapped into the points $\xi = (0, \pm H)$, the original problem (2), (11), (10) about the plate with the clamped peak converts into the following mixed boundary-value problem for the Lame system in the strip $-\partial_1 \sigma_{j1}(w;\xi) - \partial_2 \sigma_{j2}(w;\xi) = 0$, $\xi \in S$, j = 1,2,

$$\sigma_{j2}\left(w;\xi_{1},\pm\frac{1}{2}\right) = 0, \ \xi_{1} > 0, \ j = 1,2,$$

$$w_{j}\left(\xi_{1},\pm\frac{1}{2}\right) = G_{j}^{\pm}, \ \xi_{1} < 0, \ j = 1,2.$$
(31)

The boundary layer $w(\xi) = (w_1(\xi), w_2(\xi))$ is intended to compensate for the main discrepancy of the vector function (28) in the Dirichlet conditions (10) and hence, the data of the problem (31) look as follows:

$$G_{2}^{\pm}(\xi_{1}) = W_{2}^{h} \coloneqq \sum_{\pm} \left(c_{(\pm)}^{im} h^{\pm it_{-}-3/2} + c_{(\pm)}^{re} x_{1}^{\pm t_{+}-3/2} \right),$$

$$G_{1}^{\pm}(\xi_{1}) = \pm W_{1}^{h} \coloneqq \mp H \sum_{\pm} \left(\left(\pm it_{-} - \frac{3}{2} \right) c_{(\pm)}^{im} h^{\pm it_{-}-3/2} + \left(\pm t_{+} - \frac{3}{2} \right) c_{(\pm)}^{re} x_{1}^{\pm t_{+}-3/2} \right).$$
(32)

Thus, the solution of the problem (31) with the finite elastic energy is nothing but the bounded displacement field with the linear dependence on the transversal coordinate ξ_2 , that is,

$$w(\xi) = \left(-H\xi_2 W_1^h, W_2^h\right).$$

This boundary layer term gets the intrinsic property of the exponential decay as $\xi_1 \to \pm \infty$ only in the case

$$W_1^h = 0, \qquad W_2^h = 0.$$
 (33)

This implies that the problem (31) must be homogeneous and the main term of the boundary layer must be absent in the asymptotics.

Let us find coefficients in the linear combination (26) which provides the relation (33). The first step looks quite unanticipated, namely we set $c_{(+)}^{re} = 0$ (34) and, therefore, exclude from the linear combination the "decent" solution in the couple (25) but keep the "undeserving" one with objectionable behavior as $x_1 \rightarrow +0$. A reason for this procedure will be explained in the end of Section 5.

At the second step, we insert the formulas (32) into the equations (33) and exclude from the obtained system of linear algebraic equations

$$c_{(+)}^{im}h^{+it_{-}-3/2} + c_{(-)}^{im}h^{-it_{-}-3/2} + c_{(-)}^{re}h^{-t_{+}-3/2} = 0,$$

$$c_{(+)}^{im}\left(it_{-}-\frac{3}{2}\right)h^{+it_{-}-5/2} - c_{(-)}^{im}\left(-it_{-}-\frac{3}{2}\right)h^{-it_{-}-5/2} - c_{(-)}^{re}\left(t_{+}+\frac{3}{2}\right)h^{-t_{+}-5/2} = 0$$
(35)

the unknown and irrelevant coefficient $c_{(-)}^{re}$. As a result, we come across the following relationship between the coefficients $c_{(-)}^{im}$ and $c_{(+)}^{im}$ of the oscillatory waves:

$$c_{(-)}^{im} = -h^{2it_{-}} \frac{t_{+} + it_{-}}{t_{+} - it_{-}} c_{(+)}^{im}.$$
(36)

We emphasize that modulo of the coefficient on the right-hand side of (36) is equal to one. It should also be noted that the equalities (35) imply that the main asymptotic terms of the displacement field (26) with the coefficient (34) vanish at the cross-section $\{x: x_1 = h, |x_2| < Hh^2\}$ of the cusp Π_d and hence can be extended by zero onto the peak Π_h with the clamped sides γ_h^{\pm} in order to satisfy the Dirirchlet conditions (10). The latter is the immediate consequence of the equalities (33) caused by our consideration of the boundary layer phenomenon.

4. Asymptotic conditions at the cusp top and the self-adjoint operator pencils

Let $\mathcal{W}(\Omega)$ be a space of vector functions in the form (9) where

$$u^{0}(x) = c_{(+)}^{im} u_{(+)}^{im}(x) + c_{(-)}^{im} u_{(-)}^{im}(x) + c_{(+)}^{re} u_{(+)}^{re}(x).$$
(37)

Notice that in contrast to (34) we now have set

$$c_{(-)}^{re} = 0$$
 (38)

and the linear combination (26) under the restriction (38) becomes nothing but (37). The norm in $\mathcal{W}(\Omega)$ is the sum of the coefficients moduli $|c_{(\pm)}^{im}| + |c_{(+)}^{im}|$ and an appropriate (see [2] and compare with (29)) weighted norm of the remainder \tilde{u} . Such spaces are called weighted spaces with detached asymptotics. Fixing some phase $\psi \in [0,2\pi)$, we impose the relationship $c_{(-)}^{im} = e^{i\psi} c_{(+)}^{im}$ (39)

and denote by $\mathcal{W}(\Omega; \psi)$ the subspace of vector functions $u \in \mathcal{W}(\Omega)$ subject to the restriction (39). Dealing with solutions of the problem (2), (3) in this space should be interpreted as imposing certain asymptotic conditions at the top \mathcal{O} of the cusp.

To investigate general properties of the problem (2), (3), (39), we first of all insert any vector functions $u^{(m)} \in \mathcal{W}(\Omega; \psi), m = 1, 2$, into the Green formula on the domain $\Omega^{\varepsilon} = \Omega \setminus \Pi^{\varepsilon}$ and perform the limit passage $\varepsilon \to +0$. Denoting by $c_{(\pm)}^{im(m)}, c_{(+)}^{re(m)}$ and $\tilde{u}^{(m)}$ the introduced attributes of $u^{(m)}$ and setting

$$w^{(m)}(x_1) = c_{(+)}^{im(m)} x_1^{it_- -3/2} + c_{(-)}^{im(m)} x_1^{-it_- -3/2} + c_{(+)}^{re(m)} x_1^{t_+ -3/2},$$
(40)
we obtain

$$-\sum_{j=1}^{2} \left(\left(\partial_{1} \sigma_{j1}(u^{(1)}), u_{j}^{(2)} \right)_{\Omega^{\varepsilon}} + \left(\partial_{2} \sigma_{j2}(u^{(1)}), u_{j}^{(2)} \right)_{\Omega^{\varepsilon}} - \left(u_{j}^{(1)}, \partial_{1} \sigma_{j1}(u^{(2)}) \right)_{\Omega^{\varepsilon}} + \left(u_{j}^{(1)}, \partial_{2} \sigma_{j2}(u^{(2)}) \right)_{\Omega^{\varepsilon}} \right) +$$

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$$+ \left(\sigma^{(n)}(u^{(1)}), u^{(2)}\right)_{\Gamma \setminus \overline{Y_{\varepsilon}}} - \left(u^{(1)}, \sigma^{(n)}(u^{(2)})\right)_{\Gamma \setminus \overline{Y_{\varepsilon}}} =$$

$$= \frac{8}{3} MH^{3} \lim_{\varepsilon \to 0} \left(\frac{d}{dx_{1}} \left(x_{1}^{6} \frac{d^{2}w^{(1)}}{dx_{1}^{2}}(x_{1})\right) \overline{w^{(2)}(x_{1})} - x_{1}^{6} \frac{d^{2}w^{(1)}}{dx_{1}^{2}}(x_{1}) \frac{\overline{dw^{(2)}(x_{1})}}{dx_{1}} + x_{1}^{6} \frac{d^{w^{(1)}}}{dx_{1}} \frac{\overline{d^{2}w^{(1)}}}{dx_{1}^{2}}(x_{1})}{dx_{1}^{2}} - w^{(1)}(x_{1}) \overline{\left(\frac{d}{dx_{1}}x_{1}^{6} \frac{d^{2}w^{(2)}}{dx_{1}^{2}}(x_{1})\right)}\right)} \right) \Big|_{x_{1}=\varepsilon} =$$

$$= 4Tit_{-} \left(c_{(+)}^{im(1)}\overline{c_{(+)}^{im(2)}} - c_{(-)}^{im(1)}\overline{c_{(-)}^{im(2)}}\right) = 0.$$

$$(41)$$

The numbers *M*, *H* and *T* are taken from (1), (6) and (21), respectively, and (,)_{Ξ} stands for the natural scalar product in the Lebesgue space $L^2(\Xi)$. In the middle of the calculation (41) we have used the formulas (23) and (24) while the last equality is due to the imposed relationship (39) which demonstrates that $c_{(+)}^{im(1)}\overline{c_{(+)}^{im(2)}} = c_{(-)}^{im(1)}\overline{c_{(-)}^{im(2)}}$.

Green's formula (41) means that the operator $\mathcal{A}_{\gamma}(\kappa)$ of the problem (2), (3) with the domain $\mathcal{W}(\Omega; \psi)$ is formally self-adjoint. It must be regarded as a holomorphic pencil, see the monographs [11; Ch. 1] and [12; Ch. 1]. Its spectrum in the half-plane $\mathbb{C}_{\dagger} = \{\kappa \in \mathbb{C}: \operatorname{Re} \kappa \ge \kappa_{\dagger}\}$ form the monotone unbounded sequence of normal real eigenvalues listed according to their multiplicity

$$\kappa_{\dagger} < k_N(\psi) \le k_{N+1}(\psi) \le \dots \le k_{N+q}(\psi) \le \dots + \infty.$$
(42)

By the relationship (39), the eigenvalues (42) depend 2π -periodically on the parameter ψ .

5. Asymptotics of eigenvalues of the problem with clamped peak

We now are in a position to formulate appropriate asymptotic conditions at the cusp top O in order to create an asymptotic model of the problem (2), (10), (11) with the help of asymptotic conditions. Comparing (39) with (36), we set

$$\psi(h) = \tau + 2t_{-} \ln h,$$
(43)
where the phase $\tau \in [0, 2\pi)$ is chosen such that

$$e^{i\tau} = -\frac{t_+ + it_-}{t_+ - it_-}.$$
(44)

The operator $\mathcal{A}_{\psi(h)}(\kappa)$ of the problem (2), (3) defined in the space $\mathcal{W}(\Omega; \psi(h))$, that is, with the asymptotic conditions (28), (37), (39), (43), differs crucially from the operator $\mathcal{M}(\kappa)$ of the same problem but with the Umov-Mandelstam radiation conditions

$$u(x) = \chi(x_1) \left(c_{(-)}^{im} u_{(-)}^{im}(x) + c_{(+)}^{re} u_{(+)}^{re}(x) \right) + \tilde{u}(x),$$
(45)

which allow only the wave $u_{(-)}^{im}$ outgoing to the top \mathcal{O} , and of course, the field $c_{(+)}^{re}u_{(+)}^{re}$ with the finite elastic energy. Indeed, the operator $\mathcal{M}(\kappa)$ get a skew-symmetric component owing to Green's formula (41) whose right-hand side gets the form

$$-4Tit_{-}c_{(-)}^{im(1)}\overline{c_{(-)}^{im(2)}}$$

In contrast to $\mathcal{M}(\kappa)$, the operator $\mathcal{A}_{\psi(h)}(\kappa)$ is self-adjoint and possesses the discrete spectrum (42) with the parameter (43). The eigenvalues (42) of $\mathcal{A}_{\psi(h)}(\kappa)$ become (π/t_{-}) periodic in the logarithmic scale, namely this period is attributed to the functions $\ln h \mapsto k_N(\psi(h)).$ (46) In the case $\kappa \in (0, \kappa_{\dagger})$ the operator of the problem (2), (3) in the energy space $E(\Omega)$ is Fredholm and self-adjoint too. Hence, it has a finite number of eigenvalues below the threshold (5)

 $0 = \kappa_1^0 = \kappa_2^0 = \kappa_3^0 < \kappa_4^0 \le \dots \le \kappa_{N-1}^0 < \kappa_{\dagger}.$ (47)

Here, the three null eigenvalues are generated by rigid motions, that is, two translations and one rotation, which are generated by the linear solutions (16) of the limit differential equation (15).

Asymptotic forms for the eigenvalues $\kappa_4^0, ..., \kappa_{N-1}^0$ in (47) are well-known, see [13-16], and we only mention that the perturbation of the null eigenvalues by the Dirichlet conditions (10) is evaluated in [15, 16] as follows:

$$\kappa_p^h = O(h), \quad p = 1,2,3$$

The justification procedure of the asymptotic forms

 $\kappa_j^h = k_j(\psi(h)) + O(h^{\delta}), \quad j = N, N+1, \dots$ (48)

for the eigenvalues in the sequence (12) above the threshold (5) is much more complicated. To construct a proper approximation pattern of an eigenmode of the problem (2), (10), (11), we add to an eigenmode $u_{(i)}^0$ with a natural frequency (19) the displacement field

$$c_{(-)}^{re}(h)\,\chi(x_1)\,u_{(-)}^{re}(x) \tag{49}$$

with the very singular behavior but the small coefficient $r^{re}(h) = O(ht_{+})$

$$c_{(-)}^{re}(h) = O(h^{r+})$$

calculated through the system (35) of linear algebraic equations with the entries $c_{(\pm)}^{im}$ taken from the representation (28), (26), (39) of the chosen vector function $u_{(j)}^0$. The term (49) brings sufficiently small discrepancy into the problem (2), (19), (11) so that general results of the spectral theory of self-adjoint operators in Hilbert space, see [5, Ch. 6], provide the desiered asymptotic representation (48) with the exponent $\delta = t_+ > 0$.

It is worth to mention that the proposed structure of the approximate eigenmode with the singular term (49) explains our procedure in Section 3 to impose the "strange" requirement (34) and to derive the algebraic system (35) which leads to the key relationship (36).

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MICRO AND NANOSHUNGITES – PERSPECTIVE MINERAL FILLERS FOR RUBBER COMPOSITES USED IN THE TIRES

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Abstract. Physical-mechanical properties of rubber filled by mineral filler (micro and nanoparticles of shungite) were studied experimentally. To date, shungite is one of the most promising materials used in the tire industry as active reinforcing fillers. Experiments on uniaxial tensile at break showed that input of this filler leads to a significant increase in rubber strength. Investigation of thermo-viscoelastic properties of these materials using dynamomechanical analyzer (DMA) were also carried out. As a result, the dynamic and viscous modulus dependences on the frequency (at 20° C) and their temperature dependences (from -50 to $+100^{\circ}$ C) were constructed.

Keywords: rubber composite, shungite filler, strength, dynamo-mechanical analyzer

1. Introduction

Carbon black (technical carbon) and white soot (hydrated silicon dioxide $mSiO_2 \cdot nH_2O$) are traditionally the most common fillers (reinforcing agents) of elastomeric composites based on natural and synthetic rubbers. The incorporation of these fillers into elastomers significantly improve their mechanical characteristics, especially the strength and stress-strain behavior of the material. To date, these effects have been well studied, and it can be said that this approach to the modifying rubber properties "has reached its ceiling" [1 – 3].

The further progress in this area requires a continuous search for new unconventional fillers [4 - 7]. One promising direction is the use of dispersed clay minerals (monmorillonite, halloysite, palygorskite, shungite, etc.) [8 - 16]. This allows to vary the shape of filler particles in a natural way depending on the task and according to the peculiar structure of these materials. For example, dispersion of montmorillonite produces ultra-thin plates [17, 18], palygorskite – needle-like particles [19 – 20], shungite – globules [21].

It should be noted that all the aforementioned mineral fillers are made from loose and soft sedimentary rocks (Mohs hardness from 1 to 4). At the same time, the filler particles obtained after dispersing the original mineral are much more rigid and durable than their progenitor. That is, the "low hardness" of the mineral is one of the signs of its good dispersibility.

The input of clay dispersed particles into rubber allows not only to improve its physical and mechanical characteristics, but also to give it a number of additional important operational properties: increased thermal stability, resistance to burning, low diffusion permeability, ecological purity and relative cheapness of production [22, 23].

At its core, these materials represent a complex structural heterogeneous systems consisting of a low-modulus highly elastic matrix, which embedded by a much more rigid and

durable particles of the particulate filler. Such materials are characterized by a complex mechanical behavior (finite deformations, nonlinear elasticity, viscoelasticity), which is caused by a different nature reversible and irreversible structural changes occurring under deformation [24, 25]. Currently, elastomer composites with various mineral fillers are the subject of intensive research, both experimental and theoretical [26 - 30]. As for application, the most promising direction of using such materials is the production of automobile tires.

2. The object of study

The main object of research were elastomeric composites with a dispersed filler made of micro and nanoshungite dispersed particles. Shungite is a sedimentary mineral formed from organic bottom sediments in freshwater reservoirs (sapropel). As for their structure, shungites are natural composites with a uniform distribution of highly disperse crystalline silicate particles in a carbon matrix [21, 31]. Depending on a deposit, the composition of shungite rocks can vary within fairly wide limits. On average, these materials contain about 60-70%-wt. of silicates and 30%-wt. of shungite carbon with an admixture of other inorganic substances (< 4%-wt., Al₂O₃, FeO, MgO, CaO, etc.) [32].

Shungite carbon is a mixture of various allotropes of carbon, whose crystal lattices are joined with amorphous carbon. It is reliably established that the shungite carbon in the rock is lined up by globules connected together (that is, particles of approximately spherical shape). The diameter of the shungite globules is about 10 nm (which is unique for materials of natural origin). There is a strong bond between the carbon and silicate components. The rock is characterized by high density $(1.9-2.4 \text{ g/cm}^3)$, chemical resistance and electrical conductivity ($(1-3)\times10^3$ S/m), hardness on mineralogical Mohs scale is 3.5-4 [33-36].

Such structure and composition impart a number of unusual physicochemical and technological properties to shungite material. The particles of the shungite powder contain different phases with respect to polarity. Due to the bipolarity, powders of shungite rocks mix well practically with all known substances (aqueous suspensions and fluoroplastics, rubbers, resins and cements, etc.). Therefore, they are one of the most promising fillers in terms of universality.

Currently, shungite is being used in the tire industry to produce active and semi-active fillers of a new generation. In general, the experimental testing of shungite in rubber compounds revealed the following main effects [37 - 40]

1) Improving the ability of rubber compounds to process (in comparison with carbon black and white soot).

2) Shungite-filled rubber has improved dynamic properties: resistance to growth of cracks in bending with puncture, reduced heat generation under alternating bending, dynamic endurance under angular rotation.

3) Filling rubber with shungite significantly increases their thermal and fire resistance.

The main goal of this work was to study experimentally the strength properties of shungite-filled rubbers depending on the size of the filler particles and their concentration, as well as their thermo-viscoelastic behavior using the dynamo-mechanical analyzer (DMA).

Experimental studies were carried out on samples of synthetic butadiene-styrene rubber SBR-1500, filled with dispersed shungite particles, shredded to micro and nano-state in the planetary ball mill. The average characteristic size of the microshungite particles was about 500 nm, nanoshungite – 60-80 nm. The volume concentration (ϕ) of microfiller was equal to 10% (phr = 25), 18% (phr = 65) and (phr = 105), for the nanofiller ϕ = 18% (phr = 65). All particles were pretreated with a surfactant (3-Mercaptopropyltriethoxysilane) to improve the interfacial adhesion between the filler and the matrix (and improving the overall strength of the composite). The elastomeric compositions were prepared in the standard laboratory mixer

HAAKE Rheomix. All samples were manufactured at the Institute of Applied Mechanics RAS (by Yu.V. Kornev).

3. Experiment and results discussion

Experimental studies of shungite-filled elastomers consisted of two stages: 1) uniaxial stretching prior to rupture; 2) tests on the dynamo-mechanical analyzer (DMA).

Experiments on uniaxial stretching were carried out using the universal tensile testing machine Testometric FS100kN CT. Samples were manufactured in accordance with the standard ISO 527-25A with working part $10 \times 2 \times 2$ mm. During the test, each sample was monotonically stretched to a break at a deformation rate of 25%/min. 9-12 samples were tested for each particle size and filler concentration. The averaged results of the experiments are shown in Fig. 1.



Fig. 1. Nominal stresses σ^0 versus extension ratio λ at stretching of elastomers filled with micro- and nanoshungite particles. Microshungite filler (black lines): $\varphi=0\%$ (1), 10% (2), 18% (3), 27% (4); nanoshungite filler (gray line) – $\varphi=18\%$ (5)

It was found that the addition of micro-shungite filler to the rubber leads to increase in the composite strength. At the same time, its deformability grew too, but not so much (by about 10-30%).

A more interesting picture is observed for nanoshungite filler. Comparison of dependencies 3 and 5 in Fig. 1 shows, that at the same volume concentration of 18%, the use of the nanoshungite filler increases the strength of material more than 2 times compared with the microshungite and 8.5 times with respect to the pure elastomer (see curve 1 in Fig. 1). The limiting deformations of micro- and nanoshungite rubbers turned out to be quite close. From the structural point of view, the main difference between micro and nano shungite is that the particles of the latter have approximately 4 times the specific surface area. That is, it can be argued that an increase in the specific surface area of the filler improves stiffness and the strength characteristics of the material (provided good adhesion (chemical affinity) between the matrix and the dispersed phase). These results are consistent with known literature data on testing of filled elastomers with other clay fillers [29].

The thermo-viscous-elastic properties of these composite materials were investigated in the second stage. The experiments were held on a dynamo-mechanical analyzer DMA/STDA861e (METTLER TOLEDO STAR^e). This device allows obtaining information about the change in the viscoelastic characteristics of the material under the action of a dynamic cyclical load (linear viscoelasticity model) for given temperature values from -150 to $+500^{\circ}$ C. Rectangular samples were used for the tests: base (working part) 10 mm, width 3 mm and thickness 2 mm. One-point loading scheme was applied: cyclic uniaxial stretching–compression of a pre-stretched sample with dynamic load applied according to a harmonic law.

The range of assigned frequencies f varied from 1 to 20 Hz, which corresponds to the rolling speed of a standard automotive wheel (landing diameter 15 inches) in the range from 6 to 136 km/h, respectively. The amplitude of specimen deformations ε_0 was set at 3% in all cases.

As a result, the dependences of the dynamic (E') and viscous (E'') modules on the loading frequency f were plotted. Their temperature dependences $(-50 \text{ to } +100^{\circ}\text{C})$ at a constant frequency of 13 Hz (which corresponds to approximately 90 km/h) were built too. The corresponding graphs are shown in Figures 2-4. The analysis of results obtained by DMA showed the following.

Frequency tests. The addition of micro-shungite filler to rubber promoted an increase in both E' and E'', and with concentration growth this effect intensified. The replacement of microparticles with a nanofiller (at the same concentration) also contributed to an increase in the values of these characteristics (curves 3 and 5 in Fig. 2). It was also found that in this frequency range the dynamic and viscous modules retained almost constant values (increasing slightly with φ rising). Thus, we can assume that the studied rubber composites have sufficiently stable viscoelastic characteristics in this frequency range of tire rotation.



Fig. 2. Frequency dependences of dynamic (*E'*) and viscous (*E''*) modules for rubbers filled with micro and nanoshungite particles. Microshungite filler (black lines): $\varphi=0\%$ (*I*), 10% (*2*), 18% (*3*), 27% (*4*); nanoshungite filler (gray line) – $\varphi=18\%$ (*5*)

Temperature tests. The conducted studies showed that all samples demonstrated the stability of their mechanical characteristics at temperatures in the range of about -25° C and above, that is, they are quite suitable for operation in temperate climates.

A sharp increase in both the dynamic and viscous modules (by several orders of magnitude) occurred in the rubbers filled with micro and nanoshungite if the temperature dropped below -30° C. The values of E' and E'' also increased with the filler concentration growth, but, interestingly, the effect of "cold amplification" on nanoparticles was somewhat weaker than for microshungite for the same concentration (curves 3 and 5 in Fig. 3). The pure

elastomer was much more stable: E' at t= -50°C increased approximately 15 times, and E' - in 70.

The analysis of the temperature dependences of the loss tangent ($\tan \delta = E''/E'$) (Fig. 4) showed that when both in case of micro and nanoshungite fillers added, the characteristic peaks corresponding to the glass transition temperature shifts toward increasing it: from -45°C (pure elastomer) to -25°C (volume concentration 27%).



Fig. 3. Temperature dependences of dynamic (*E'*) and viscous (*E''*) modules for rubbers filled with micro and nanoshungite particles. Microshungite filler (black lines): $\varphi=0\%$ (*1*), 10% (*2*), 18% (*3*), 27% (*4*); nanoshungite filler (gray line) – $\varphi=18\%$ (5)



Fig. 4. Temperature dependences of loss tangent for rubbers filled with micro and nanoshungite. Microshungite filler (black lines): $\varphi=0\%$ (1), 10% (2), 18% (3), 27% (4); nanoshungite filler (gray line) – $\varphi=18\%$ (5)

Consequently, the use of tires with only such fillers in such low temperatures is quite problematic – some special additives are needed in the tire compound in this case.

4. Conclusions

The addition of dispersed mineral filler from micro and nanoshungite to tire rubber improves their strength and deformability, moreover in the case of nanoparticles this effect is enhanced. Studies of these rubber composites on dynamo-mechanical analyzer showed that they have stable viscoelastic properties at temperatures above -25 $^{\circ}$ C, that is, they are quite suitable for operation in temperate climates.

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OPTIMIZATION OF SURFACE ROUGHNESS OF DUPLEX STAINLESS STEEL IN DRY TURNING OPERATION USING TAGUCHI TECHNIQUE

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Abstract. This paper presents the results of experimental work carried out in dry turning operation of nitrogen alloyed duplex stainless steel ASTM A 995 Grade 5A. In this investigation, the cutting parameters considered were cutting speed, feed rate and depth of cut. The effects of these cutting parameters on the surface roughness were analyzed using Taguchi technique. The results revealed that the feed rate is the most important parameter affecting the surface roughness, followed by cutting speed and depth of cut. The minimum surface roughness was obtained when the process parameters were set at their optimum values.

Keywords: duplex stainless steel, dry turning, surface roughness, Taguchi technique

1. Introduction

Stainless steels are iron-base alloys that contain a minimum of approximately 11% Cr, the amount needed to prevent the formation of rust in unpolluted atmospheres. Duplex stainless steels (DSSs) are chromium-nickel-molybdenum alloys that are balanced to contain a mixture of austenite and ferrite and are magnetic. But their machinability is more difficult than other alloy steels due to the reasons like low heat conductivity, high built up edge formation tendency, high deformation hardening and so on. DSS combines the benefits of both Ferritic stainless steel (FSS) and austenitic stainless steels (ASS) by proper balancing of ferrite and austenite. [1]. Machinability aspect is importance for manufacturing engineers to know about the machinability of a work material so that the processing can be planned in an efficient manner. Modern DSS grades tend to be difficult to machine, by virtue of their higher austenite and nitrogen contents. The use of DSSs has been increased because of their high strength, higher pitting corrosion resistance equivalent and stress corrosion resistance. DSSs are used in desalination plants and other industrial applications [2]. DSSs are extensively being used within a number of industry sectors outside desalination, e.g. chemical tankers, pressure vessels, storage tanks and oil and gas, petrochemical, pulp and paper, pollution control industries and civil engineering applications. The DSSs are less costly due to lower contents of mainly nickel and molybdenum, and they are excellent engineering materials [3].

Ciftci [4] investigated the machining characteristics of AISI 304 and AISI 316 ASSs using coated carbide tools. They reported that the increase in cutting speed decreased the surface roughness values until a minimum value and beyond which they increase. Korkut et al. [5] carried out turning tests to determine optimum machining parameters for machining of ASS. They reported that the Surface roughness values were found to decrease with increasing cutting speeds. Xavior et al. [6] investigated the influence of cutting fluids on tool wear and

surface roughness during turning of AISI 304 with carbide tool. The use of coconut oil as cutting fluid improved the surface roughness during turning process. Kaladhara et al. [7] used Taguchi method to determine the optimum process parameters for turning of AISI 304 ASS on CNC lathe using coated cemented carbide cutting insert. Their results revealed that the cutting speed was the dominant parameter which affects the surface roughness. Koyee et al. [8] conducted turning tests on ASS and DSSs applying Taguchi coupled Fuzzy Attribute Decision Making (FMADM) methods for optimize the surface roughness. They found that the feed rate was the predominant parameter which affects the surface roughness. Selvaraj et al. [9] conducted turning experiments to optimize the cutting force, surface finish, and tool wear of cast DSS. They reported that higher cutting speed and lower feed rate gave lower surface roughness and cutting force.

From the literature stated above, it is clear that many research works have been carried out in the machining of ASS. But few reports could be found on the machining of DSS and the machining of nitrogen alloyed DSS are yet to be investigated. Surface roughness is the vital machinability index to evaluate the machining characteristics of the materials. Therefore in this work the machining studies of nitrogen alloyed DSS are carried out to understand the influence of the cutting speed, feed rate and depth of cut on the surface roughness using Taguchi technique.

2. Taguchi method

Taguchi method provides a simple, efficient and systematic approach to determine optimal machining parameters. Taguchi method uses an orthogonal array (OA) to study the entire process with only a small number of experiments. The Taguchi design method can be divided into three stages: system design, parameter design, and tolerance design. The second stage-the parameter design-is considered to be the most important stage [10, 11]. Several researchers have been applied Taguchi technique to optimize the cutting parameters in various machining operations like turning, end milling, drilling, flow forming etc in various alloys [11-16].

3. Experimental procedure

Work Piece Material. The work piece material selected for investigation was the cast nitrogen alloyed DSS ASTM A 995 grade 5A with the chemical composition as shown in Table 1. The mechanical properties of the material investigated are given in Table 2.

Tuble 1. Chemieur composition of the first 11,990 grade of 1,000 (((++,0))									
С	Si	Mn	S	Р	Cr	Ni	Mo	Ν	Fe
0.028	0.67	0.87	0.005	0.028	25.10	6.63	4.16	0.17	Bal

Table 1. Chemical composition of ASTM A 995 grade 5A DSS (Wt %)

Table 2. Mechanical	properties of ASTM	A 995 grade 5A DSS
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Tensile Strength (MPa)Yield Strength (MPa)		Elongation (%)	Hardness (BHN)	
741	546	32.2	223	

Machining process. The turning tests are conducted on a Kirloskar Turn master-35 Lathe with a power rating of 3HP. The power rating of the variable feed motor is 1HP. The variable speed and feed controller are used to adjust the speed and feed rates. The diameter and length of the cylindrical work piece used in the turning experiments are 80 mm and 300 mm, respectively.

The cutting tools used are carbide inserts (Taegu Tec make) coated with TiC and TiCN with a specification of SNMG 120408 MT TT5100. The inserts are clamped on a pin and hole

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type tool holder (Taegu Tec make) with a specification of PSBNR 2525M12. The tool holder is shown in Fig. 1. The basic forms and geometries of the tool insert are shown in Fig. 2. The dimensions of the inserts are given in mm. Surface roughness was measured using a portable TIME surface roughness tester (TR100). A cut-off length of 2.5 mm was used for taking the surface roughness measurements. The experiments were conducted without the application of cutting fluid (dry turning).



Fig. 1. Tool holder



l = 12.7, d = 12.7, t = 4.76 and R = 0.8

Fig. 2. Turning tool insert

Plan of experiments. There are several parameters that could be considered for machining of a particular material in turning operation. However, the review of literature shows that cutting speed, feed rate and depth of cut are the most significant cutting parameters to control the turning process. Hence in the present study cutting speed, feed rate and depth of cut are selected as the machining parameters while the other parameters such as nose radius and tool angles are kept as constant [11, 17, 18]. For 3 levels and 3 factor experiments, the turning tests are planned using the Taguchi's L₉ OA. For turning DSS material using carbide cutting tool, the cutting speed range is 80-120 m/min as per the standard published by International Molybdenum Association (IMOA 1999). Based on the tool manufacturer recommendation, preliminary experiments are conducted and feasible range of feed rate (0.04)

to 0.12 mm/rev) and depth of cut (0.4 to 1.2 mm) are selected for the present study. The experiments are conducted at three different cutting speeds (80, 100 and 120 m/min) with three different feed rates (0.04, 0.08 and 0.12 mm/rev) and three different depth of cuts (0.4, 0.8 and 1.2 mm). The cutting parameters and their levels in dry turning operation are indicated in Table 3. The experimental layout using L₉ OA for dry turning is shown in Table 4.

Symbol	Cutting parameters	Level 1	Level 2	Level 3
V	Cutting speed (m/min)	80	100	120
F	Feed rate (mm/rev)	0.04	0.08	0.12
D	Depth of cut (mm)	0.4	0.8	1.2

Table 3. Cutting parameters and their levels in dry turning operation

Table 4. Experimental layout using L_9 OA for dry turning operation					
Experimental number	Cutting parameter level				
	V	F	D		
1	1	1	1		
2	1	2	2		
3	1	3	3		
4	2	1	2		
5	2	2	3		
6	2	3	1		
7	3	1	3		
8	3	2	1		
9	3	3	2		

Table 4	Experimental	lavout using	L ₀ OA	for dry	<i>i</i> turning	operation
1 auto 4.	Барегинсица	layout using	LgOA	101 ul y	, turning	operation

4. Analysis of Experimental Results

The experiments are conducted according to a 3-level and 3-factor L₉ OA. The experimental results for surface roughness during dry turning of 5A grade DSS is given in Table 5. The experimental results are analyzed to find out the main effects and their difference between level 1 and 2, level 2 and 3 and level 3 and 1 of the input parameters on the surface roughness. In the present study, Taguchi analysis is conducted using average-of-results methodology. Design of experiment software Qualitek-4 is used for this analysis.

In order to calculate the main effects and their differences, first the overall mean of the surface roughness is calculated by using the equation (1) discussed by Phadke [19].

Mean Ra $=\frac{1}{9}\sum_{i=1}^{9}$ Ra $= 1.249 \,\mu\text{m}.$ (1)

The main effect of cutting speed, V at level 1 (i.e., = 80 m/min), on surface roughness is calculated by using the Equation (2) discussed by Phadke [19].

Mean Ra for V at level 1 =
$$\frac{Ra1 + Ra2 + Ra3}{3}$$
 = 1.293 µm. (2)

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Exp. No.		$R_{a}(\mu m)$		
	V	F	D	
1	1	1	1	1.18
2	1	2	2	1.29
3	1	3	3	1.41
4	2	1	2	1.12
5	2	2	3	1.21
6	2	3	1	1.24
7	3	1	3	1.22
8	3	2	1	1.23
9	3	3	2	1.34

Table 5. Experimental results for surface roughness during dry turning operation

The main effects and their difference between levels associated with the surface roughness of 5A grade DSS during dry turning operation is given in Table 6.

Eastars	Level 1	Level 2	Level 3	Difference between levels			
Factors	(L ₁)	(L ₂)	(L ₃)	L_2 - L_1	L_3-L_1	L_3-L_2	
V (mm/min)	1.293	1.189	1.263	-0.104	-0.030	0.073	
F(mm/rev)	1.173	1.243	1.330	0.070	0.157	0.086	
D (mm)	1.216	1.250	1.279	0.034	0.062	0.028	

Table 6. Main effects and their differences on the surface roughness in dry turning operation

During dry turning of 5A grade DSS, the change of cutting speed from 80 to100 m/min decreases the main effects of surface roughness from a mean value of 1.293 to 1.189 µm. The change of cutting speed from 100 to 120 m/min increases the main effects of surface roughness from a mean value of 1.189 to 1.263 µm. Generally surface finish increases with increase of cutting speed. At lower cutting speed (80 m/min), surface finish is poor due to built-up edge formation tendency. When the cutting speed is increased from 80 to 100 m/min, the built-up edge size starts decreasing and disappears owing to increased tool temperature. However, as the cutting speed increases from 100 to 120 m/min, the tool temperature increased and softened the tool materials. Hence abrasive, adhesive and diffusive wear are occurred in the tool. Hence, at higher cutting speed, surface finish is reduced due to the tool wear [9, 20]. Therefore, medium cutting speed (100 m/min) is the optimal cutting speed which gives better surface finish in the present work. The change of feed rate from 0.04 to 0.08 mm/rev increases the main effects of surface roughness from a mean value of 1.173 to 1.243 µm. The change of feed rate from 0.08 to 0.12 mm/rev increases the main effects of surface roughness from a mean value of 1.243 to 1.330 µm. The change of depth of cut from 0.4 to 0.8 mm increases the main effects of surface roughness from a mean value of 1.216 to 1.250 µm. The change of depth of cut from 0.8 to 1.2 mm increases the main effects of surface roughness from a mean value of 1.250 to 1.279 µm. The surface roughness value increases with increase in feed rate and depth of cut. As the feed rate and depth of cut is increased, the area of contact between tool and work and the volume of material removed by the tool increases. Hence cutting force increases which leads to increase in surface roughness.

The main effects and their difference between levels of the cutting parameters on the surface roughness of 5A grade DSS during dry turning operation is shown in Fig. 3. The

relative slopes of linear graphs indicate significance of the cutting parameters [15]. Here the slope of the line showing the influence of the feed rate is higher compared to the slope of the cutting speed and depth of cut. Hence, the feed rate is the most significant cutting parameter for surface roughness followed by the cutting speed and the depth of cut. The lowest main effect for surface roughness is obtained when the cutting speed is at level 2, feed rate at level 1 and depth of cut at level 1. Therefore the optimal cutting parameters for surface roughness are the cutting speed at level 2 (100 m/min), the feed rate at level 1 (0.04 mm/rev) and depth of cut at level 1 (0.4 mm).



Fig. 3. Main effects of the design parameters on surface roughness during dry turning operation

At lower cutting speed, the built-up edge formation tendency is more. Therefore, the cutting speed has more influence on the surface roughness at lower cutting speed. At higher cutting speed, the built-up edge formation tendency is decreased and disappeared. Therefore, the cutting speed has less influence on the surface roughness at higher cutting speed.

The average surface roughness, Ra is given by the following equation discussed by Juneja et al. [21].

Average surface roughness,
$$Ra = \frac{0.2566 f^2}{r_n}$$
. (3)

Here, f is the feed rate in mm/rev and r_n is the nose radius in mm.

In the present work nose radius (r_n) is kept as constant. Hence, from the equation (3) surface roughness depends only on feed rate. The equation (3) does not consider the effects of cutting speed and depth of cut. Hence, this equation does not give correct results in practical applications. Basically, surface roughness is correlated strongly with machining parameters such as cutting speed, feed rate and depth of cut in turning operation. Hence, for more accurate results surface roughness model is developed by researchers using regression method and Response surface methodology (RSM).

The results of the ANOVA for the surface roughness of 5A grade DSS in dry turning operation is given in Table 7. It can be observed that the feed rate is the most significant cutting parameter affecting the surface roughness in dry turning operation of DSS. The contribution order of the cutting parameters for affecting the surface roughness is feed rate, cutting speed and then depth of cut. ANOVA results show that the feed rate, cutting speed and depth of cut affect the surface roughness by about 61%, 28% and 10%, respectively.

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Cutting Parameter	DOF	SS	MS	F-Ratio	Contribution (%)
V	2	0.016	0.008	107.761	27.95
F	2	0.036	0.018	234.897	61.24
D	2	0.006	0.003	32.278	9.76
Error	2	0.002	0.001		1.05
Total	8	0.060			100

 Table.7 ANOVA results for surface roughness during dry turning operation

Table 8 Or	otimum	condition	for	minimum	surface	roughness	during a	drv	turning	operation
1 4010.0 0	Junum	contantion	101	mmmun	Surface	rouginess	uuring	ur y	turning	operation

Factor	Level description	Level	Contribution
V	100	2	-0.059
F	0.04	1	-0.076
D	0.4	1	-0.033

Table 8 gives the optimum cutting conditions for achieving minimum surface roughness for 5A grade DSS during dry turning operation. It reveals that for optimal surface roughness, the cutting speed should be at level 2, the feed rate should be at level 1 and the depth of cut should be at level 1. The total contribution from the three input parameters is -0.168. It provides the contribution that a parameter has made to improve the expected response. The current grand average of performance is 1.249 μ m. It is the overall mean of all trials. Expected surface roughness value at optimum condition is 1.08 μ m. Experimental surface roughness value at optimum condition is 1.03 μ m.

5. Conclusions

The Taguchi technique was applied to find the optimal process parameters of nitrogen alloyed duplex stainless steel during dry turning process. The variables affecting the surface roughness according to their relative significance were the feed rate, the cutting speed and the depth of cut.

The ANOVA results revealed that the feed rate, the cutting speed and the depth of cut were affecting the surface roughness by about 61%, 28% and 10%, respectively. The optimum surface roughness was obtained when the cutting speed was at 100 m/min, the feed rate at 0.04 mm/rev and the depth of cut at 0.4 mm. It was found that the optimum levels of cutting parameters ensured significant improvement in the surface finish.

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FULLERENE MOLECULE AS A NANOSIZE QUANTUM SYSTEM

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Abstract. It is shown that a strong Coulomb and exchange interactions between π electrons in a fullerene molecule lead to the localization of these electrons, quantization of their energies, and a highly correlated state manifesting itself in the formation of electron crystals. In this approximation the fullerene molecule is a nanosize quantum system consisting of a positively charged rolled-up carbon backbone surrounded by three electron crystals: (i) two crystals formed by π electrons in the 2 p_z state that participate in the π bond formation through the resonance of structures and are located on the convex and concave sides of the molecule, and (ii) the crystal formed by pairs of π^* electrons excited into the 2p_z 3s state and participating in the formation of nonresonant π^* bonds. The chemical activity and physical properties of such a system are determined by the crystal formed by electron pairs.

Keywords: fullerenes, highly correlated electron state, electron crystals, nanosize quantum system

1.Introduction

The π electron state in the fullerene molecule is typically considered in the approximation of weakly interacting particles and is characterized by a set of molecular energy levels for π electrons near E_F.

However, it is difficult to explain a number of rather unusual experimentally observed properties of the molecule in this approach. First of all, this concerns the molecule chemical activity. In contrast to benzene which consists of one carbon hexagon and is characterized by a negative electron affinity (-1.1eV), a fullerene molecule containing 20 hexagons shows a positive electron affinity (+2.7eV) [1]. As a consequence, the molecule is capable of accepting up to 12 additional electrons (without noticeably changing its icosahedral shape), but hardly loses electrons [2, 3].

In addition, the molecule demonstrates a pronounced selectivity of attachment sites [4], a high polarizability [5], and the ability to pass into an excited state [6]. The molecule is also characterized by a complex multistage ionization process when exposed to a laser radiation. This process is often accompanied by the formation of a short-lived triplet state [7], delayed ionization [8], and fragmentation of the molecule through the loss of neutral C_2 molecules [8, 9]. Besides, the absorption of one energy quantum often results in a simultaneous emission of two electrons [10].

It is also difficult to explain: (i) the rotation of molecules when they come closer to each other (a disordered rotation at high temperatures and a synchronous rotation at low temperatures) [11, 12]; (ii) excitation of Ridberg states [13]; (iii) a considerable scatter in the lengths of bonds between carbon atoms observed by neutron diffraction [14].

The attempts to explain these experimental facts led to the assumption that strong electron correlations can exist in the molecule [10]. The assumption of the presence of strong

intramolecular interactions resulted also from the observation of superconductivity in doped solid fullerenes [15]. However, the character of the interactions still remains unclear.

The hypothesis has recently been put forward [16] that the exchange and strong Coulomb interactions between π electrons in an atomically flat carbon monolayer (graphene) can lead to their strongly correlated state which manifests itself in the formation of electron crystals.

Since the basis of the fullerene molecule is a carbon monolayer with π electrons that perform the same function of resonant π bonding as in a flat monolayer, it can be supposed that the state of π electrons in the molecule must be similar to their state in the monolayer.

The goal of our study was to show that in the approximation of strongly interacting π electrons the fullerene molecule, as well as the flat carbon monolayer, is a quantum system with π electrons that form electron crystals.

2. Fullerene molecule in the approximation of strongly interacting π electrons

It was shown in [16] that under the influence of exchange and strong Coulomb interactions between the π electrons these electrons are localized on carbon atoms and form a spinpolarized electron crystal on each side of the carbon backbone. It would seem that exactly the same state of π electrons and on the same terms as in [16] could also be expected in a fullerene molecule, since the molecule is formed by the rolled-up carbon monolayer. However, as also shown in [16], the process of rolling up of the carbon backbone under the condition of a strong interaction between electrons is accompanied by a change in the state of a part of π electrons: they are pushed out from the π electron crystal plane to the convex side of the curved carbon backbone and are excited from the $2p_z$ state into the hybrid $2p_z$ 3s one. The $2p_z$ 3s state is more extended in space and is higher in energy. The carbon atoms to which such excited electrons belong pass into a new hybridization state sp² + $2p_z$ 3s (see Fig. 1).



Fig. 1. Two states of hybridization of carbon atom in the fullerene molecule: sp^2+2p_z (a) and sp^2+2p_z3s (b)

According to [16], the ordering of such excited carbon atoms in the lattice can be accompanied by the formation of nonresonant π bonds between neighboring atoms, i.e., the formation of pairs by the excited π electrons, and also the formation of quasi-1D crystals from these pairs. By analogy, it can be expected that quasi-1D π -electron pair crystals will be formed on the convex side of the fullerene molecule whose carbon backbone is rolled-up to a truncated icosahedron.

As for the two spin-polarized π -electron crystals in the $2p_z$ state, mentioned above, they will have a quasi-spherical shape in the fullerene molecule since they will repeat the shape of the carbon backbone. Under a strong Coulomb interaction between π -electrons the ratio of squares of radii for these quasi-spherical crystals will be determined by the equality of electron densities on both sides of the rolled-up backbone. In order to achieve this equality of densities, a part of π electrons of the internal electron crystal must pass to the convex side of

the molecule and must be excited into the hybrid $2p_z$ 3s state (Fig. 1). Thus, the number of π electrons on two sides of the carbon backbone of the molecule will be different.

It is possible to find the number of such excited π electrons and their location in the fullerene molecule by constructing resonant structures of the Kekule type. It is known that the number of such structures for the fullerene molecule is very high. However, if we take into account the spin ordering of π electrons which arises due to the exchange interaction between them, the number of such resonant structures for the molecule decreases to nine. One of such structures is presented in Fig. 2a, where the projection diagram of the molecule is shown.



Fig. 2. Projection diagram of fullerene molecule: a) One of resonance structures of the molecule. Black circles show the carbon atoms the π electrons of which participate in resonant π bonding. Open circles are carbon atoms the π^* electrons of which do not participate in resonant π bonding. Double and single lines denote double ($\sigma + \pi$) and single bonds (σ) of the resonant bond state, respectively. Heavy lines correspond to double bonds between excited carbon atoms ($\sigma + \pi^*$). Dashed lines are single bonds between excited and unexcited atoms (σ). The arrows show the electron spin direction. b) Schematic representation of distortions of hexagons and pentagons, and the arrangement of quasi-1D crystal formed by π^* electron pairs. Single lines correspond to resonant bonds ($\sigma + \pi^*$)

The construction of such resonant structures which differ only in the arrangement of double and single bonds proved to be surprisingly informative. It allowed us to determine the multiplicity and, hence, the length of each of 90 bonds and their location in the molecule. The bond multiplicity was calculated from the frequency of occurrence of double and single bonds

in nine resonant structures. The bond length was determined by extrapolating the known bond lengths in benzene and graphite under the assumption of a linear dependence of the length on multiplicity. Certainly, the accuracy of determining the bond length in this way is not high, but, as will be seen below, the accurate estimation of the bond lengths was not as important as revealing of the fact that there is a scatter in the bond lengths. The calculated scatter in the lengths and multiplicities is presented in Table 1.

Bond multiplicity	Number of bonds	Bond length, Å
1.0	24	1.52
1.14	18	1.48
1.29	12	1.43
1.50	12	1.41
1.57	12	1.37
1.85	6	1.35
2.00	6	1.33

Table 1. Scatter in lengths and multiplicities of bonds

It can be seen that most of the bonds (60 of 90) are characterized by different nonintegral multiplicities, which points, in particular, to a non-equivalence of positions of carbon atoms in the fullerene molecule. The remaining 30 bonds proved to be either double bonds with a nonresonant π bond (6) or single bonds (24). The scatter in the bond lengths also points to distortions of all hexagons and pentagons, except for two hexagons located at opposite points of the molecule. Their planes are parallel to each other and perpendicular to the same axis passing through their centers. These two undistorted hexagons with a bond multiplicity of ~1.30 and a bond length of ~1.43 Å form as if two poles of the fullerene molecule. In Fig. 2a, b these hexagons are developed on the plane and form the lines that limit the projection diagram of the molecule from above and below.

The presence of distorted hexagons and pentagons means that the fullerene molecule is not a regular truncated icosahedron. It can be seen from Fig. 2b that double and single bonds, i.e., the shortest and longest bonds, are located in the equatorial region relative to the molecule poles which are formed by two undistorted hexagons. It can also be seen that each distorted pentagon contains two single bonds belonging to one and the same carbon atom. This atom differs from the neighboring ones: the spin direction of its π electron cannot be determined because the spin directions of the neighboring electrons are oppositely directed (Fig. 3). In other words, the π electron of this atom cannot be spin-ordered relative to the π electrons of neighboring atoms and, hence, cannot take part in resonant π bonding.

It is this π electron that will be pushed out by the Coulomb interaction with the remaining π electrons of spin-polarized electron crystals and will be excited into the hybrid 2p_z3s state (Fig. 1). There will be 12 of such excited π electrons. Under the influence of the same Coulomb repulsion, each excited π electron will be forced to occupy only one of two hybrid 2p_z3s states located on the convex side of the molecule. As a result, the total number of electrons on the convex side of the molecule will exceed by 12 electrons their number on the concave side, i.e., there will be 36 electrons on the convex side and 24 electrons on the concave one. In all probability, this difference will ensure the equality of electron densities on both sides of the rolled-up carbon backbone under the conditions of a strong Coulomb interaction between electrons.



Fig. 3. Fragment of projection diagram of fullerene molecule. Impossibility of spin ordering of π electrons of carbon atoms (C₁ and C₂) at pentagon apexes is demonstrated. π^* electrons can form only a π^* bond between these atoms

In order to distinguish between the excited π electrons and the π electrons forming the resonant π bonds, we will denote them as π^* electrons, and the bonds they form will be denoted as π^* bonds.

The ordered arrangement of distorted pentagons and hexagons leads to an ordered arrangement of π^* bonds between excited carbon atoms and, hence, an ordered arrangement of π^* electron pairs. As a result, a quasi-1D crystal from π^* electron pairs is formed in the equatorial region of the molecule. Such a crystal consists of six electron pairs and has a peculiar zigzag-like shape (Fig. 2b).

The π^* -electron pairs of this quasi-1D crystal form negatively charged "protrusions" on the molecule surface that increase the diameter of the fullerene molecule in its equatorial region. This unscreened π^* -electron pair crystal, along with the unscreened π -electron crystal and unscreened (in some places) carbon ions, make the electric field around the molecule highly inhomogeneous.

The crystallization of all π and π^* electrons which are in definite quantum states (2p_z and 2p_z3s, respectively) makes the fullerene molecule a nanoscale quantum system of ~10 Å in diameter. The system consists of a positively charged rolled-up carbon backbone (including 12 excited carbon atoms) and the three electron crystals considered above. In contrast to the extremely unstable quantum system of a flat carbon monolayer [16], the quantum system of the fullerene molecule is stable. This stability is first of all due to the presence of the π^* electron pair crystal on the convex surface of the fullerene molecule. This crystal (i) lowers the free energy of the system by the amount of energy of π^* bonds, (ii) ensures the equality of electron densities on both sides of the rolled-up carbon backbone, (iii) partly screens the underlying π -electron crystal from external influences, (iv) converts the molecule from a radical to a non-radical (by pairing π^* electrons).

3. On properties of a nanosize quantum fullerene system

The consideration of the quantum fullerene system structure described above and the state of π electrons in it leads to some conclusions on its chemical and physical properties. Below we compare the properties predicted by our model with the properties observed experimentally.

As shown above, the carbon backbone rolling up under the conditions of exchange and Coulomb interactions between π electrons is accompanied by distortions of hexagons and pentagons and, hence, a significant scatter in bond lengths. Neutron scattering experiments with crystalline fullerene at low temperatures [14] confirm the presence of a scatter in the bond lengths. It turns out that the lengths of the bonds shared by two hexagons and hexagon-pentagon lie in the ranges 1.366-1.412 Å and 1.420-1.487 Å, respectively. These values somewhat differ from the calculated ones (see Table 1). However, an exact coincidence in the

bond lengths cannot be expected because, on the one hand, the calculation of the bond length from its multiplicity is inaccurate and, on the other hand, the accuracy of the neutron scattering data can be affected by a permanent rotation of molecules relative to each other in the crystalline phase.

It is fairly obvious that the chemical activity of the quantum system should be determined by the electron crystal formed by pairs of π^* electrons which are in the $2p_z3s$ state and are the farthest from the carbon backbone and less tightly bound to it than the π electrons in the $2p_z$ state (the difference in bond energies depends on the energy of the 3s state for carbon atom and is likely to be several electron volts). Since the hybrid $2p_z3s$ states of excited atoms are occupied incompletely, the electron affinity of this system must be positive. Moreover, in accordance with the number of free hybrid states on the convex side of the molecule, the system can be capable of accepting at least 12 more electrons. This conclusion agrees well with the experimental observation of a positive electron affinity [1] and the attachment of 12 electrons not accompanied by noticeable changes in the molecule shape [2].

The presence of π^* electrons must lead to a decrease in the work function of electron at the sites of their localization and also to a nonhomogeneity of the work function on the molecule surface. The location of π^* electrons only in the equatorial region of the molecule must result in a highly nonhomogeneous polarizability of the molecule and also the selectivity of attachment sites for other atoms. All these features were observed experimentally [4, 5].

Because of the presence of π^* -electron pairs, simultaneous emission of two electrons of one pair can occur at absorption of one quantum of energy. In all probability, this was observed in [10] and is known as a double photoemission.

Since π^* electrons belong to excited carbon atoms which are strongly coupled to each other via double bonds ($\sigma + \pi^*$) but are coupled much weaker to the carbon backbone (via single σ bonds) (Fig. 3), the molecule ionization can result in a simultaneous loss of two excited atoms. Perhaps that is why a molecule fragmentation with a loss of C₂ was observed during its ionization [9].

In addition to the twelve $2p_z 3s$ states on the convex side of the molecule, there are 12 completely unoccupied similar states on the concave side. Therefore, if an additional electron is accepted by the molecule, it can occupy one of free states, and then (in the case of π^* bond rupture) triplet electron pair can appear in an excited carbon atom (in accordance with the Hund's rule for hybrid state filling). However, such a triplet state in the fullerene molecule will be extremely unstable due to a strong Coulomb repulsion of the accepted electron from the electron crystal formed by π electrons on the concave side of the molecule. Such instability of the triplet state can apparently explain the observation of a short-lived highly reactive triplet state that appeared during electron bombardment of a fullerene molecule [7].

A strong nonhomogeneity of the electric field on the surface of the quantum fullerene system can result in a Coulomb interaction between molecules as they approach each other, i.e., the so-called configuration forces which depend on the mutual arrangement of charges in neighboring molecules arise. Possibly, these forces can cause clustering of molecules and their rotation when they come nearer to each other, which was observed in [11, 12]. Besides, the Coulomb interaction between molecules must also promote the crystallization of molecules in the structures which are more typical of ionic crystals, which is also observed experimentally (fcc at room temperature and sc at low temperatures) [14].

As for the magnetic properties of the quantum fullerene system in which there are no unpaired π electrons, the system can show only the diamagnetism associated with the orbital rotation of π electrons forming resonant bonds, like in a flat carbon monolayer [16]. However, the diamagnetic susceptibility of a fullerene molecule must be very weak because the curvature of the carbon backbone violates the parallelism of the planes of electron rotation

orbits which prevails in a flat monolayer [16]. A low diamagnetic susceptibility was observed experimentally in [17].

4. Conclusions

It has been shown that in the approximation of strongly interacting π electrons the fullerene molecule C₆₀ proves to be a nanoscale quantum system consisting of a positively charged rolled-up carbon backbone and three electron crystals with quantized energies. Two of these crystals consist of spin-polarized π electrons, have a quasi-spherical shape, and are located on opposite sides of the carbon backbone. The third crystal is quasi-1D, it consists of six pairs of π^* electrons excited into the $2p_z3s$ state and is located on the convex side of the molecule (it encircles the molecule in the equatorial region). This crystal, which is the farthest from the carbon backbone, is responsible for the chemical activity of the fullerene molecule and its physical properties, including stability. It has been shown that the chemical activity and the physical properties of such a quantum system are in good agreement with the experimental data obtained.

The possibility to explain the set of available experimental data on the fullerene molecule properties demonstrated in this paper is a serious argument speaking in favor of the proposed approach.

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RELATION OF THE OPTICAL PROPERTIES OF BORON COPPER-CONTAINING GLASSES ON THE CONCENTRATION OF LITHIUM

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Abstract. In this work, optical properties of a variety of boron host glasses with copper in relation to the lithium content from 0 to 25 % are studied. It is shown that with the increase of the lithium concentration the absorption band of Cu^{2+} increases. This fact is associated with the interaction of lithium ions in the melt with atmospheric oxygen. It is shown that the photoluminescence band shifts by more than 20 nm upon excitation at 320 nm with increasing lithium concentration. This is can be explained by the high splitting of the levels of Cu(I) under the action of lithium ions, and also with the formation of Cu^+ - Cu^+ dimers in the glass structure.

Keywords: boron copper-containing glasses, lithium content, optical properties

1. Introduction

The development and investigation of new photonic materials for «down converters» is a new research trend that grows rapidly. These materials convert the UV solar radiation to visible radiation due their luminescence by UV radiation, which allows to improve efficiency of solar cell. Silicon solar cells are not susceptible to the UV radiation. Thus, the converting of UV radiation to visible radiation increases the absorption of solar cell and consequence its efficiency.

There are several types of glass hosts that can be used for down converters. First one, there are borate-barium glasses with ions of rare earth [1]. These glasses production is expensive since the cost of rare earth reagents. Another one type of glass compositions are silicate glass with ions and clusters of silver [2]. The melt temperatures of such glasses are high (1550°C), the requirements for chemical purity of reagents are also high; in addition; cerium ions are present in their composition. Thus, glasses with ions and clusters of silver are also not cheap.

In this work, boron glasses with copper ions are proposed as an alternative to reviewed glasses [3-5]. These glasses have not expensive components, and their synthesis temperatures are 1300-1400°C. In these glasses basic luminescent components are copper ions and clusters. As shown in [6], such type of glasses can be efficient converters of solar UV radiation.

We should say a few words about the states of copper ions in glass. Copper ions can be in three states: atomic (Cu^0) , Cu(I), Cu(I). When the oxidation-reduction potential of the melt is shifted toward the reduction, an atomic copper [7] occurs in the glass. At the shift towards oxidation the bivalent Cu(II) will be released. Ions of bivalent copper have an absorption band at 800 nm. The main factor determining in which state will be the copper ions in the glass is the concentration of oxygen in the melt [8, 9].

Let us consider the luminescent properties of copper ions and clusters more in detail. The absorption bands of Cu^+ ions for different glass hosts can range from 250 to 300 nm [10], and the photoluminescence from 460 to 475 nm, 485-500 nm [11].

It has reason to suppose that the blue luminescence of 485-500 nm corresponds to a transition from the lower triplet energy level ${}^{3}E_{g}$ " formed by the splitting of the ${}^{3}Eg$ level due to the tetragonal stretching of the oxygen octahedron [11]. The change in the level splitting of the ${}^{3}E_{g}$ level (12) determines the energy of the ${}^{3}E_{g}$ level, as a result, the blue luminescence band shifts. The 540-nm luminescence band is referred to the Cu ⁺-Cu⁺ dimers (13, 14), as well as to the Cu⁺ (15) ions in a planar environment.

In [16] it is shown that lithium in potassium-alumina borate glasses promotes the crystallization and the separation of nanoparticles. Such processes occur at temperatures above the glass transition temperature. As concerns clusters, there may be a separation of copper clusters during the primary cooling of the glass after synthesis. S.A. Stepanov in his work [17] notes that for each type of glass host the pore size is different, that determines the size of the separated clusters [17].

In addition, according to the electronegativity table, lithium ions have a high field strength in comparison with sodium and potassium ions. That can lead to the destruction of covalent bonds in the glass, to the formation of non-bridging oxygens, to the deformation of structural groups in the glass, and thus to change the environment of copper ions. The changes of copper environment contributes to the changes of character of the copper ions luminescence and to the formation of copper clusters.

2. Experimental

In this work, glasses obtained by standard melting methods in a quartz crucible were investigated. The glasses were melt at 1400°C for 2 hours with a quartz stirrer mixing. Further, the glasses were cooled in a muffle from 400 °C to room temperature for 12 hours. The glass composition was $(25-x)K_2O-xLi_2O-50B_2O_3-25Al_2O_3$ (molar %). There were additions in excess of 100% of 0.5 Cu₂O and four weight percent of ground coal as a reducing agent. The content of lithium ions was varied from 0 to 25% in steps of 5%.

For further measurements from synthesized glasses, flat-parallel samples were made. The absorption spectra from 300 to 800 nm were measured by the Avaspec 2048 spectrometer complex, photoluminescence spectra were measured on the same complex upon excitation of 320 nm. The quantum yield was measured by the Hamamatsu C9920-02G quantum yield measuring device at the same excitation wavelength.

3. Discussion

The absorption spectra of the samples are shown in Fig. 1. As can be seen, depending on the concentration of lithium, the maximum of absorption in the visible range has the glass, in which the potassium is completely replaced by lithium. It is seen from the Fig. 1 that there is an absorption band at 800 nm due to the presence of bivalent copper in the glass. With an increase in the potassium concentration, the absorption band decreases, which negates the green color of the glass, due to the transition of ions to the Cu⁺ state. As can be seen all synthesized glasses have a short-wavelength absorption edge at 350 nm, which is typical for boron glasses with copper [8, 9]. The short-wavelength absorption edge can be coupled with the presence of copper ions in the state of Cu⁺, as well as Cu⁺ -Cu⁺ dimers [10].

Also shown in the figure 2 (left), that at the concentration of 5% of lithium oxide, the absorption band at 600 nm exists, as consequence of copper nanocrystals plasmon absorption. According to [18], it is possible to shift the absorption toward larger wavelengths with an

increase in the refractive index of the surrounding medium. The absorption peak with several absorption bands is possible in the presence of elliptical nanoparticles or particles with dimensions larger than 50 nm. Under this work, this effect was not investigated in details. It should be noted that there is an anomalous formation of these copper nanoparticles just at the announced concentration of lithium ions. One can suppose that the presence of small concentration of lithium contributes to an additional increase of ability of nanoparticle formation in glass, that is, liquation. In this case, lithium exists as a liquation agent [16] rather than the component of a glass net.



Fig. 1. Optical absorption spectra of glass samples with various concentration of lithium oxide (digits)

In Figure 2 (right), the dependence of the absorption bands of bivalent copper for glasses with different concentrations of lithium ions is shown. As can be seen, the dependence is practically linear, consequently with the increase of lithium concentration the intensity of the absorption band of Cu^{2+} increases. For obvious reasons, there are no results for the glass composition with 5 % of lithium are shown since in this case the plasmon absorption band of copper nanoparticles also appears. Thus, one can say that with an unchanged concentration of the reducing agent (coal) and copper in the glass compositions, an increase in the concentration the lithium content occurs an increase in the concentration of copper ions (II).

This can be explained by the high chemical reactivity of the lithium. In a melt during the glass synthesis, lithium easy interacts with oxygen from the atmosphere above the melt, and thereby displaces the oxidation-reduction equilibrium in the melt toward the oxidation, and therefore also increases the content of bivalent copper in the melt.

The photoluminescence spectra of the samples are shown in Fig. 3. It should be taken into account that these spectra only the structure of the bands should be determined. It can be seen that all the bands have a half-width of 125 nm and have one maximum. The dependence of the magnitude of the maximum on the concentration of lithium ions is shown in Fig. 4 (left).



Fig. 2. Opticalabsorption spectra of a glass with 5 % Li₂O (left) and dependence of intensity of optical absorption Cu(II) from the Li₂O concentration (right)



Fig. 3. Photoluminescence emission spectra of glass samples with various concentration of lithium oxide (digits)

As can be seen from the luminescence bands, with a change in the lithium concentration, the maximum of the luminescence intensity shifts by 30 nm from 480 nm to 510 nm. According to the data we can suppose [6] that the peak at 480 nm in the spectrum corresponds to the luminescence of Cu^+ . For the abnormal shift more than 30 nm of the luminescence maximum in spectrum both the Cu^+-Cu^+ dimer bands and the above-mentioned tetragonal stretching of the oxygen octahedron under the action of lithium ions [11] can be responsible. Therefore, in an increase of lithium ions concentration occurs to an increase in the concentration of copper dimers and to the splitting of the levels of univalent copper.

Figure 4 (right) shows the dependence of the quantum yield on the concentration of lithium ions in the glass. It can be seen that the quantum yield decreases by more than 3 times. It can be explained by increasing of the absorption band of bivalent copper ions with the concentration of lithium increases. In this case, part of the copper ions, which could be univalent, became divalent, thereby reducing the number of luminescent centers. The

absorption centers of Cu^{2+} block the luminescence of the remaining univalent copper ions. Owing to these two factors, shown above, the quantum yield of glasses decreases as the concentration of lithium ions increases.

Thus, we can detail the basic results of this work:

1. There is an increase in the concentration of bivalent copper in glass at the transition from lithium to potassium.

2. The quantum yield decreases at the transition from potassium to lithium.

3. The maximum of the luminescence spectra changes by 30 nm - a shift to a longer wavelength occurs.

4. An increase in the concentration of lithium ions in boron glass leads to the transition of Cu^+ ions to the state of Cu^+ -Cu+ dimers, as well as to anomalous stretching of bonds of oxygen-containing octahedral groups, into which univalent copper ions enter.



Fig. 4. Photoluminescence peak wavelength dependence from lithium oxide concentration (left) and quantum yield dependence from lithium oxide concentration (right)

4. Conclusions

With an increase in the concentration of lithium in the borate glass with copper, the concentration of bivalent copper ions increases, and the luminescence band shifts from 480 to 510 nm. We suppose that lithium ions contribute to an increase in the content of oxygen groups in the melt, and contribute to a high degree of splitting of the energy levels of univalent copper ions in the glass and, possibly, to the formation of Cu^+-Cu^+ dimers.

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EFFECT OF NON-HOMOGENEITY IN A MAGNETO ELECTRO ELASTIC PLATE OF POLYGONAL CROSS-SECTIONS

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Abstract. The effect of non-homogeneity in a magneto electro elastic plate of polygonal cross sections is studied using the linear theory of elasticity. The wave equation of motion based on two-dimensional theory of elasticity is applied under the plane strain assumption of plate of polygonal shape, composed of non-homogeneous transversely isotropic material. The frequency equations are obtained by satisfying the irregular boundary conditions of the polygonal plate using Fourier expansion collocation method. The analytical results obtained in the physical domain have been computed numerically for Triangle, Square, Pentagon and Hexagonal plates. The results for stress, strain, displacements, induced electric and magnetic fields have been presented graphically.

Keywords: magneto-electro elastic cylinder, solid with polygonal cross sections, Fourier expansion collocation method, stresses/vibration, transducers, sensors/actuators, MEMS/NEMS

I. Introduction

The three dimensional vibration in plates of polygonal cross section made of smart and intelligent materials has considerable importance for a long time. The electro-magneto-elastic materials exhibit a desirable coupling effect between electric and magnetic fields, which are useful in smart structure applications. These materials have the capacity to react corresponding response due to the external stimulation and impulse load. The advantages of non homogeneous material still remain the structural integrity than the conventional composite materials under severe conditions. The composite consisting of piezoelectric and piezomagnetic have found increasing application in engineering structures, particularly in smart/intelligent structure system. The magneto-electro-elastic materials are used as magnetic field probes, electric packing, acoustic, hydrophones, medical, ultrasonic image processing, sensors and actuators with the responsibility of magnetic-electro-mechanical energy conversion.

Recently, many researchers have devoted their attention to the mechanics problems of transversely isotropic material connected with magneto-electro-elasticity. Ahmadi and Eskandari [1] investigated the vibration analysis of a rigid circular disk embedded in a transversely isotropic solid. Green's functions of a surface-stiffened transversely isotropic half-space were developed by Eskandari and Ahmadi [2]. Ahmadi and Eskandari [3] studied the axisymmetric circular indentation of a half-space reinforced by a buried elastic thin film. Eskandari et al. [4] analyzed the time-harmonic response of a surface stiffened transversely isotropic half-space. Weaver et al. studied the transient elastic waves in a transversely

isotropic Plate, Haojiang et al. [5] investigated the free axisymmetric vibration of transversely isotropic piezoelectric circular plates

Pan [6] and Pan and Heyliger [7] analyzed the three-dimensional behavior of magnetoelectroelastic laminates under simple support boundary conditions. An exact solution for magnetoelectroelastic laminates in cylindrical bending has also been obtained by Pan and Heyliger [8]. Pan and Han [9] studied the exact solution for functionally graded and layered magneto-electro-elastic plates. Feng and Pan [10] discussed the dynamic fracture behavior of an internal interfacial crack between two dissimilar magneto-electro-elastic plates. Buchanan [11] developed the free vibration of an infinite magneto-electro-elastic cylinder. Dai and Wang [12, 13] have studied thermo-electro-elastic transient responses in piezoelectric hollow structures and hollow cylinder subjected to complex loadings. Annigeri et al. [14 - 15]studied respectively, the free vibration of clamped-clamped magneto-electro-elastic cylindrical shells, free vibration behavior of multiphase and layered magneto-electro-elastic beam, free vibrations of simply supported layered and multiphase magneto-electro-elastic cylindrical shells. Gao and Noda [16] presented the thermal-induced interfacial cracking of magnetoelectroelastic materials. Hon et al. [17] analyzed a point heat source on the surface of a semi-infinite transversely isotropic electro-magneto-thermo-elastic material. The dynamic response of a heat conducting solid bar of polygonal cross section subjected to moving heat source is discussed by Selvamani [18] using the Fourier expansion collocation method (FECM). The wave propagation in a magneto-thermo elastic wave in a transversely isotropic cylindrical panel using the wave propagation approach were investigated by Ponnusamv and Selvamani [19]. Recently, Selvamani and Ponnusamy [20] have studied the wave propagation in a generalized piezothermoelastic rotating bar of circular cross-section using threedimensional linear theory of elasticity.

Bin et al. [21] analyzed the wave propagation in non-homogeneous magneto-electroelastic plates. Chen et al. [22] worked on free vibration of non-homogeneous transversely isotropic magneto-electro-elastic plate. Chakraverty et al. [23] studied the flexural vibrations of non-homogeneous elliptic plates. Tanigawa [24] presented some basic thermoelastic problems for nonhomogeneous structural materials. Li [25] discussed the magnetoelectroelastic multi-inclusion and inhomogeneity problems and their applications in composite materials. Kong et al. [26] presented the thermo-magneto-dynamic stresses and perturbation of magnetic field vector in a non-homogeneous hollow cylinder. Ding et al. [27] and Hou et al. [28] presented an analytical solution to solve the transient responses of a special non-homogeneous pyroelectric hollow cylinder for piezothermoelastic axisymmetric plane strain dynamic problems. Ibrahim [29] provided a finite element method to solve the thermal shock problem in a non-homogeneous isotropic hollow cylinder with two relaxation times.

In this paper, the effect of magnetic field and non-homogeneity in a piezoelectric plate of polygonal cross sections is studied using the linear theory of elasticity. The frequency equations are obtained by satisfying the irregular boundary conditions of the polygonal plate using Fourier expansion collocation method. The analytical results obtained in the physical domain have been computed and the numerically analyzed results for the stress, strain, displacements and induced electric and magnetic fields have been presented graphically.

2. Formulation of the Problem

We consider a homogeneous transversely isotropic magneto-electro-elastic plate of polygonal cross-sections as shown in Fig. 1. The system displacements and stresses are defined by the cylindrical coordinates r, θ and z. The governing equations of motion of the electric and magnetic conduction in the absence of body force are taken from Selvamani and Ponnusamy [22]

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{1}{r} (\sigma_{rr} - \sigma_{\theta\theta}) = \rho \frac{\partial^2 u}{\partial t^2},$$

$$\frac{\partial \sigma_{r\theta}}{\partial \sigma_{r\theta}} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2}{r^2} = \frac{\partial^2 v}{\partial t^2},$$
(1)

 $\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2}{r} \sigma_{r\theta} = \rho \frac{\sigma_{r\theta}}{\partial t^2}.$ The equation of electric conduction is given by:

$$D_{r,r} + r^{-1}D_{,r} + r^{-1}D_{\theta,\theta} = 0.$$
(2)

The equation of Magnetic conduction is given by: $B_{r,r} + r^{-1}B_r + r^{-1}B_{\theta,\theta} = 0,$ (3)

where:

$$\sigma_{rr} = c_{11}e_{rr} + c_{12}e_{\theta\theta},$$

$$\sigma_{\theta\theta} = c_{12}e_{rr} + c_{11}e_{\theta\theta},\tag{4}$$

$$\sigma_{r\theta} = 2c_{66}e_{r\theta}.$$

$$D = 2e_{-\theta}e_{-\theta} + \varepsilon_{-}F_{-} + m_{-}H_{-}$$

$$D_r = 2e_{15}e_{rz} + \varepsilon_{11}E_r + m_{11}H_r,$$

$$D_{\theta} = 2e_{15}e_{\theta z} + \varepsilon_{11}E_{\theta} + m_{11}H_{\theta}.$$
And:
(5)

$$B_{r} = 2q_{15}e_{rz} + m_{11}E_{r} + \mu_{11}H_{r},$$

$$B_{\theta} = 2q_{15}e_{\theta z} + m_{11}E_{\theta} + \mu_{11}H_{\theta},$$
(6)

where $\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{r\theta}$ are the stress components, c_{11}, c_{12} and c_{66} are elastic constants, ε_{11} are the dielectric constants, μ_{11} are the magnetic permeability coefficients, e_{31}, e_{33}, e_{15} are the piezoelectric material coefficients, m_{11} are the magnetoelectric material coefficients, ρ is the density of the material, D_r, D_{θ} are the electric displacements, B_r, B_{θ} are the magnetic displacements corresponding to the cylindrical coordinates are given by

$$e_{rr} = \frac{\partial u}{\partial r}, e_{\theta\theta} = \frac{1}{r} \left(\frac{\partial v}{\partial \theta} + \frac{u}{r} \right),$$

$$e_{r\theta} = \frac{1}{2} \left(\frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial r} - \frac{v}{r} \right),$$
(7)

where u and v are the mechanical displacements along the radial and circumferential directions.

The Electric field vector E_i is related to the electric potential E as:

$$E_r = -\frac{\partial E}{\partial r}, \ E_\theta = -\frac{1}{r}\frac{\partial E}{\partial \theta}.$$
(8)

Similarly, the magnetic field vector H_i is related to the magnetic potential H as

$$H_r = -\frac{\partial H}{\partial r}, \ H_\theta = -\frac{1}{r}\frac{\partial H}{\partial \theta}.$$
(9)

Substituting Eqs. (7) - (9) in Eqs. (1) - (6), we obtain the following stress displacement relations:

$$\sigma_{rr} = c_{11} \frac{\partial u}{\partial r} + c_{12} \left(\frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right),$$

$$\sigma_{\theta\theta} = c_{12} \frac{\partial u}{\partial r} + c_{11} \left(\frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right),$$

$$\sigma_{r\theta} = c_{66} \left(\frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial r} - \frac{v}{r} \right),$$

and

$$D_{r} = -\varepsilon_{11} \frac{\partial E}{\partial r} - m_{11} \frac{\partial H}{\partial r},$$

$$D_{\theta} = -\frac{\varepsilon_{11}}{r} \frac{\partial E}{\partial \theta} - \frac{m_{11}}{r} \frac{\partial H}{\partial \theta},$$

$$B_{r} = -m_{11} \frac{\partial E}{\partial r} - \mu_{11} \frac{\partial H}{\partial r},$$

$$B_{\theta} = -\frac{m_{11}}{r} \frac{\partial E}{\partial \theta} - \frac{\mu_{11}}{r} \frac{\partial H}{\partial \theta}.$$
(10)

The elastic constants c_{11}, c_{12}, c_{66} , magnetic permeability coefficient μ_{11} , electromagnetic material coefficient m_{11} , density ρ are characterized in terms of non-homogeneity of the material as follows:

$$c_{11} = (L+V)r^{2m}, c_{12} = Lr^{2m}, c_{66} = \frac{V}{2}r^{2m},$$

$$\mu_{11} = V'r^{2m}, m_{11} = m'_{11}r^{2m},$$

$$\varepsilon_{11} = \varepsilon'_{11}r^{2m}, \rho = \rho_0 r^{2m},$$
(11)

where L, V, V' and $\rho_0, m'_{11}, \varepsilon'_{11}$ are constants of homogeneous matter and *m* is the rational number. Substituting Eq. (11) in Eq. (10) we obtain the stress displacement equations for nonhomogeneous medium:

$$\begin{aligned} \sigma_{rr} &= r^{2m} \left[\left(\left(L+V \right) \frac{\partial u}{\partial r} + L \left(\frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right) \right) \right], \\ \sigma_{rr} &= r^{2m} \left[\left(L \frac{\partial u}{\partial r} + \left(L+V \right) \left(\frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right) \right) \right], \\ \sigma_{rr} &= \frac{V}{2} r^{2m} \left[\left(\frac{\partial v}{\partial r} - \frac{v}{r} + \frac{1}{r} \frac{\partial u}{\partial \theta} \right) \right], \\ D_{r} &= r^{2m} \left(-\varepsilon_{11} \cdot \frac{\partial E}{\partial r} - m_{11} \cdot \frac{\partial H}{\partial r} \right), \\ D_{\theta} &= r^{2m} \left(-\frac{\varepsilon_{11}}{r} \cdot \frac{\partial E}{\partial \theta} - \frac{m_{11}}{r} \cdot \frac{\partial H}{\partial \theta} \right), \\ B_{r} &= r^{2m} \left(-m_{11} \cdot \frac{\partial E}{\partial r} - \mu_{11} \cdot \frac{\partial H}{\partial r} \right), \\ B_{\theta} &= r^{2m} \left(-\frac{m_{11}}{r} \cdot \frac{\partial E}{\partial \theta} - \frac{\mu_{11}}{r} \cdot \frac{\partial H}{\partial \theta} \right). \end{aligned}$$
(12)

Substituting the Eq. (12) in the Eqs. (1) - (3), we obtain the set of displacement equations

$$(L+V)\left(\frac{\partial^{2}u}{\partial r^{2}} + \frac{1}{r}\frac{\partial u}{\partial r} - \frac{1}{r^{2}}u\right) + \frac{V}{2}\frac{1}{r^{2}}\frac{\partial^{2}u}{\partial \theta^{2}} + \left(\frac{2L+V}{2}\right)\frac{1}{r}\frac{\partial^{2}v}{\partial r\partial \theta} - \left(\frac{2L+3V}{2}\right)\frac{1}{r^{2}}\frac{\partial v}{\partial \theta} + \left(\frac{2m}{r}\right)\left((L+V)\frac{\partial u}{\partial r} + L\left(\frac{1}{r}\frac{\partial v}{\partial \theta} + \frac{u}{r}\right)\right) = \rho\frac{\partial^{2}u}{\partial t^{2}}$$
(13a)

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$$\begin{pmatrix} \frac{V}{2} \end{pmatrix} \left(\frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} - \frac{1}{r^2} v \right) + \left(\frac{2L+V}{r} \right) \frac{\partial^2 u}{\partial r \partial \theta} - \left(\frac{2L+3V}{2} \right) \frac{1}{r^2} \frac{\partial u}{\partial \theta}$$

$$+ \left(\frac{L+V}{r^2} \right) \frac{\partial^2 v}{\partial \theta^2} + \left(\frac{Vm}{r} \right) \left(\frac{\partial v}{\partial r} - \frac{v}{r} + \frac{1}{r} \frac{\partial u}{\partial \theta} \right) = \rho \frac{\partial^2 v}{\partial t^2}$$

$$\varepsilon_{11}^{'} \left(\frac{\partial^2 E}{\partial r^2} + \frac{1}{r} \frac{\partial E}{\partial r} + \frac{1}{r^2} \frac{\partial^2 E}{\partial \theta^2} \right) + m_{11}^{'} \left(\frac{\partial^2 H}{\partial r^2} + \frac{1}{r} \frac{\partial H}{\partial r} + \frac{1}{r^2} \frac{\partial^2 H}{\partial \theta^2} \right) + \left(\frac{2m}{r} \right) \left(\varepsilon_{11}^{'} \frac{\partial E}{\partial r} + m_{11}^{'} \frac{\partial H}{\partial r} \right) = 0$$
(13c)
$$m_{11}^{'} \left(\frac{\partial^2 E}{\partial r^2} + \frac{1}{r} \frac{\partial E}{\partial r} + \frac{1}{r^2} \frac{\partial^2 E}{\partial \theta^2} \right) + V^{'} \left(\frac{\partial^2 H}{\partial r^2} + \frac{1}{r} \frac{\partial H}{\partial r} + \frac{1}{r^2} \frac{\partial^2 H}{\partial \theta^2} \right) + \left(\frac{2m}{r} \right) \left(m_{11}^{'} \frac{\partial E}{\partial r} + V^{'} \frac{\partial H}{\partial r} \right) = 0$$
(13d)

3. Solution of the problem

The Eqs. (13) is a coupled partial differential equation with three displacements and magnetic and electric conduction components. To uncouple the Eqs. (13), we seek the solution in the following form:

$$u(r,\theta) = \sum \varepsilon_n \left(r^{-1} \psi_{n,\theta} - \phi_{n,r} \right),$$

$$v(r,\theta) = \sum \varepsilon_n \left(-r^{-1} \phi_{n,\theta} - \psi_{n,r} \right),$$

$$w(r,\theta) = \sum \varepsilon_n W_{n,z},$$

$$E(r,\theta) = \sum \varepsilon_n E_{n,z},$$

$$H(r,\theta) = \sum \varepsilon_n H_{n,z},$$

(14)

where $\phi_n(r,\theta)$, $\psi_n(r,\theta)$, $W_n(r,\theta)$, $E_n(r,\theta)$ and $H_n(r,\theta)$ are the displacement potentials. Substituting the Eq. (14) in (13), we get

$$(L+V)\nabla_1^2\varphi_n + 2m\left(\frac{L+V}{r}\frac{\partial\varphi_n}{\partial r} - \frac{L}{r^2}\varphi_n\right) - \rho_0\frac{\partial^2\varphi_n}{\partial t^2} = 0, \qquad (15a)$$

$$\varepsilon_{11}^{'}\nabla_{1}^{2}E_{n} + m_{11}^{'}\nabla_{1}^{2}H_{n}\frac{2m}{r}\left(\varepsilon_{11}^{'}\frac{\partial E_{n}}{\partial r} + m_{11}^{'}\frac{\partial H_{n}}{\partial r}\right) = 0, \qquad (15b)$$

$$m_{11}^{'}\nabla_{1}^{2}E_{n} + V^{'}\nabla_{1}^{2}H_{n} + \frac{2m}{r}\left(m_{11}^{'}\frac{\partial E_{n}}{\partial r} + V^{'}\frac{\partial H_{n}}{\partial r}\right) = 0, \qquad (15c)$$

and

$$\frac{V}{2}\nabla_1^2 \psi_n + Vm \left(\frac{1}{r}\frac{\partial \psi_n}{\partial r} - \frac{\psi_n}{r}\right) = 0, \qquad (16)$$

where

$$\nabla_1^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}.$$

We consider the free vibration of non homogeneous polygonal cross-sectional plate and we seek the displacement function, electric and magnetic displacement function as:

$$\phi_n(r,\theta,t) = r^{-m}\phi_n(r)\cos n\theta e^{i\omega t},$$

$$E_n(r,\theta,t) = r^{-m}E_n(r)\cos n\theta e^{i\omega t},$$

$$H_n(r,\theta,t) = r^{-m}H_n(r)\cos n\theta e^{i\omega t},$$
and
$$w_n(r,\theta,t) = -\frac{m}{2}w_n(r)\cos n\theta e^{i\omega t},$$

$$(17)$$

Using the Eqs. (17) and (18) in the Eqs. (15) and (16), we get

$$\varphi_{n}^{'}(r) + \frac{1}{r}\varphi_{n}^{'}(r) \left(\frac{\rho_{0}\omega^{2}a^{2}}{L+V} - \frac{\left(\left(m^{2}+n^{2}\right)2mL\right)}{L+V}\varphi_{n}(r) \right) = 0, \qquad (19)$$

which is reduced as

$$\varphi_{n}^{"}(r) + \frac{1}{r} \varphi_{n}^{'}(r) \left(\alpha^{2} r^{2} - \beta^{2}\right) \varphi_{n}(r) = 0, \qquad (20)$$
where $\alpha^{2} = \frac{\rho_{0} \omega^{2} a^{2}}{L + V}, \quad \beta^{2} = \frac{\left(\left(m^{2} + n^{2}\right) 2mL\right)}{L + V}.$

Equation (20) is Bessel equation with order β and its solution is given by:

$$\varphi_n(r) = \left(A_{1n}J_\beta(\alpha r) + A_{1n}Y_\beta(\alpha r)\right)\cos n\theta = 0, \qquad (21)$$

where A_{In} and A'_{In} are arbitrary constants and $J_{\beta}(\alpha r)$ and $Y_{\beta}(\alpha r)$ are the Bessel functions of first and second kind of order β respectively.

Substituting Eq. (18) in to Eq. (16), we get

$$\psi_{n}^{*}(r) + \frac{1}{r}\psi_{n}^{*}(r) \left(\frac{2\rho_{0}\omega^{2}a^{2}}{V} - \frac{1}{r^{2}}\left(4m^{2} + 4n + n^{2}\right)\right)\psi_{n}(r) = 0, \qquad (22)$$

which is reduced to

$$\psi_{n}^{''}(r) + \frac{1}{r}\psi_{n}^{'}(r)(k^{2}r^{2} - \delta^{2})\psi_{n}(r) = 0.$$
(23)
Equation (23) is Passel equation with order S and its solution is given by

$$\psi_n(r) = \left(A_{4n}J_{\delta}(\alpha r) + A_{4n}Y_{\delta}(\alpha r)\right)\sin n\theta = 0, \qquad (24)$$

where A_{4n} and A_{4n} are arbitrary constants and $J_{\delta}(\alpha r)$ and $Y_{\delta}(\alpha r)$ are the Bessel functions of first and second kind of order δ respectively.

Substituting Eq. (17) in to Eqs. (15), we get

$$\left(\varepsilon_{11}^{'}\frac{\partial^{2}E_{n}}{\partial r^{2}} + \frac{\varepsilon_{11}^{'}}{r}\left(2m+1\right)\frac{\partial E_{n}}{\partial r} + \frac{\varepsilon_{11}^{'}}{r^{2}}\frac{\partial^{2}E_{n}}{\partial \theta^{2}}\right) + \left(m_{11}^{'}\frac{\partial^{2}H_{n}}{\partial r^{2}} + \frac{m_{11}^{'}}{r}\left(2m+1\right)\frac{\partial H_{n}}{\partial r} + \frac{\varepsilon_{11}^{'}}{r^{2}}\frac{\partial^{2}H_{n}}{\partial \theta^{2}}\right) = 0, \quad (25)$$

$$m_{11}^{'}\left(E_{n}^{''}(r)+\frac{1}{r}E_{n}^{'}(r)-\frac{(m^{2}+n^{2})}{r^{2}}E_{n}(r)\right)+V^{'}\left(H_{n}^{''}(r)+\frac{1}{r}H_{n}^{'}(r)-\frac{(m^{2}+n^{2})}{r^{2}}H_{n}(r)\right)=0, \quad (26)$$
which will reduced in to the convenient form:

which will reduced in to the convenient form:

$$\varepsilon_{11}^{'}\left(E_{n}^{''}(r)+\frac{1}{r}E_{n}^{'}(r)-\frac{p^{2}}{r^{2}}E_{n}(r)\right)+m_{11}^{'}\left(H_{n}^{''}(r)+\frac{1}{r}H_{n}^{'}(r)-\frac{p^{2}}{r^{2}}H_{n}(r)\right)=0,$$
(27)

$$m_{11}^{'}\left(E_{n}^{''}(r)+\frac{1}{r}E_{n}^{'}(r)-\frac{p^{2}}{r^{2}}E_{n}(r)\right)+V^{'}\left(H_{n}^{''}(r)+\frac{1}{r}H_{n}^{'}(r)-\frac{p^{2}}{r^{2}}H_{n}(r)\right)=0,$$
(28)

where

 $p^2 = m^2 + n^2.$

Solving Eq. (27) and Eq. (28), we can get

$$E_{n}^{*}(r) + \frac{1}{r}E_{n}^{'}(r) - \frac{p^{2}}{r^{2}}E_{n}(r) = 0, \qquad (29)$$

$$H_{n}^{"}(r) + \frac{1}{r}H_{n}^{'}(r) - \frac{p^{2}}{r^{2}}H_{n}(r) = 0.$$
(30)

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The general solution of Eqs. (29) and (30) are as follows:

$$E_n(r,\theta,t) = \left(A_{2n}r^p + A'_{2n}r^{-p}\right)\cos n\theta e^{iwt},\tag{31}$$

$$H_n(r,\theta,t) = (A_{3n}r^p + A'_{3n}r^{-p})\cos n\theta e^{iwt}, \qquad (32)$$

where $A_{2n}, A'_{2n}, A_{3n}, A'_{3n}$ are the arbitrary constants.

The general solution of the non-homogeneous solid plate of polygonal cross sections is as:

$$\phi_n(r,\theta,t) = A_{1n}J_\beta(\alpha r)\cos n\theta, \qquad (33a)$$

$$E_n(r,\theta,t) = A_{2n}r^p \cos n\theta, \qquad (33b)$$

$$H_n(r,\theta,t) = A_{3n}r^p \cos n\theta, \qquad (33c)$$

$$\psi_n(r,\theta,t) = A_{\ln}J_{\delta}(kr)\sin n\theta.$$
(33d)

4. Boundary condition and frequency equations

In this problem, the vibration of polygonal cross-sectional plate is considered. Since the boundary is irregular in shape, it is difficult to satisfy the boundary conditions along the surface of the plate directly. Hence, the Fourier expansion collocation method is applied to satisfy the boundary conditions. For the plate, the normal stress σ_{xx} and shearing stresses σ_{xy}, σ_{xz} , the electric field D_r and the magnetic field B_r is equal to zero for stress free boundary, and for rigidly fixed boundary, the displacements along the radial direction u_r , along the circumferential direction u_{θ} , and the electric field E, and the magnetic field H is equal to zero. Thus the following types of boundary conditions are assumed for the plate of polygonal cross-section is

- (i) Stress free(unclamped edge), which leads to $(\sigma_{xx})_i = (\sigma_{xy})_i = (\sigma_{xz})_i = (D_r)_i = (B_r)_i = 0;$ (34)
- (ii) Rigidly fixed(clamped edge), implies that $(u_r)_i = (u_\theta)_i = (E)_i = (H)_i = 0,$ (35)

where σ_{xx} is the normal stress, σ_{xy}, σ_{xz} are the shearing stresses, D_r is the electric field, B_r is the magnetic field and the bracket ()_i is the value at the boundary Γ_i . Similarly u_r, u_θ are displacements along the radial and circumferential direction, E and H are respectively the electric and magnetic displacements in the *i*th segment of the polygonal cross-sectional plate. Since the vibration displacements are expressed in terms of the coordinates r and θ , it is convenient to treat the boundary conditions when the derivatives in the equations of the stresses are transformed in terms of the coordinates r and θ instead of the coordinates x_i and

 y_i . The relations between the displacements are as follows for i^{th} segment of straight-line boundaries

$$u_{x} = u_{r} \cos(\theta - \gamma_{i}) - u_{\theta} \sin(\theta - \gamma_{i}),$$

$$u_{y} = u_{\theta} \cos(\theta - \gamma_{i}) - u_{r} \sin(\theta - \gamma_{i}).$$
(36)

Since the angle γ_i between the reference axis and normal of the *i*th boundary has a constant value in a segment Γ_i , we obtain:

$$\frac{\partial r}{\partial x_i} = \cos(\theta - \gamma_i), \ \frac{\partial \theta}{\partial x_i} = -\left(\frac{1}{r}\right)\sin(\theta - \gamma_i),$$

$$\frac{\partial r}{\partial y_i} = \sin(\theta - \gamma_i), \ \frac{\partial \theta}{\partial y_i} = \left(\frac{1}{r}\right)\cos(\theta - \gamma_i).$$
Using the Eqs. (36) and (37), the normal and shearing stresses are transformed as:

$$\sigma_{xx} = c_{11} \cos^{2} (\theta - \gamma_{i}) + c_{12} \sin^{2} (\theta - \gamma_{i}) u_{,r} + r^{-1} (c_{11} \sin^{2} (\theta - \gamma_{i}) + c_{12} \cos^{2} (\theta - \gamma_{i})) (u + v_{,\theta}) + c_{66} (r^{-1} (v - u_{,\theta}) - v_{,r}) \sin 2(\theta - \gamma_{i}) + c_{13} w_{,z} + e_{31} E_{,zz} + q_{31} H_{,zz} = 0 \sigma_{xy} = c_{66} ((u_{,r} - r^{-1} (v_{,\theta} + u))) \sin 2(\theta - \gamma_{i}) + (r^{-1} (u_{,\theta} - v) + v_{,r}) \cos 2(\theta - \gamma_{i})) = 0 \sigma_{xz} = c_{44} ((u_{,z} + w_{,r}) \cos (\theta - \gamma_{i}) - (v_{,z} + r^{-1} w_{,\theta}) \sin (\theta - \gamma_{i})) + e_{15} (E_{,r} \cos (\theta - \gamma_{i}) - r^{-1} E_{,\theta} \sin (\theta - \gamma_{i})) + q_{15} (H_{,r} \cos (\theta - \gamma_{i}) - r^{-1} H_{,\theta} \sin (\theta - \gamma_{i})) = 0 D_{x} = -\varepsilon_{11} \frac{\partial E}{\partial r} - m_{11} \frac{\partial H}{\partial r} = 0, B_{x} = -m_{11} \cdot \frac{\partial E}{\partial r} - \mu_{11} \cdot \frac{\partial H}{\partial r} = 0.$$
(38)

Imposing non-homogeneity to the Eq. (38), we can get the following mechanical, magnetic and electric stress equations :

$$\sigma_{xx} = (L+V)\cos^{2}(\theta - \gamma_{i}) + L\sin^{2}(\theta - \gamma_{i})u_{,r} + r^{-1}((L+V)\sin^{2}(\theta - \gamma_{i}) + L\cos^{2}(\theta - \gamma_{i}))(u + v_{,\theta}) + c_{66}(r^{-1}(v - u_{,\theta}) - v_{,r})\sin 2(\theta - \gamma_{i}) + c_{13}w_{,z} + e_{31}E_{,zz} + q_{31}H_{,zz} = 0 \sigma_{xy} = \frac{V}{2}((u_{,r} - r^{-1}(v_{,\theta} + u)))\sin 2(\theta - \gamma_{i}) + (r^{-1}(u_{,\theta} - v) + v_{,r})\cos 2(\theta - \gamma_{i})) = 0 D_{x} = -\varepsilon_{11}\frac{\partial E}{\partial r} - m_{11}\frac{\partial H}{\partial r} = 0 B_{x} = -m_{11}\frac{\partial E}{\partial r} - \mu_{11}\frac{\partial H}{\partial r} = 0.$$
(39)

Substituting the Eqs. (33a) - (33d) in the Eq. (34), the boundary conditions are transformed for stress free non-homogeneous polygonal cross-sectional plate as follows:

$$\begin{split} \left[\left(S_{xx} \right)_{i} + \left(\overline{S}_{xy} \right)_{i} \right] e^{i\omega t} \\ \left[\left(S_{xy} \right)_{i} + \left(\overline{S}_{xy} \right)_{i} \right] e^{i\omega t} \\ \left[\left(E_{x} \right)_{i} + \left(\overline{E}_{x} \right)_{i} \right] e^{i\omega t} \\ \left[\left(H_{x} \right)_{i} + \left(\overline{H}_{x} \right)_{i} \right] e^{i\omega t} , \\ \text{where} \\ \\ S_{xx} &= 0.5 \left(A_{10} e_{0}^{1} + A_{20} e_{0}^{2} + A_{30} e_{0}^{3} \right) + \sum_{n=1}^{\infty} \left(A_{1n} e_{n}^{1} + A_{2n} e_{n}^{2} + A_{30} e_{n}^{3} + A_{4n} e_{n}^{4} \right) \\ S_{xy} &= 0.5 \left(A_{10} f_{0}^{1} + A_{20} f_{0}^{2} + A_{30} f_{0}^{3} \right) + \sum_{n=1}^{\infty} \left(A_{1n} f_{n}^{1} + A_{2n} f_{n}^{2} + A_{30} f_{n}^{3} + A_{4n} f_{n}^{4} \right) \\ S_{xz} &= 0.5 \left(A_{10} g_{0}^{1} + A_{20} g_{0}^{2} + A_{30} g_{0}^{3} \right) + \sum_{n=1}^{\infty} \left(A_{1n} g_{n}^{1} + A_{2n} g_{n}^{2} + A_{30} g_{n}^{3} + A_{4n} g_{n}^{4} \right) \end{split}$$

$$E = 0.5 \left(A_{10} h_0^1 + A_{20} h_0^2 + A_{30} h_0^3 \right) + \sum_{n=1}^{\infty} \left(A_{1n} h_n^1 + A_{2n} h_n^2 + A_{30} h_n^3 + A_{4n} h_n^4 \right)$$

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$$H = 0.5 \left(A_{10} i_0^1 + A_{20} i_0^2 + A_{30} i_0^3 \right) + \sum_{n=1}^{\infty} \left(A_{1n} i_n^1 + A_{2n} i_n^2 + A_{30} i_n^3 + A_{4n} i_n^4 \right)$$
(40)

$$\overline{S}_{xx} = 0.5 \overline{e_0}^5 \overline{A}_{50} + \sum_{n=1}^{\infty} \left(A_{1n} \overline{e_n}^1 + A_{2n} \overline{e_n}^2 + A_{30} \overline{e_n}^3 + A_{4n} \overline{e_n}^4 \right)$$

$$\overline{S}_{xy} = 0.5 \overline{f_0}^5 \overline{A}_{50} + \sum_{n=1}^{\infty} \left(A_{1n} \overline{f_n}^1 + A_{2n} \overline{f_n}^2 + A_{30} \overline{f_n}^3 + A_{4n} \overline{f_n}^4 \right)$$

$$\overline{S}_{xz} = 0.5 \overline{g_0}^5 \overline{A}_{50} + \sum_{n=1}^{\infty} \left(A_{1n} \overline{g_n}^1 + A_{2n} \overline{g_n}^2 + A_{30} \overline{g_n}^3 + A_{4n} \overline{g_n}^4 \right)$$

$$\overline{E} = 0.5 \overline{h_0}^5 \overline{A}_{50} + \sum_{n=1}^{\infty} \left(A_{1n} \overline{h_n}^1 + A_{2n} \overline{h_n}^2 + A_{30} \overline{h_n}^3 + A_{4n} \overline{h_n}^4 \right)$$

$$\overline{H} = 0.5 \overline{i_0}^5 \overline{A}_{50} + \sum_{n=1}^{\infty} \left(A_{1n} \overline{i_n}^1 + A_{2n} \overline{i_n}^2 + A_{30} \overline{i_n}^3 + A_{4n} \overline{i_n}^4 \right).$$
(41)

The coefficients $e_n^i \sim \overline{i_n}^{-i}$ are given in the Appendix A.

Performing the Fourier series expansion to Eq. (35) along the boundary, the boundary conditions along the surface are expanded in the form of double Fourier series. In the symmetric mode, the boundary conditions are obtained as:

$$\sum_{m=0}^{\infty} \mathcal{E}_{m} \left[E_{m0}^{1} A_{10} + E_{m0}^{2} A_{20} + E_{m0}^{3} A_{30} + E_{m0}^{4} A_{40} + \sum_{n=1}^{\infty} \left(E_{nm}^{1} A_{1n} + E_{nm}^{2} A_{2n} + E_{nm}^{3} A_{3n} + E_{nm}^{4} A_{4n} + E_{nm}^{5} A_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \mathcal{E}_{m} \left[F_{m0}^{1} A_{10} + F_{m0}^{2} A_{20} + F_{m0}^{3} A_{30} + F_{m0}^{4} A_{40} + \sum_{n=1}^{\infty} \left(F_{nm}^{1} A_{1n} + F_{nm}^{2} A_{2n} + F_{nm}^{3} A_{3n} + F_{nm}^{4} A_{4n} + F_{nm}^{5} A_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \mathcal{E}_{m} \left[G_{m0}^{1} A_{10} + G_{m0}^{2} A_{20} + G_{m0}^{3} A_{30} + G_{m0}^{4} A_{40} + \sum_{n=1}^{\infty} \left(G_{nm}^{1} A_{1n} + G_{nm}^{2} A_{2n} + G_{nm}^{3} A_{3n} + G_{nm}^{4} A_{4n} + G_{nm}^{5} A_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \mathcal{E}_{m} \left[H_{m0}^{1} A_{10} + H_{m0}^{2} A_{20} + H_{m0}^{3} A_{30} + H_{m0}^{4} A_{40} + \sum_{n=1}^{\infty} \left(H_{mn}^{1} A_{1n} + H_{mn}^{2} A_{2n} + H_{mn}^{3} A_{3n} + H_{mn}^{4} A_{4n} + H_{mn}^{5} A_{5n} \right) \right] = 0.$$

$$\sum_{m=0}^{\infty} \mathcal{E}_{m} \left[I_{m0}^{1} A_{10} + I_{m0}^{2} A_{20} + I_{m0}^{3} A_{30} + H_{m0}^{4} A_{40} + \sum_{n=1}^{\infty} \left(I_{mn}^{1} A_{1n} + I_{mn}^{2} A_{2n} + I_{mn}^{3} A_{3n} + I_{mn}^{4} A_{4n} + I_{mn}^{5} A_{5n} \right) \right] = 0.$$

$$(42)$$

Similarly, for the antisymmetric mode, the boundary conditions are expressed as:

$$\sum_{m=0}^{\infty} \left[\overline{E}_{m0}^{5} \overline{A}_{50} + \sum_{n=1}^{\infty} \left(\overline{E}_{nn}^{1} \overline{A}_{1n} + \overline{E}_{mn}^{2} \overline{A}_{2n} + \overline{E}_{nm}^{3} \overline{A}_{3n} + \overline{E}_{nm}^{4} \overline{A}_{4n} + \overline{E}_{nm}^{5} \overline{A}_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \left[\overline{F}_{m0}^{5} \overline{A}_{50} + \sum_{n=1}^{\infty} \left(\overline{F}_{nn}^{1} \overline{A}_{1n} + \overline{F}_{nn}^{2} \overline{A}_{2n} + \overline{F}_{nn}^{3} \overline{A}_{3n} + \overline{F}_{nn}^{4} \overline{A}_{4n} + \overline{F}_{nn}^{5} \overline{A}_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \left[\overline{G}_{n0}^{5} \overline{A}_{50} + \sum_{n=1}^{\infty} \left(\overline{G}_{nn}^{1} \overline{A}_{1n} + \overline{G}_{nn}^{2} \overline{A}_{2n} + \overline{G}_{nn}^{3} \overline{A}_{3n} + \overline{G}_{nn}^{4} \overline{A}_{4n} + \overline{G}_{nn}^{5} \overline{A}_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \left[\overline{H}_{n0}^{5} \overline{A}_{50} + \sum_{n=1}^{\infty} \left(\overline{H}_{nn}^{1} \overline{A}_{1n} + \overline{H}_{nn}^{2} \overline{A}_{2n} + \overline{H}_{nn}^{3} \overline{A}_{3n} + \overline{H}_{nn}^{4} \overline{A}_{4n} + \overline{H}_{nn}^{5} \overline{A}_{5n} \right) \right] = 0$$

$$\sum_{m=0}^{\infty} \left[\overline{I}_{n0}^{5} \overline{A}_{50} + \sum_{n=1}^{\infty} \left(\overline{I}_{nn}^{1} \overline{A}_{1n} + \overline{I}_{nn}^{2} \overline{A}_{2n} + \overline{I}_{nn}^{3} \overline{A}_{3n} + \overline{I}_{nn}^{4} \overline{A}_{4n} + \overline{I}_{nn}^{5} \overline{A}_{5n} \right) \right] = 0,$$
(43)
where

$$E_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} e_{n}^{j} \left(R_{i},\theta\right) \cos m\theta d\theta$$
$$F_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} f_{n}^{j} \left(R_{i},\theta\right) \sin m\theta d\theta$$

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$$G_{nn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{l} \int_{\theta_{i-1}}^{\theta_{i}} g_{n}^{j}(R_{i},\theta) \cos m\theta d\theta$$

$$H_{nm}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{l} \int_{\theta_{i-1}}^{\theta_{i}} h_{n}^{j}(R_{i},\theta) \cos m\theta d\theta$$

$$\overline{E}_{nm}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{l} \int_{\theta_{i-1}}^{\theta_{i}} \overline{e}_{n}^{j}(R_{i},\theta) \sin m\theta d\theta$$

$$\overline{F}_{nm}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{l} \int_{\theta_{i-1}}^{\theta_{i}} \overline{f}_{n}^{j}(R_{i},\theta) \cos m\theta d\theta$$

$$\overline{G}_{nm}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{l} \int_{\theta_{n-1}}^{\theta_{i}} \overline{g}_{n}^{j}(R_{i},\theta) \sin m\theta d\theta$$

$$\overline{H}_{nm}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{l} \int_{\theta_{i-1}}^{\theta_{i}} \overline{h}_{n}^{j}(R_{i},\theta) \sin m\theta d\theta ,$$

$$(45)$$

where j=1,2,3,4, I is the number of segments, R_i is the coordinate r at the boundary and N is the number of truncation of the Fourier series. The frequency equations are obtained by truncating the series to N+1 terms, and equating the determinant of the coefficients of the amplitude $A_{in} = 0$ and $\overline{A}_{in} = 0$ (i=1,2,3,4), for symmetric and anti symmetric modes of vibrations. When the plate is symmetric about more than one axis, the boundary conditions in the case of symmetric mode can be written in the form of matrix as given below:

Similarly, the matrix for the antisymmetric mode is obtained as:

5. Homogeneous electro-elastic plate of polygonal cross-sections

The result for homogeneous transversely isotropic electro-elastic plate of polygonal crosssections can be obtained by omitting the magnetic conductions $B_i = 0$ (i= r, θ , z) in the corresponding relations and expressions. Thus the displacement potential for this problem is obtained by setting piezomagnetic material coefficients $q_{15} = q_{31} = q_{33} = 0$, magnetic material coefficients $m_{11} = m_{33} = 0$ and the magnetic permeability coefficients $\mu_{11} = \mu_{33} = 0$. Therefore the Eqs. (13a)- (13d) are reduced to

$$\left(\overline{c}_{11}\nabla_{2}^{2} - t_{L}^{2} + \Omega^{2}\right)\overline{\phi}_{n} + \left(1 + \overline{c}_{13}\right)t_{L}^{2}\overline{W}_{n} + \left(\overline{e}_{31} + \overline{e}_{15}\right)t_{L}^{2}\overline{E}_{n} = 0$$

$$\left(\nabla_{2}^{2} + \Omega^{2} - \overline{c}_{33}t_{L}^{2}\right)\overline{W}_{n} + \left(1 + \overline{c}_{13}\right)\nabla_{2}^{2}\overline{\phi}_{n} + \left(\overline{e}_{15}\nabla_{2}^{2} - t_{L}^{2}\right)\overline{E}_{n} = 0$$

$$\left(\overline{e}_{15}\nabla_{2}^{2} - t_{L}^{2}\right)\overline{W}_{n} - \left(\overline{e}_{31} + \overline{e}_{15}\right)\nabla_{2}^{2}\overline{\phi}_{n} + \left(\overline{\varepsilon}_{33}t_{L}^{2} - \overline{\varepsilon}_{11}\nabla_{2}^{2}\right)\overline{E}_{n} = 0$$

$$and \left(\nabla_{2}^{2} + \frac{\Omega^{2} - t_{L}^{2}}{\overline{c}_{66}}\right)\overline{\psi}_{n} = 0.$$

$$(49)$$

Solving the Eq. (48), we obtain a trivial solution. To obtain the non-trivial solutions, put the determinant of the coefficient of the matrix is equal to zero. Thus we get

$$\begin{vmatrix} (\bar{c}_{11}\nabla_{2}^{2} + \Omega^{2} - t_{L}^{2}) & (1 + \bar{c}_{13})t_{L}^{2} & (\bar{e}_{31} + \bar{e}_{15})t_{L}^{2} \\ (1 + \bar{c}_{13})\nabla_{2}^{2} & (\nabla_{2}^{2} + \Omega^{2} - \bar{c}_{33}t_{L}^{2}) & (\bar{e}_{15}\nabla_{2}^{2} - t_{L}^{2}) \\ - (\bar{e}_{31} + \bar{e}_{15})\nabla_{2}^{2} & (\bar{e}_{15}\nabla_{2}^{2} - t_{L}^{2}) & (\bar{\varepsilon}_{33}t_{L}^{2} - \bar{\varepsilon}_{11}\nabla_{2}^{2}) \end{vmatrix}$$
(50)

Simplifying the Eq. (50), we get a six order partial differential equation, that is $\left(P\nabla_2^6 + Q\nabla_2^4 + R\nabla_2^2 + S\right)\phi_n = 0,$ where
(51)

$$P = -\bar{c}_{11}\left(\bar{\varepsilon}_{11} + \bar{e}_{15}^{2}\right)$$
$$Q = \bar{c}_{11}\left(g_{7} - g_{5}\bar{\varepsilon}_{11} + 2g_{6}\bar{e}_{15}\right) - g_{1}\left(\bar{\varepsilon}_{11} + \bar{e}_{15}^{2}\right) + t_{L}^{2}\left(-g_{2}\left(g_{2}\bar{\varepsilon}_{11} + 2g_{3}\bar{e}_{15}\right) + g_{3}^{2}\right)$$

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$$R = \overline{c}_{11} \left(g_5 g_7 - g_6^2 \right) + g_1 \left(g_7 - g_5 \overline{c}_{11} + 2g_6 \overline{e}_{15} \right) + t_L^2 \left(g_2 \left(g_2 g_7 + 2g_3 g_6 \right) + g_3^2 g_5 \right)$$

$$S = g_1 \left(g_5 g_7 - g_6^2 \right).$$
(52)

Solving the Eq. (51), the solution for the symmetric mode is obtained as

$$\overline{\phi}_{n}(r) = \sum_{i=1}^{3} A_{in}J_{n}(\alpha_{i}r)\sin(m\pi\zeta)\sin n\theta e^{i\omega t}$$

$$\overline{W}_{n}(r) = \sum_{i=1}^{3} d_{i}A_{in}J_{n}(\alpha_{i}r)\sin(m\pi\zeta)\sin n\theta e^{i\omega t}$$

$$\overline{E}_{n}(r) = \sum_{i=1}^{3} e_{i}A_{in}J_{n}(\alpha_{i}r)\sin(m\pi\zeta)\sin n\theta e^{i\omega t}.$$
(53)

The constants d_i and e_i defined in the Eq. (53) are given by

$$d_{i} = \frac{\left(\bar{c}_{11}\alpha_{i}^{2} - g_{1}\right)\left(\bar{e}_{15}\alpha_{i}^{2} + g_{6}\right) - g_{3}g_{6}\alpha_{i}^{2}t_{L}^{2}}{t_{L}^{2}\left(g_{2}\left(\bar{e}_{15}\alpha_{i}^{2} + g_{6}\right) + g_{3}\left(g_{5} - \alpha_{i}^{2}\right)\right)}$$

$$e_{i} = \frac{\left(\bar{c}_{11}\alpha_{i}^{2} - g_{1}\right)\left(g_{5} - \alpha_{i}^{2}\right) + g_{2}^{2}\alpha_{i}^{2}t_{L}^{2}}{t_{L}^{2}\left(g_{2}\left(\bar{e}_{15}\alpha_{i}^{2} + g_{6}\right) + g_{3}\left(\alpha_{i}^{2} - g_{5}\right)\right)}.$$
(54)

Similarly solving the Eq. (49), we obtain the solution for the symmetric mode as $\overline{\psi}_n(r) = A_{4n}J_n(\alpha_4 r)\sin(m\pi\zeta)\sin n\theta e^{i\omega t}$. (55)

The boundary condition for a electro-elastic plate of polygonal cross-section is obtained as (i) Stress free(unclamped edge)

(i) Sites inecluleramped edge)

$$(\sigma_{xx})_i = (\sigma_{xy})_i = (\sigma_{xz})_i = (D_r)_i = 0;$$
(ii) Rigidly fixed (clamped edge)
(56)

(57) Rigidly fixed (clamped edge)

$$(u_r)_i = (u_\theta)_i = (E)_i = 0,$$

where σ_{xx} is the normal stress, σ_{xy} , σ_{xz} are the shearing stresses, D_r is the electric potential as discussed in the section A. By using the same procedure as discussed in the section A, the boundary conditions (56) and (57) are transferred as

$$\sigma_{xx}' = c_{11}\cos^{2}(\theta - \gamma_{i}) + c_{12}\sin^{2}(\theta - \gamma_{i})u_{,r} + r^{-1}(c_{11}\sin^{2}(\theta - \gamma_{i}) + c_{12}\cos^{2}(\theta - \gamma_{i}))(u + v_{,\theta}) + c_{66}(r^{-1}(v - u_{,\theta}) - v_{,r})\sin 2(\theta - \gamma_{i}) + c_{13}w_{,z} + e_{31}E_{,zz} = 0 \sigma_{xy}' = c_{66}((u_{,r} - r^{-1}(v_{,\theta} + u)))\sin 2(\theta - \gamma_{i}) + (r^{-1}(u_{,\theta} - v) + v_{,r})\cos 2(\theta - \gamma_{i})) = 0 \sigma_{xz}' = c_{44}((u_{,z} + w_{,r})\cos(\theta - \gamma_{i}) - (v_{,z} + r^{-1}w_{,\theta})\sin(\theta - \gamma_{i})) + e_{15}(E_{,r}\cos(\theta - \gamma_{i}) - \frac{1}{r}E_{,\theta}\sin(\theta - \gamma_{i})) = 0 D_{x} = 0$$
(58)

Substituting the Eq.v(53) in the Eq. (56) the boundary conditions are transformed for stress free polygonal cross-sectional plate is obtained as

$$\begin{bmatrix} \left(S'_{xx}\right)_{i} + \left(\overline{S'}_{xx}\right)_{i} \end{bmatrix} \sin\left(m\pi\zeta\right) \sin n\theta e^{i\omega t} \\ \begin{bmatrix} \left(S'_{xy}\right)_{i} + \left(\overline{S'}_{xy}\right)_{i} \end{bmatrix} \sin\left(m\pi\zeta\right) \sin n\theta e^{i\omega t} \\ \begin{bmatrix} \left(S'_{xz}\right)_{i} + \left(\overline{S'}_{xz}\right)_{i} \end{bmatrix} \sin\left(m\pi\zeta\right) \sin n\theta e^{i\omega t} \end{bmatrix}$$

$$\begin{bmatrix} (E'_{x})_{i} + (\overline{E'}_{x})_{i} \end{bmatrix} \sin(m\pi\zeta) \sin n\theta e^{i\omega t},$$
(59)
where $S'_{xx} = 0.5 \Big(A_{10} p_{0}^{1} + A_{20} p_{0}^{2} + A_{30} p_{0}^{3} \Big) + \sum_{n=1}^{\infty} \Big(A_{1n} p_{n}^{1} + A_{2n} p_{n}^{2} + A_{3n} p_{n}^{3} + A_{4n} p_{n}^{4} \Big)$
 $S'_{xy} = 0.5 \Big(A_{10} q_{0}^{1} + A_{20} q_{0}^{2} + A_{30} q_{0}^{3} \Big) + \sum_{n=1}^{\infty} \Big(A_{1n} q_{n}^{1} + A_{2n} q_{n}^{2} + A_{3n} q_{n}^{3} + A_{4n} q_{n}^{4} \Big)$
 $S'_{xz} = 0.5 \Big(A_{10} r_{0}^{1} + A_{20} r_{0}^{2} + A_{30} r_{0}^{3} \Big) + \sum_{n=1}^{\infty} \Big(A_{1n} r_{n}^{1} + A_{2n} r_{n}^{2} + A_{3n} r_{n}^{3} + A_{4n} r_{n}^{4} \Big)$
 $E'_{x} = 0.5 \Big(A_{10} s_{0}^{1} + A_{20} s_{0}^{2} + A_{30} s_{0}^{3} \Big) + \sum_{n=1}^{\infty} \Big(A_{1n} r_{n}^{1} + A_{2n} s_{n}^{2} + A_{3n} s_{n}^{3} + A_{4n} r_{n}^{4} \Big)$
 $E'_{x} = 0.5 \Big(A_{10} s_{0}^{1} + A_{20} s_{0}^{2} + A_{30} s_{0}^{3} \Big) + \sum_{n=1}^{\infty} \Big(A_{1n} s_{n}^{1} + A_{2n} s_{n}^{2} + A_{3n} s_{n}^{3} + A_{4n} r_{n}^{4} \Big)$
 $\overline{S'}_{xx} = 0.5 \overline{p_{0}^{4}} \overline{A}_{40} + \sum_{n=1}^{\infty} \Big(\overline{A}_{1n} \overline{p}_{n}^{1} + \overline{A}_{2n} \overline{p}_{n}^{2} + \overline{A}_{3n} \overline{p}_{n}^{3} + \overline{A}_{4n} \overline{p}_{n}^{4} \Big)$
 $\overline{S'}_{xy} = 0.5 \overline{q_{0}^{4}} \overline{A}_{40} + \sum_{n=1}^{\infty} \Big(\overline{A}_{1n} \overline{q}_{n}^{1} + \overline{A}_{2n} \overline{q}_{n}^{2} + \overline{A}_{3n} \overline{q}_{n}^{3} + \overline{A}_{4n} \overline{q}_{n}^{4} \Big)$
 $\overline{E'}_{x} = 0.5 \overline{s_{0}^{4}} \overline{A}_{40} + \sum_{n=1}^{\infty} \Big(\overline{A}_{1n} \overline{s}_{n}^{1} + \overline{A}_{2n} \overline{s}_{n}^{2} + \overline{A}_{3n} \overline{s}_{n}^{3} + \overline{A}_{4n} \overline{s}_{n}^{4} \Big)$
(61)

The boundary conditions along the irregular shape cannot be satisfied directly. To satisfy the boundary conditions, the Fourier expansion collocation method is applied along the boundary. Performing the Fourier series expansion to the transformed expression in Eq. (56) along the boundary, the boundary conditions are expanded in the form of double Fourier series for symmetric and antisymmetric modes of vibrations. For the symmetric mode, the equation which satisfies the boundary condition, is obtained in matrix form as follows

(62)

$$P_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} p_{n}^{j}(R_{i},\theta) \cos m\theta d\theta$$
$$Q_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} q_{n}^{j}(R_{i},\theta) \sin m\theta d\theta$$

where

$$R_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} r_{n}^{j} \left(R_{i},\theta\right) \cos m\theta d\theta$$

$$S_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} s_{n}^{j} \left(R_{i},\theta\right) \cos m\theta d\theta \qquad (63)$$
Similarly for the antisymmetric mode, we get

Similarly, for the antisymmetric mode, we get

where
$$\overline{P}_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} \overline{p}_{n}^{j}(R_{i},\theta) \sin m\theta d\theta$$

 $\overline{Q}_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} \overline{q}_{n}^{j}(R_{i},\theta) \cos m\theta d\theta$
 $\overline{R}_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} \overline{r}_{n}^{j}(R_{i},\theta) \sin m\theta d\theta$
 $\overline{S}_{mn}^{j} = \left(\frac{2\varepsilon_{n}}{\pi}\right) \sum_{i=1}^{I} \int_{\theta_{i-1}}^{\theta_{i}} \overline{s}_{n}^{j}(R_{i},\theta) \sin m\theta d\theta$, (65)

where j=1,2,3 and 4, I is the number of segments, R_i is the coordinate r at the boundary and N is the terms in the Fourier series. The frequency equation for determining the frequencies may be obtained by equating the coefficient of the system of Eq. (62) or Eq. (64) to zero.

6. Numerical results and discussion

The frequency equations obtained in symmetric and antisymmetric cases given in Eq. (46) and (47) are analyzed numerically for magneto electro elastic plate of polygonal (triangular, square, pentagonal and hexagonal) cross-sections. The material properties of the electromagnetic material based on graphical results of Aboudi [33] are $c_{11} = 218 \times 10^9 N/m^2$, $c_{12} = 120 \times 10^9 N/m^2$, $c_{13} = 120 \times 10^9 N/m^2$, $c_{33} = 215 \times 10^9 N/m^2$, $c_{44} = 50 \times 10^9 N/m^2$, $c_{66} = 49 \times 10^9 N/m^2$, $e_{15} = 0$, $e_{31} = -2.5 C/m^2$, $e_{33} = 7.5 C/m^2$, $q_{15} = 200 C/m^2$, $q_{31} = 265 C/m^2$, $q_{33} = 345 C/m^2$, $\varepsilon_{11} = 0.4 \times 10^{-9} C/Vm$, $\varepsilon_{33} = 5.8 \times 10^{-9} C/Vm$,

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 $\mu_{11} = -200 \times 10^{-6} Ns^2/C^2 , \quad \mu_{33} = 95 \times 10^{-6} Ns^2/C^2 , \quad m_{11} = 0.0074 \times 10^{-9} Ns/VC ,$ $m_{33} = 2.82 \times 10^{-9} Ns/VC .$

The geometric relations for the polygonal cross-sections given by Nagaya [32] as $R_i/b = \left\lceil \cos(\theta - \gamma_i) \right\rceil^{-1},$ (66)

where b is the apothem. The relation given in Eq. (66) is used directly for the numerical calculation. The dimensionless wave numbers, which are complex in nature, are computed by fixing Ω for $0 < \Omega \le 1.0$ using secant method (applicable for complex roots). The basic independent modes like longitudinal and flexural modes of vibration are analyzed and the corresponding non-dimensional wave numbers are computed. The polygonal cross-sectional bar in the range $\theta = 0$ and $\theta = \pi$ is divided into many segments for convergence of wave number in such a way that the distance between any two segments is negligible. The computation of Fourier coefficients given in Eq. (44) is carried out using the five point Gaussian quadrature.



Fig. 1. Geometry of ring shaped polygonal plates

Longitudinal modes of polygonal plates. In case of longitudinal vibration of square and hexagonal cross-sectional plates, the displacements are symmetrical about both major and minor axes, since both the cross-sections are symmetric about both the axes. Therefore the frequency equation is obtained by choosing both terms of n and m as 0, 2, 4, 6... in Eq. (46). During flexural motion, the displacements are anti-symmetrical about the major axis and symmetrical about the minor axis. Hence the frequency equation is obtained by choosing n, m=1, 3, 5 in Eq. (46).

Flexural modes of polygonal plates. In flexural mode of square and hexagonal crosssection, the vibration and displacements are antisymmetrical about the major axis and symmetrical about the minor axis The vibrational displacements are symmetrical about the x axis for the longitudinal mode and anti-symmetrical about the y axis for the flexural mode in the triangular and pentagonal cross-sectional plates, since the cross-section is symmetric about only one axis. Therefore n and m are chosen as 0, 1, 2, 3... in Eq. (47) for the longitudinal mode and n, m=1, 2, 3... in Eq. (47) for the flexural mode.

Dispersion analysis. The variation of circumferential stress $\sigma_{\theta\theta}$ with the nonhomogeneous parameter m is discussed for different cross section of the magneto electro elastic plate in Fig. 2. It is clear that, the circumferential stress propagation behavior which is caused by the non-homogeneous parameter m is decreasing in all the cross section of the plates. Fig. 3 shows the variation of the radial stress σ_{rr} with respect to the non-homogeneous parameter m of the magneto electro elastic plate for various cross section of the magneto electro elastic plate. From the curves in Fig. 3, it is clear that the radial stresses are higher in lower non-homogeneous parameter m and decreases slowly in the remaining range with small oscillation in the hexagonal plate. The parameter m is effective in the stress distribution of the entire cross sectional plate.

Figure 4 depicts the variation of the radial strain e_{rr} with respect to the nonhomogeneous parameter m of the magneto electro elastic polygonal cross sectional plate. In Fig. 4, the radial strain obtain the positive values in the range $0 \le m \le 0.075$ for all cross sectional plates, then the radial strain distribution goes on increasing and vanishes on the domain $m \ge 0.25$. The trend is same in circumferential strain $e_{\theta\theta}$ in Fig. 5 for all type of cross sectional plates, except there is a small deviation in the starting range of the nonhomogeneous parameter m.



Fig. 2. Variation of circumferential stress versus parameter m for different cross sections of the plate



Fig. 3. Variation of radial stress versus parameter m for different cross sections of the plate



Fig. 4. Variation of radial strain versus parameter m for different cross sections of the plate



Fig. 5. Variation of circumferential strain versus parameter m for different cross sections of the plate



Fig. 6. Variation of induced electric field versus parameter m for different cross sections of the plate



Fig. 7. Variation of induced magnetic field versus parameter m for different cross sections of the plate

A graph is drawn between the variations of induced electric field versus the nonhomogeneous parameter m of magneto electro elastic plate of polygonal cross sections in Fig.6. From the Fig.6, it is clear that the displacement of induced electrical energy is getting negative values in the range $0 \le m \le 0.1$, but for the higher values of m it becomes constant for all the cross sections of the plate. The transfer of electrical energy is higher in the lower values of the parameter m as compared to the higher values and this cross over point represents the transfer of electrical energy between modes of vibration of polygonal plates. The variation of the induced magnetic field versus the non-homogeneous parameter m of magneto electro elastic polygonal plates is analyzed in Fig. 7. From these curves it is clear that in the entire cross sectional plates, the induced magnetic field takes negative values in the range $0.01 \le m \le 0.15$ but for $m \ge 0.15$ slowly it vanishes.

7. Conclusion

The effect of magnetic field and non-homogeneity in a piezoelectric plate of polygonal cross sections is studied using the linear theory of elasticity. The wave equation of motion based on two-dimensional theory of elasticity is applied under the plane strain assumption of plate of polygonal shape, composed of homogeneous transversely isotropic material. The frequency equations are obtained by satisfying the irregular boundary conditions of the polygonal plate using Fourier expansion collocation method. The analytical results obtained in the physical domain have been computed numerically for a magneto electro elastic material. The numerically analyzed results for the stress, strain, displacements and induced electric and magnetic fields have been presented graphically. The polygonal plates, as structural elements, are widely used in construction of oil pipes, submarine and flight structures to ensure the strength and reliability, acted upon by nonuniform loads.

Appendix A

$$\begin{split} e_{n}^{1} &= \begin{bmatrix} (\beta(\beta-1)J_{\beta}(\alpha r) + (\alpha r)J_{\beta+1}(\alpha r))(\overline{L} + \sin^{2}(\theta - \gamma_{i})) - (\beta(\beta+1)J_{\beta}(\alpha r) + (\alpha r)J_{\beta+1}(\alpha r)) \\ (\overline{L} + \cos^{2}(\theta - \gamma_{i})) + (\alpha r)^{2}((1 + \overline{L})\cos^{2}(\theta - \gamma_{i}) + \overline{L}\sin^{2}(\theta - \gamma_{i}))J_{\beta}(\alpha r) \\ &- n\{(\beta-1)J_{\beta}(\alpha r) + (\alpha r)J_{\beta+1}(\alpha r)\}\sin 2(\theta - \gamma_{i})\sin n\theta \\ e_{n}^{1} &= \begin{bmatrix} (\beta(\beta-1)J_{\beta}(\alpha r) + (\alpha r)J_{\beta+1}(\alpha r))(\overline{L} + \sin^{2}(\theta - \gamma_{i})) - (\beta(\beta+1)J_{\beta}(\alpha r) + (\alpha r)J_{\beta+1}(\alpha r)) \\ (\overline{L} + \cos^{2}(\theta - \gamma_{i})) + (\alpha r)^{2}((1 + \overline{L})\cos^{2}(\theta - \gamma_{i}) + \overline{L}\sin^{2}(\theta - \gamma_{i}))J_{\beta}(\alpha r) \\ &- n\{(\beta-1)J_{\beta}(\alpha r) + (\alpha r)J_{\beta+1}(\alpha r)\}\sin 2(\theta - \gamma_{i})\sin n\theta \\ e_{n}^{2} &= 0 \qquad e_{n}^{3} = 0 \\ e_{n}^{4} &= \begin{bmatrix} (n(\delta-1)J_{\delta}(kr) + (kr)J_{\delta+1}(kr))\cos 2(\theta - \gamma_{i})\cos n\theta \\ - (\delta(\frac{\delta+1}{2}) + (\frac{n^{2}-(kr)^{2}}{2})J_{\delta}(\alpha r) + (\alpha r)J_{\delta+1}(\alpha r) \end{bmatrix} \end{bmatrix}\sin 2(\theta - \gamma_{i})\sin n\theta \\ f_{n}^{1} &= \begin{bmatrix} 2(\beta J_{\beta}(\alpha r) - (\alpha r)J_{\beta+1}(\alpha r)) + ((\alpha r)^{2} - \beta^{2} - n^{2})J_{\beta}(\alpha r) \\ - \cos n\theta \sin 2(\theta - \gamma_{i})\sin n\theta \end{bmatrix} \\ f_{n}^{1} &= \begin{bmatrix} 2n(\delta J_{\delta}(kr) - (kr)J_{\delta+1}(kr)) \cos n\theta \sin 2(\theta - \gamma_{i}) \\ + 2n\{(\beta-1)J_{\beta}(\alpha r) - (\alpha r)J_{\beta+1}(\alpha r)\}\cos n\theta \sin 2(\theta - \gamma_{i}) \\ + 2n\{(\beta-1)J_{\beta}(\alpha r) - (\alpha r)J_{\beta+1}(kr))\cos n\theta \sin 2(\theta - \gamma_{i}) \\ + 2n\{(\beta-1)J_{\beta}(\alpha r) - (\alpha r)J_{\beta+1}(kr)\}\cos 2(\theta - \gamma_{i})\sin n\theta \end{bmatrix} \\ \sin n\theta \cos 2(\theta - \gamma_{i}) \\ + 2n\{(\beta-1)J_{\beta}(\alpha r) - (\alpha r)J_{\beta+1}(\alpha r)\}\cos 2(\theta - \gamma_{i})\sin n\theta \end{bmatrix}$$

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STATISTICAL CHARACTERISTICS OF A QUASI-BREATHER WITH A HARD TYPE OF NONLINEARITY IN A CUAU CRYSTAL

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Abstract. By the method of molecular dynamics a study in the work is made of the statistical characteristics of a quasi-breather in a model CuAu crystal. The phonon spectrum of this model crystal, the dependences of mean-square deviation, the coefficient of variation and the average frequency of the model quasi-breather on the time of its existence are obtained. The statistical data analysis allows for the conclusion that the quasi-breather model solution in the model considered (which uses the interatomic potential obtained by means of embedded atom method (EAM)) slightly differs from the one in the corresponding exact breather. **Keywords:** quasi-breather, discrete breather, nonlinear dynamics, soliton

1. Introduction

Solitary waves are among the most interesting and important objects of nonlinear physics relevant for practical applications [1, 2]. Despite the fact that solitons were discovered more than 180 years ago, the number of studies devoted to their properties is still growing. Recently, there has been growing interest in the investigation of discrete nonlinear systems where the existence of dynamic solitons is possible. High-amplitude, spatially localized time-periodic vibrational modes in nonlinear crystals with translational symmetry called discrete breathers (DBs) belong to the class of the above mentioned dynamical solitons [3].

There are experimental evidences of formation of such localized excitations in different physical systems, including spin lattices in antiferromagnets [4], the lattices of coupled nonlinear optical waveguides [5], the assemblies of micromechanical oscillators [6]. The application of such systems as an element base of promising radio-frequency filters, magnetometers and other devices [7] determines not only a fundamental but also a practical interest for the breathers.

Discrete breathers can be divided into two types based on the nature of their frequency dependence on the amplitude [8]. In soft-type discrete breathers the frequency decreases as its amplitude grows (such discrete breathers can only exist in the crystals having a slot in the phonon spectrum: their frequency lies in the phonon spectrum slot, and therefore they are called slotted), while a reverse situation occurs with the hard-type discrete breathers (they may have frequencies both in the slot and above the phonon spectrum). Discrete breathers with a soft-type of nonlinearity can be excited in diatomic crystals, for example, in NaCl [8], Pt₃Al [9-14], as well as in graphene and grafane [15]. Breathers with a hard type of nonlinearity exist in pure metals with FCC –, BCC –, and HCP – structures.

Depending on the problem formulation we speak of the discrete breathers with either an infinite lifetime (in this case, the solution is always periodic in time [15] and the corresponding family of trajectories has a null measure) or with a finite lifetime, so-called

quasi-breathers - such solutions have a non-zero probability measure and can be implemented in physical systems or in statistical numerical experiments [16]. A discrete breather, as a strictly time-periodic object, is obtained by means of numerical simulation only provided that the initial conditions of the Cauchy problem are perfectly set for a certain diversity of small dimension in the multidimensional space of all possible initial values of coordinates of individual particles and their velocities. Such fine-tuning is difficult to fulfill even within a computational experiment. Moreover, it is practically impossible to do when performing any physical experiments, particularly in cases when the breather-like objects arise spontaneously.

Therefore, the paper [16] proposed the concept of quasi-breathers as some dynamic objects localized in space, but not strictly time-periodic. For that purpose, a certain criterion of proximity of a quasi-breather to its corresponding exact breather was formulated. It is based on the calculation of mean-square deviation $\eta(t_k)$ of the oscillation frequencies of selected breather particles found at some interval in the vicinity of time t_k , and calculating the mean-square deviation of the oscillation frequencies of a selected j-th breather particle at different time intervals.

The objective of this paper is to fulfill a statistical evaluation of quasi-breathers characteristics in a model CuAu crystal. In this formulation, we will identify the concept of quasi-breather and quasi-breather model solution. The molecular dynamics method was selected as a research method in our paper. The choice of the method is due to a number of factors. Discrete breathers are very difficult to observe in a full-scale experiment given the fact that they are not topological defects; they have a lifetime of several thousand periods of atomic oscillations, which is about 0.1ns. Besides, they can move at high velocities in metals. At the same time, computer simulation has become a very successful research method in condensed matter physics and materials science. This fact is due to the continuous power growth and availability of computers, development and software implementation of numerical methods. Being based on the well-tested interatomic potentials, the molecular dynamics method is one of the most effective methods of studying discrete breathers. When we speak of the molecular dynamics method in more detail, it should be noted that it provides an opportunity to solve the issues related to the problems of structural energy transformations both in crystalline and non-crystalline materials. Besides, this method makes it possible to design many properties of the system both thermodynamical (e.g., energy, pressure, entropy) and kinetic (diffusion coefficients, frequencies of atom oscillations). Moreover, the process dynamics is studied on a real time basis in this method.

2. Model description and experimental procedure

We considered the biatomic system CuAu. As it has already been mentioned above, the investigation was performed by means of the well-known molecular dynamics method. This method was implemented using LAMMPS Molecular Dynamics Simulation, the package for modular dynamic modeling [17], which uses well-tested many-body interatomic potentials built according to the embedded atom method (EAM-potentials).

We considered a three-dimensional crystal containing 48000 atoms (Fig. 1). Periodic boundary conditions were imposed along all directions.



Fig. 1. The view of a 3D CuAu crystal containing 48000 atoms

The potential obtained by the method described in [18] for the Cu-Au system was used in the calculations. The process of selecting the interatomic potentials is an important task worth a detailed consideration. The home-made software [18] generates EAM-potentials of alloys using the rapid fitting procedure by combining the previously developed elemental potentials. More specifically, we applied the Finnis-Sinclair potentials for alloys determining the energy of each atom in the system, using the expression:

$$U_{i} = F_{\alpha} \left(\sum_{i \neq j} \rho_{\alpha} \beta(r_{ij}) \right) + \frac{1}{2} \sum_{i \neq j} \phi_{\alpha} \beta(r_{ij}).$$

$$\tag{1}$$

This equation consists of three types of functions: embedding functions (F), electron density functions (ρ), and pairwise interaction functions (φ). In this formula there is an embedding function for each element type, one electron density function for each permutation of two types of atoms (a, p), and a pairwise interaction function for each combination. For binary potentials, there are only three functions that need to be selected in case of using elementary conditions from existing potentials: $\rho_{\alpha\beta}$, $\rho_{\beta\alpha}$, and $\varphi_{\alpha\beta}$. Since there are no triple conditions in the Finnis-Sinclair formula, potentials with more than two elements can be created by combining all the information contained in the binary files. The method proposed by the authors of the article allows to combine elemental EAM potentials and to establish the potentials for alloys using the density functional theory (DFT) data.

Firstly, the approach of simple "rule of mixtures" is used for compensation of the difference between the lattice parameters and elasticity modulus predicted by the DFT and measured experimentally. The elastic moduli and lattice parameters calculated for intermetallic compounds are multiplied by the effective correction factor, which is the average of the elementary correction factors taken in the proportion of elements fractions. Secondly, single-element potentials are adapted to improve compatibility in binary and multicomponent potentials in such a way as to preserve all the initial states of the system. Thirdly, in the case of bonding of two elemental potentials, the maximum cut off distance is adopted for the binary potential. The electron density functions and the interaction of the original pair potentials are available in a tabular format with functions defined at discrete points, this implementation uses cubic spline interpolation in order to calculate the values of functions in between the tabulated points.

The next step was the installation of cross-potentials. The Finnis-Sinclair composition for the EAM potential is used for every alloy potential considered. For a binary system, two embedding functions (F_{α} , F_{β}), four electron density functions ($f_{\alpha\alpha\beta}$, $f_{\beta\beta}$, $f_{\beta\beta}$) and three pair interaction functions ($\phi_{\alpha\alpha\beta}$, $\phi_{\beta\beta}$) are used. Similarly to the case of single-component potentials, two-component ones are combined by converting the embedded function so that it exists on the same interval and assumes the maximum cut off radius. While the "pure" elemental potentials are used to create each double file, the electron density and interaction functions of the pair contained in the original binaries are sufficient to create higher-order potentials without any additional equipment. In addition, the properties of each binary system and the original pure elements remain in these new potentials. The potentials created by means of the proposed technique were confirmed by comparison with the experimental results and existing potentials for the alloys. In addition, the dependence of the accuracy of binary potentials on the source of elementary potentials was estimated.

In order to analyze the possibility of the existence of DBs in CuAu crystal, the density of the phonon states of the crystal was calculated (see Fig. 2). The absence of a gap in the CuAu phonon spectrum dictates the impossibility of DB with soft nonlinearity type in this system. [19, 20]. This was confirmed in [21].



Fig. 2. The density of phonon states of CuAu crystal

The process of searching for discrete breathers in crystals involves selecting initial conditions-deviations of atoms from the equilibrium position or setting initial velocities.

For pure metals or alloys with a small difference in the atomic masses of the components, the excitation of DBs with a hard type of nonlinearity has some peculiarities. Thus, the authors of [19] proposed an ansatz for excitation of DBs in pure fcc and bcc metals, setting the DB profile in a closely packed atomic row by setting atomic displacements and velocities according to physically motivated functions. The displacements of the atoms were realized in such a way that the neighboring atoms oscillated in antiphase [22].

The Gaussian function (2), adapted for crystal conditions was used to excite a DB in the CuAu crystal

$$f(x) = A_0 e^{-\frac{x^2}{2C^2}},$$
(2)

where A_0 defines the initial amplitude of the central atoms of a DB, x is the relative coordinate of a pair of atoms in a row, and parameter C is the degree of spatial localization of DB. Varying the values A_0 and C, we select the profile of the discrete breather, thereby setting the initial deviations from the equilibrium position for the atoms included in the DB oscillations.

Unlike the exact discrete breathers, quasi-breathers are not dynamic objects strictly periodic in time, although they are localized in space. They arise in any sufficiently small deviations from the exact breather solutions in multidimensional space of any and all initial conditions while solving the Cauchy problem for the original differential equations, since there is no complete suppression of contributions from the oscillations of peripheral particles with their natural frequencies in this case. Thus, "dictatorship weakening" on the part of the breather nucleus (a single central particle forms a nucleus as well in case of a symmetric breather considered by us, and it is being formed by its two central particles in case of an antisymmetrical breather) leads to the presence of small contributions with different frequencies in the breather solution. These small contributions may be detected in the oscillations of all chain particles including the central ones. If we estimate (with reasonable precision) the oscillation frequencies of all quasi-breather particles calculated at a certain time interval near $t = t_k$, they will not be strictly identical. In light of this, let us find the mean-square deviations $\eta(t_k)$ of the oscillation frequency of different breather particles from the average breather frequency ϖ :

$$\overline{\omega}(t_k) = \frac{1}{N} \sum_{i=1}^{N} \omega_i(t_k), \qquad (3)$$

$$\eta(t_k) = \sqrt{\frac{\sum_{i=1}^{N} (\omega_i(t_k) - \overline{\omega}(t_k))^2}{N(N-1)}}. \qquad (4)$$

The more the value $\eta(t_k)$, the more the quasi-breather solution differs from the exact breather solution, for which $\eta(t_k)=0$ at any particular time t_k .

3. Results and discussion

The distribution of the phonon modes, i.e. the crystal phonon spectrum is important for the existence of quasi-breather on a first-priority basis. The reduced density of the phonon states of CuAu was compared with the oscillation frequencies of the quasibreather. Below is a calculation of the statistical characteristics of a quasi-breather.

The dependence of the model quasi-breather mean-square deviation η on its lifetime t_k is shown in Fig. 3.



Fig. 3. Dependence of the model quasi-breather mean-square deviation η on its lifetime t_k (in picoseconds (ps))

Statistical characteristics of a quasi-breather with a hard type of nonlinearity in a CuAu crystal

The mean-square deviation characterizes the measure of data scattering. In our case, this is a deviation of peripherical atom frequencies of model quasi-breather from the quasi-breather nucleus frequency. It is apparent from Fig. 3 that the quasi-breather mean-square deviation ranges from 0.01261065 to 0.02610272, which is equivalent to slight scattering of peripheral atom frequency from the model quasi-breather nucleus frequency.

The mean-square deviation gives an absolute estimation of the measure of spread. Therefore, in order to understand how much variation is large relative to the values themselves (i.e., regardless of their scale), a relative index is required. Such an indicator is called the coefficient of variation and is calculated by the following formula:

$$V = \frac{\eta}{\omega_{cp.}}.$$
(5)

By this indicator, it is possible to compare the homogeneity of the most diverse phenomena, regardless of their scale and units of measurement. Table 1 shows the exponents of the coefficient of variation of V from the lifetime of the quasi-breather t_k .

Table 1. The exponent of the coefficient of variation of V from the lifetime of the quasibriser tk (in ps)

t_k	V	
5	0.00220377958477173	
10	0.00286022261352874	
15	0.00374032727309376	
20	0.00435946841613917	
25	0.00491586066089457	
		_

The dependence of the model quasi-breather mean frequency ω_{mean} on its lifetime t_k is shown in Fig. 4.



Fig. 4. Dependence of the model quasi-breather mean frequency ω_{mean} (in THz) on its lifetime t_k (in ps)

It is apparent from Fig. 3 and 4 that the deviation of the model quasi-breather frequency of peripherical atoms from the quasi-breather nucleus frequency is extremely negligible. Moreover, the medium frequency ranges from 5.30989773163211 THz to 5.72228656205187 THz.

For a group of atoms contained in the model quasi-breather, the mathematical expectation (the sample mean) of an ungrouped sample of the mean frequencies (5.72228656205187, 5.60811384473751, 5.39908960106847, 5.39342834099743, 5.30989773163211) is calculated by the formula:

$$M = \frac{1}{N} \sum_{i=1}^{N} X_i \,.$$
(5)

The mathematical expectation of the initial sample is 5.486563 THz, which is slightly higher than the upper limit of the phonon spectrum of the CuAu crystal (see Fig. 2).

The variance of the same ungrouped sample is calculated by the formula:

$$D = \frac{1}{N-1} \sum_{i=1}^{N} (X_i - M).$$
(6)

The result of the calculation by the formula above is 0.0229469. The obtained values show that within the framework of this model of the CuAu crystal, one can speak of the proximity of the model quasi-breather to the corresponding exact breather. Besides, the following statistical characteristics and functions were calculated within the limits of this model: grouped statistical array of absolute and relative frequencies, range of absolute and relative frequencies, histogram of relative frequencies, empirical distribution function.

4. Conclusion

The statistical characteristics of a quasi-breather with the hard type of nonlinearity were calculated by means of the molecular dynamics method. The main characteristics include the mean square deviation of the frequencies of some particular atoms in the breather from the mean value of the quasi-breather core frequency, as well as the coefficient of variation at different stages of life of the object under study.

It should be noted that the final quasi-breather destruction occurs at the moment when the frequencies mean square deviation exceeds the difference between the quasi-breather mean frequency and the crystal phonon spectrum upper boundary. At this moment the oscillations delocalization and the energy dissipation through the crystal in the form of lowamplitude thermal lattice vibrations occur. It is shown that the obtained quasi-breather is slightly different from the corresponding exact breather. This may indicate the stability of the obtained discrete breather in the model cells and the possibility of its excitation in real alloys of the composition examined in the work

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AB INITIO CALCULATIONS OF STRUCTURAL AND THERMAL PROPERTIES OF WURTZITE ZN_{1-X}CD_XO ALLOYS WITH DEBYE-GRUNEISEN MODEL

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Abstract. In this paper, structural and thermal properties of Zn1-xCdxO alloys for x=0, 0.125, 0.25, 0.375, 0.5, and 0.625 have been investigated by Ab initio calculations method. Both lattice constants a and c of wurtzite structure follow Vegard's law and are in a good agreement with the experimental data for x=0. The diagrams of specific heat at constant volume versus temperature for different values of x have been plotted and values of specific heat at constant pressure for different concentrations of x at 300K, 600K and 900K have been obtained. The value of specific heat at constant pressure for ZnO has a good consistency with experimental data. Specific heat at constant volume increased by increasing temperature and specific heat at constant pressure decreased by increasing x. The diagrams of Debye temperature versus x at 0K, 300K, 600K and 900K have been plotted, too. These diagrams state that Debye temperature decreases by increasing x or increasing temperature.

Keywords: ab initio calculations, thermal properties, Debye-Gruneisen model, $Zn_{1-x}Cd_xO$ alloy.

1. Introduction

Wurtzite Zn1-xCdxO ternary alloys were investigated because of applications for the light emitting diodes. For this reason, the study of the thermodynamic properties of the $Zn_{1-x}Cd_xO$ ternary alloy is very significant in the point of view of the fabrication of effective LEDs [1].

So far, Wang Zhi et al. [2], have obtained structural and corrected band properties of $Zn_{1-x}Cd_xO$ by first principle study. They found that the band gap decreases by increasing concentration of Cd. Xin Tang et al. [3], have investigated the doping stability and electronic structure of $Zn_{1-x}Cd_xO$. They found that by increasing Cd concentration, formation enthalpy of $Zn_{1-x}Cd_xO$ alloy increases. I.I. Shtepliuk et al. obtained the critical temperature for $Zn_{1-x}Cd_xO$ system about 1140K. Yabin Chen et al. [4], have investigated pressure-induced structural transition of $Zn_{1-x}Cd_xO$ alloys. According to their experiment, at x=0.67 where the alloy is intrinsically stable in the rock-salt phase even at ambient pressure.

Since theoretical works on electronic properties were successful [2, 3], we decided to investigate the structural and thermal properties of $Zn_{1-x}Cd_xO$ for x=0, 0.125, 0.25, 0.375, 0.5, 0.625 by Debye-Gruneisen model that scarcely has been paid attention by researchers.

In this paper, in addition to obtaining the related lattice constants and testing the correction of Vegard's law about them the thermal quantities like, specific heats at constant volume and pressure, Debye temperature at different temperatures and concentration of x have been investigated.

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2. Computational Details

The calculations are on the basis of Density Functional Theory (DFT). Ab initio calculations have been done by Quantum Espresso [5] package. The exchange correlation functional GGA(PBE) has been used. In these calculations the cut off energy equals 60 Rydberg and uniformed k-mesh 5*5*5 has been considered. Using third-order Brich-Murnaghun Eos, the fitting of energy versus volume data was done by code Gibbs 2 [6, 7] and the thermal properties also were calculated by this code.

In code Gibbs 2, non-equilibrium Gibbs function is written in the following form: $G^{*}(V; P, T) = E(V) + PV + A_{vib}[\theta_{D}(V), T],$ (1)

where E(V) is the total energy per unit cell, PV is corresponding hydrostatic pressure conditions, $\theta_D(V)$ is Debye temperature and A_{vib} is vibration term which can be written as:

$$A_{vib} = nk_B T \left[\frac{9\theta}{8T} + 3\ln(1 - e^{\frac{-\theta}{T}}) - D(\frac{\theta}{T})\right].$$
(2)

In above relation $D(\frac{\theta}{T})$ is Debye integral. In quasi-harmonic model Debye temperature

can be obtained by:

$$\theta_{D}(V) = \theta_{D}(V_{0}) \frac{(B_{Stat} / B_{0})^{b}}{(V / V_{0})^{a}},$$
(3)

where V_0 and B_0 are equilibrium volume and bulk modulus, respectively. The values of parameters *a* and *b* are assumed to be -0.5 and 0.5, respectively in the Dugdale-McDonald approximation [7].

By minimizing non-equilibrium Gibbs Free energy proportional to volume, the thermal properties of the system like C_v and C_p can be calculated.

3. Results and Discussions

Structural Properties. The diagrams of lattice constants of $Zn_{1-x}Cd_xO$ alloy versus *x* have been shown in Fig.1.



Fig. 1. The diagrams of lattice constants of $Zn_{1-x}Cd_xO$ alloy versus x

It is obvious that the lattice constants increase by increasing concentration of Cd. It is because of weaker bonding of CdO than ZnO due to more ionic bonding of ZnO than CdO caused by higher difference of electronegativity between Zn (1.65) and O (3.44) than Cd (1.69) and O (3.44). Also, more atomic radius of Cadmium and more distance of valence electrons from nucleus of Cd might be the other reasons of weaker bonding of wurtzite ZnO. The experimental results confirm above sentences where binding energy of wurtzite ZnO is 7.52(ev/pair) [9], while, as we know, the highest calculated value of wurtzite CdO binding energy equals 5.97(ev/pair) [9].

Our calculated lattice constants a and c at different concentration of Cd together with experimental and other theoretical values results are listed in Table 1.

experimental and medicilear results in ringstrom unit						
	X=0	X=0.125	X=0.25	X=0.375	X=0.5	X=0.625
Present work	a=3.2496,	a=3.31,	a=3.3767,	a=3.4323,	a=3.4831,	a=3.514,
	c=5.1993	c=5.3	c=5.4027	c=5.4917	c=5.5729	c=5.622
Experimental	a=3.2496,					
work [8]	c=5.2042	-	-	-	-	-
Theoretical	a=3.286,					
work [8]	c=5.241	-	-	-	-	-

Table 1. Calculated lattice constants *a* and *c* at different concentration of Cd together with experimental and theoretical results in Angstrom unit

Lattice constants of $Zn_{1-x}Cd_xO$ alloy follow Vegard's law and experiment confirms this result up to *x*=0.69[2]. The reasons of following lattice constants from Vegard's law include:

i) The relative atomic sizes of the elements;

ii) The relative volume per valence electron in crystals of the pure elements;

iii) Brillouin-zone effects;

iv) electrochemical differences between the elements [10].

Thermal properties. The diagrams of specific heat at constant volume versus temperature for different values of x for $Zn_{1-x}Cd_xO$ have been plotted in Fig. 2. The diagrams at low temperatures have T^3 behavior and at high temperatures tend to saturation limit.



Fig. 2. The diagrams of variations of specific heat at constant volume by increasing temperature at different concentration of Cd

The diagrams of specific heat at constant pressure of $Zn_{1-x}Cd_xO$ at 300K, 600K and 900K and different Cd concentrations have been shown in Fig. 3. At low temperatures, the specific heat depends on strength of bonding between atoms and their molecular mass. Because of weaker bonding between cadmium and oxygen in comparison with zinc and oxygen plus heavier molecular mass of cadmium oxide than zinc oxide that decreases the velocity of phonon vibrations, the Specific heat at constant pressure and low temperatures decreases linearly by doping of Cd atoms as it is confirmed with our calculations. At higher temperatures due to ionic nature of these bonding, Coulomb interactions have the most important role in optical modes. Hence, the specific heats of this alloy decrease with increasing Cd concentration because of higher lattice constants, higher difference of electronegativity of ZnO wurtzite than CdO wurtzite and more screening of ionic potential in cadmium.



Fig. 3. The diagrams of variations of specific heat at constant pressure of $Zn_{1-x}Cd_xO$ at 300K, 600K and 900K



Fig. 4. The diagrams of Debye temperature versus x at 0K, 300K, 600K and 900K

As we know from literatures, Debye temperature is the highest temperature that can be achieved due to a single vibration in alloys and has a direct relation with static bulk modulus. The diagrams of Debye temperature of $Zn_{1-x}Cd_xO$ versus *x* at different temperatures have been shown in Fig. 4. As it is seen, Debye temperature decreases by increasing the concentration of Cd in $Zn_{1-x}Cd_xO$ so that the difference of this parameter is about 130K when *x* varies between 0 and 0.67.

4. Conclusion

and thermal properties of $Zn_{1-x}Cd_xO$ In this paper, structural alloy for x=0, 0.125, 0.25, 0.5, 0.625 have been investigated. The values of lattice constants a and cwere calculated 3.2496 and 5.1993, respectively, for x=0 which are in good agreement with the experimental and theoretical reports. Also lattice constants for different values of x follow Vegard's law. The diagrams of specific heat at constant volume at low temperatures have T^3 behavior and at high temperatures tend to saturation limit. Specific heat at constant pressure versus x at 300K, 600K and 900K has been plotted. Specific heat at constant pressure decreases linearly by increasing x and specific heats increases by increasing temperature. Debye temperature diagram versus x at different temperature shows to be decreased by increasing x and temperature.

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ADAPTATION OF THE MAGNETIC PULSE METHOD FOR CONDUCTIVE MATERIALS TESTING

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Abstract. The paper presents the results of experimental testing by magnetic-pulse method of Cu-ETP samples with crack type macro defect. Three-dimensional modeling of the magnetic field in the loading device -sample system was performed, on the basis of which the magnetic pressure was calculated and mechanical simulation was performed with Johnson-Cook plasticity model and fracture criteria. Comparison of the obtained results of residual deformation indicates the applicability of Johnson Cook plasticity model for OFHC copper for describing the behavior of Copper ETP in the deformation rate range up to 10^4 1/s. **Keywords:** high speed deformation, magnetic-pulse loading, Johnson-Cook plasticity model

1. Introduction

Using of the magnetic-pulse method for creation controlled pressure pulses with microsecond duration for study of pulse strength of brittle nonconductive materials allowed to reveal a number of general consistent patterns of deformation process [1, 2, 3]. Applying of the thermodynamic approach for analysis of the results allowed to obtain the characteristic relation between extreme deformation loads and their duration, and specific for each material parameter - the time of energy accumulation [4]. Main feature of magnetic-pulse method of loading is the ability to form stress states, in which there are no loading modes with preliminary material compression, typical for spalling deformation tests. The realization of this feature is especially important in the testing of composite and laminate materials with an explicit spatial anisotropy of deformation characteristics.

The aim of the work is to substantiate and experimentally confirm the possibility of testing conductive samples in high-speed deformation modes and to identify possible limitations associated with the influence of the current induced in the sample on the deformation curves of the metal.

2. Pressure forming by the magnetic-pulse loading

The use of magnetic-pulse method, described in [4], for forming a load on a conducting sample can lead to a change in the ratios of the current pulse parameters flowing along the magnetic-pulse driver (hereinafter MPD) and the parameters of the pressure transferred to the sample.

The impact of conducting sample presence was studied with the use of numerical simulation in the environment Comsol Multiphysics. Process of generating a magnetic field in a MPD-sample system with geometric dimensions corresponding to dimensions of the sample used in the experiment. Simulation was performed for the MPD with length 15 mm. The main view of test sample with installed MPD is shown in Fig. 1.



Fig. 1. Test sample (O) with installed magnetic-pulse driver (insulation is not shown)

The results of magnetic field simulation for simple and quasi-coaxial MPD with the width c_{mpd} =7.8 mm and samples with different conductivity are shown in Fig. 2.



Fig. 2. Distribution of magnetic field induction at the moment of current maximum: a) simple MPD, conductive sample; b) quasi-coaxial MPD, conductive sample; c) simple MPD, conductive sample

Analysis of the results revealed some influence of the MPD width on the parameters of the pressure acting on the sample. This is due to the fact that in the system of flat busbars, under condition $c_{mpd} >> h_{mpd}$, magnetic pressure P_m is related to the MPD current I with a simple relation:

$$P_m = \mu_0 \cdot (I/c_{mpd})^2 / 2, \qquad (1)$$
where $\mu_0 = 4\pi \cdot 10^{-7}$ H/m, but this condition is not always satisfied during the experiment.
Real relations between ratio of magnetic pressure acting on the groove and calculated with the use of (1), during the impulse current flowing through MPD
 $i(t) = I_m sin\left(\frac{2\pi t}{T}\right)$
(2)
with the period $T=8$ us, close to the experimental one, and geometry peremeters of MPD are

with the period $T=8 \ \mu$ s, close to the experimental one, and geometry parameters of MPD are shown in Fig. 3. Simulation was provided varying the width of MPD c_{mpd} and saving the value of current density $I_m/c_{mpd} = 10 \ \text{kA/mm}$, where I_m - amplitude value of current for test sample with thickness c=2 mm, width and length b=a=30 mm, height of the groove h=3 mm, length of the groove l=15 mm (Fig. 1).



Fig. 3. Relations between ratio of magnetic pressure acting on the groove and calculated with the use of (1) and ratio of MPD busbars width and length between those busbars; 1 - simple MPD, 2 - quasi-coaxial MPD

The relations shown in Fig. 3 reveal that the increase of ratio c_{mpd}/h_{mpd} makes closer magnetic pressure to the pressure calculated with the use of (1). Since the calculation was performed for the experimental configuration of the sample, where groove height is constant, magnetic pressure formed by quasi-coaxial MPD exceeds the pressure formed by simple MPD with the same current in the branch of MPD.

3. Process of sample deformation under pulse loading

The simulation of elastic–plastic deformation of a copper busbar with macro defect of type of crack in the three-dimension setting was carried out using the ANSYS Autodyn environment [5]. Johnson-Cook (JC) plasticity model for OFHC copper [6] was selected as a calculation model of deformation.

JC plasticity model describes deformation process up to fracture, and the validity of use of JC plasticity model is confirmed by the good correspondence between calculated and experimental deformation curves for different plastically deformable materials at strain rates up to ~ 2000 1/s. The reliability of mentioned model for various metals is supported by its implementation in different programming environments, e.g. [5]. For instance, the applicability of JC model for description of the high-speed deformation process for steel 09G2S at strain rates up to 1500 1/s is shown in [7].

According to JC model the elastic limit of material varies depending on plastic strain, strain rate v_p , which must be equal or more then 1 s⁻¹, and temperature is described by the next expression

$$\sigma = \left[A + B\varepsilon_p^n\right] \cdot \left[1 + Cln\dot{\varepsilon}_p^*\right] \cdot \left[1 - T^{*m}\right],\tag{3}$$

where ε_p – is an effective plastic strain, $\dot{\varepsilon}_p^* = \dot{\varepsilon}_p / \dot{\varepsilon}_p^0$ is a standardized effective plastic strain rate ($\dot{\varepsilon}_p^0 = 1 \text{ s}^{-1}$), T^* is homologous temperature

$$T^* = (T - T_{room}) / (T_{melt} - T_{room}), \tag{4}$$

A = 90 MPa, B = 292 MPa, n = 0.31, C = 0.025, m = 1.09, $T_{melt} = 1082.9$ °C are model parameters.

JC fracture model similar to plasticity model is applied as the failure criterion: $D = \sum \frac{\Delta \varepsilon}{cf},$

$$\varepsilon^{f} = \left[D_{1} + D_{2} e^{D_{3} \sigma^{*}} \right] \cdot \left[1 + D_{4} ln \dot{\varepsilon}_{p}^{*} \right] \cdot \left[1 + D_{5} T^{*} \right], \tag{6}$$

(5)

where ε^{f} is an effective fracture strain, $D_{1} = 0.54$, $D_{2} = 4.89$, $D_{3} = -3.03$, $D_{4} = 0.014$, $D_{5} = 1.12$ – deformation model parameters. When the parameter *D* reaches the value 1, the material is destroyed.

As it is presented in [8], the character of the stress state is defined by the characteristic size of the sample *b* and the loading wavelength $\lambda = c_1 T$, where the condition $\lambda \ll b$ allows to realize a shock-wave mode of loading, otherwise quasi-static mode. Maximum von Mises stress forms in the zone near the top of the groove at uniform distribution of pulse pressure.

Deviation of deformation curve from linear as a result of plastic flow leads to sufficient reduce of acceptable stress, as it is shown in figure 4a in the case of shock-wave loading mode (curves 1, 2, 3). Herewith it is not possible to ensure high strain rate ε_p (Fig. 4). Transition to the quasi-static loading mode allows to expand the range of reachable stress and ensure greater deformations of material in the top of the groove, up to the fracture (Fig. 4, curve 4).



Fig. 4. Von Mises Stress (a) and strain (b) at the groove top. $1 - P_m = 250$ MPa, T = 8 µs (excluding plastic deformation); $2 - P_m = 250$ MPa, T = 8 µs, $\dot{\varepsilon}_p = 1600$ 1/s; $3 - P_m = 85$ MPa, T = 8 µs, $\dot{\varepsilon}_p = 500$ 1/s; $4 - P_m = 250$ MPa, T = 50 µs, $\dot{\varepsilon}_p = 90000$ 1/s; $5 - P_m = 85$ MPa, T = 50 µs, $\dot{\varepsilon}_p = 14000$ 1/s

The results of numerical simulation show that the impact of uniformly distributed pulse pressure on groove, created by MPD, allow to expand strain rate up to 10^5 1/s.

4. Experiment

The experimental setup - the pulse current generator GIT-50/12 was used for experimental study of deformation process [9] with the simple MPD loading scheme (Fig. 1). Current form, measured by Rogowski coil, was damped sinusoid, which can be described by $i(t) = I_m sin\left(\frac{2\pi t}{T}\right) \cdot e^{\left(\frac{-t}{\tau}\right)}$, (7) where $T = 5.9 \,\mu\text{s}$, $\tau = 5.6 \,\mu\text{s}$, the amplitude was determined by the test setup charging voltage, e.g. $I_m = 352 \,\text{kA}$ for No₂4.

Variation of pressure amplitude was reached by changing relation between current amplitude and MPD width. The dependence graph of relative values of groove opening -1 and precrack -2 to their initial height $D_i = h_e / h_i$, where h_e , h_i – height of a groove (a

precrack) after the experiment and initial respectively, and pressure amplitude, applied to the groove, relative to the yield stress is shown in Fig. 5.



Fig. 5. Dependence graph of relative values of precrack-I groove opening-II and applied pressure relative to the yield stress $-\sigma_y = 90$ MPa; *P* - pulse pressure form; A – photo of precrack opening of experimental samples; *JC* – calculated points

Correlation between experimental and simulation results of plastic deformation is shown in figure 5, wherein average calculated strain rate for the sample N_{2} was ~ 3 300 1/s and for the sample N_{4} was ~ 10000 1/s.

Complete fracture after the experiment of the sample N_{25} is observed (orange points in Fig. 5), whereas the results of calculation with the use of Johnson-Cook criterion for OFHC copper do not correspond conditions of fracture.

Induced current density in the top of the groove of the sample No4 reached ~ 35 kA/mm^2 , oscillation period ~ $5.7 \,\mu$ s, ratio of near amplitudes ~ 1.29. Joule heating caused the raise of temperature in the zone with induced current less than 18° C, which according to Johnson-Cook deformation model leads to the reduce of yield stress less than ~ 2 %.

Maximum of magnetic field induction in the top of sample groove reached 4.2 T, which corresponds the amplitude of magnetic pressure equal ~ 9 MPa, while the amplitude of magnetic pressure applied to the shores of the groove reached 421 MPa.

Analysis of experimental results revealed that thermal and force impact of induced currents was insufficient. Since the simulation does not include the impact of electroplastic effect and in the range of relatively low strain rates, experimental data and simulation results have a good correlation; it can be assumed that the impact of electroplastic effect during the action of currents with microsecond duration is not observed within the framework of used method.

It should be noted that in contrast with the data presented in [10–13] where the electroplastic effect was observed at current density 1 kA/mm² and impulse duration 60 μ s and more, the results of experiments with parameters described in this work revealed no impact of electroplastic effect at current densities ~ 20–40 kA/mm². This may be due to sufficiently less impulse duration or higher strain rate obtained in the experiment.

Further research implies the use of quasi-coaxial MPD, which will allow to exclude the impact of induced currents in the deformation zone, and external current source with the wide range of impulse parameters.

4. Conclusion

Analysis of simulation results showed the possibility of using magnetic-pulse method of deformation of conductive materials at strain rates up to $\sim 100\ 000\ 1/s$.

The results of experimental study have a good correlation with Johnson-Cook model up to strain rate 10^3 - 10^4 1/s, however deviation of calculated parameters from experimental data at the increase of a strain rate can be observed.

Experimental transition to higher strain rates will allow to receive data for Johnson-Cook model verification in a wider range of influences.

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ACCURACY IMPROVEMENT FOR COMBINED STATIC STRENGTH CRITERION FOR STRUCTURES UNDER COMPLEX LOADING E.V. Zenkov^{1*}, L.B. Tsvik²

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Abstract. The article deals with the relevance of the stress strain state (SSS) in areas of potential destruction for the assessment of deformed structures strength. The article develops a calculation and experimental method for building a combined strength criterion equation involving strength coefficients, introduced by Pisarenko-Lebedev criterion equation with regard to the real SSS type. The proposed method has been implemented and experimental mechanical tests were carried out for the selected samples which follow the idea that the SSS type in the active zone is identical to the SSS of the analyzed structure in the area of interest. Results of the calculations and experimental tests demonstrate a significant decrease in the limit strength value for 50CrV (high quality) under biaxial tension in comparison with the conventional limit strength value.

Keywords: modeling, stress strain state, limit state equation, prismatic sample, finite element method, strength parameters, biaxial stretching

1. Introduction

Strength analysis for deformed structures under multidirectional loads has to be carried out with regard to the stress strain state (SSS) type in the areas of potential destruction [1 - 6]. A large number of vital parts and elements with stress concentrators are used in machines and units of the transport, energy and petrochemical industries. Stress concentration near structural irregularities of different size and shape (fillets, holes, roundings, slots) is typical. Examples of such parts are choke parts of capacitive equipment [5], suspension system elements (levers, axes) [6], compressor and turbine discs [7], wrought wheels of the rolling stock [8], etc. The SSS near these concentrators is biaxial, and its most dangerous case is biaxial tension that affects the parts lifecycle and is able to cause the destruction under quasistatic loading [1 - 6].

According to the experimental data, the material strength under biaxial tension is different from the one under uniaxial tension [1, 9 - 11]. In this case, the static strength of the part calculated with regard to the traditional criteria can be erroneous if its material is under biaxial loading. The result of this error can cause premature destruction of the structure in the area where the stress level is not maximum for the whole structure. It can also cause an unjustified increase in the specific amount of metal per structure [3]. Thus, the SSS type which is ignored by conventional criteria, affects the strength.

The SSS type can be used by two methods. The first method is based on the Pisarenko-Lebedev, Yagna-Buzhinsky, and Drucker-Pragger strength criteria [1, 3]. The method involves the preliminary calculation of material strength properties by destroying the samples under different loads in a quasi-static way. The properties are as follows: uniaxial

Increasing the reliability the combined criteria of the static strength of a material of complexly loaded...

tension, compression and shear (respectively, determination of the values of σ_t , σ_c and τ_s). These criteria combine various weight factors and two summands corresponding to the shear destruction (the first summand) and the cleavage destruction (the second summand). A factor limiting the accuracy of the combined strength criteria is the difference of the real SSS type of the structure and the SSS type of the samples tested before destruction when calculating σ_t , σ_c and τ_s . Moreover, calculations of these values and the need for various laboratory tools complicate the implementation of the method.

Let us analyze the Pisarenko-Lebedev limit state equation [1, 3] which is used for the assessment of structures strength. The condition under which the quasi-static destruction of the material accompanied by crack formation occurs is as follows

$$\alpha \sigma_i^{lim} + (1 - \alpha) \sigma_1^{lim} A^{1-P} \le \sigma_t, \qquad (1)$$

where σ_i^{lim} is the stress intensity in the area of potential destruction

$$\sigma_{i}^{lim} = \frac{1}{\sqrt{2}} \sqrt{\left(\sigma_{1}^{lim} - \sigma_{2}^{lim}\right)^{2} + \left(\sigma_{2}^{lim} - \sigma_{3}^{lim}\right)^{2} + \left(\sigma_{3}^{lim} - \sigma_{1}^{lim}\right)^{2}}, \qquad (2)$$

 σ_1^{um} , σ_2^{um} , σ_3^{um} are primary stresses occurring in this area; *P* is the Smirnov-Alyaev coefficient [4, 5] characterizing the SSS type at the point under study. The coefficient is calculated by formula

$$P = \frac{\sigma_1^{lim} + \sigma_2^{lim} + \sigma_3^{lim}}{\sigma_i^{lim}},\tag{3}$$

(for biaxial tension P = 2, for uniaxial tension P = 1, for uniaxial compression P = -1, for uniaxial shearing P = 0); α and A are empirical constants characterizing the material strength independent of the SSS (*P*) and the SSS level (σ_i^{lim}) of the material in the area of destruction (hereinafter referred to as strength coefficients) calculated by formulas

$$\alpha = \frac{\sigma_{t}}{\sigma_{c}}, \quad A = \frac{\phi - \sqrt{3}\alpha}{1 - \alpha}, \quad \phi = \frac{\sigma_{t}}{\tau_{s}}.$$
(4)

Equation (1) takes into account the structural irregularity of the material, the ability to resist shearing and normal stresses. As mentioned above, in some cases, the accuracy of the criterion (1) is not sufficient due to differences between the real SSS type in the area of potential destruction and the SSS type for the samples tested before destruction when calculating σ_t , σ_c , τ_s and α and A. In [10 – 11], the authors argue that P calculated by equation (3) affects the area of destruction: with an increase in P (according to Smirnov-Alyaev, the rigidity of the SSS type), the limit stress intensity values and the first primary stress decrease.

The second method is based on the results of laboratory experiments carried out using special samples with the SSS type in the area of destruction similar to the SSS type in the area of potential destruction of the structure element. The results were accounted for in the deformation criteria [3]. The second method was implemented using special test equipment with several power drives (Fig. 1-a) creating multidirectional forces affecting the sample and special leverage mechanisms (Fig. 1-b) transforming a uniaxial force impact of the one-drive machine by levers linked to the sample into multidirectional forces affecting the sample. These samples, machines and mechanisms improve the accuracy of strength simulation and calculations but limit opportunities for carrying out the experiments.

The present article describes calculations and experiments carried out to improve the strength criterion which combines the elements of two methods. The combined criterion takes into account the real SSS type of the structure element in the area of potential destruction using typical one-drive testing machines. The use of experimental data on destruction of laboratory samples improved the calculations whose stress state at the moment of destruction simulates the stress state of the real structure in the working zone.



Fig. 1. Biaxial loading unit (a) and leverage mechanisms (b) for static tests under biaxial tension

2. Methods

The mathematical simulation method and modern engineering technologies can be used to solve the task set in the article. The FEM can be used for solving the task of body mechanics. To improve the strength criteria for structures under complex loading and strength calculation accuracy, strength coefficients α and A can be calculated by equation (1) with regard to the real type of the SSS of the loaded area of the structure. The general scheme of the method is presented in Fig. 2.



Fig.2. The scheme of improved strength calculations with regard to the real SSS type based on the combined strength criterion

Equation (1) shows that α and A are coefficients of the formula which describe the structural strength of amaterial with certain calculation values of σ_1^{lim} , σ_i^{lim} and P^{lim} (parameters σ_1^{lim} , σ_i^{lim}) at the moment of destruction at P^{lim} . From this perspective, the Pisarenko-Lebedev criterion can be transformed into the following equation:

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$$\alpha \sigma_i^{lim} + (1 - \alpha) \sigma_1^{lim} A^{1 - P^{lim}} \leq \sigma_t,$$

where α and A can be calculated from equation (5) with regard to its other parameters σ_1^{lim} , σ_i^{lim} and P^{lim} . That implies that α and A calculated from (1) do not have a conventional physical meaning resulting from the Pisarenko-Lebedev criterion. They depend on the SSS type of the material. Thus, α and A are coefficients of the empirical formula (hereinafter referred to as strength coefficients) considering the results for samples tested before destruction. They simulate the SSS type of the area of assessment.

The present article as well as the Pisarenko-Lebedev equation assumes the independence of α and A on the stress intensity σ_i and the first primary stress σ_1 in the area of potential destruction. Equation (5) approximates the real limit state equation built for a specific (or a relatively narrow range of modifications) value of P describing the SSS type. This type is determined by structural properties of samples tested before destruction. The area of destruction has to be characterized by P equal or close to P for the area of the structure.

After the value of *P* has been determined by the FEM used for solving the tasks of body mechanics to determine α and *A* from equation (5), it is necessary to match the type of the SSS of the samples and the type of the SSS of the structure. To this end, it is sufficient to test two samples before destruction. The samples have to have different sizes and SSS characteristics at the moment of destruction. Strength coefficients α and *A* can be calculated by the following algorithm:

- matching geometrical parameters of two different structural samples of special shapes with the values of P^{lim} which are close to the values of P for the area of the structure under study– $P^{1 lim}$ and $P^{2 lim}$;
- testing structural variants of the samples before destruction;
- calculating σ_1^{lim} and σ_i^{lim} which are the characteristics of the SSS level of equation (5) in the working area of the samples;
- calculating values of α and A from the system of equations

$$\alpha \sigma_{i}^{1 \lim} + (1 - \alpha) \sigma_{1}^{1 \lim} A^{1 - P^{1 \lim}} = \sigma_{t}$$

$$\alpha \sigma_{i}^{2\lim} + (1-\alpha) \sigma_{1}^{2\lim} A^{1-P^{2\lim}} = \sigma_{t},$$

where values of $\sigma_1^{1 \ lim}$, $\sigma_i^{1 \ lim}$ and $P^{1 \ lim}$ correspond to the experimentally determined moment of destruction of the first sample, $\sigma_1^{2 \ lim}$, $\sigma_i^{2 \ lim}$ and $P^{2 \ lim}$ correspond to the experimentally determined moment of destruction of the second sample. In this case, equations of type (5) corresponding to two selected structural variants form the system of two non-linear algebraic equations with unknown variables α and A which can be solved by the successive approximation method. The use of experimental data on destruction of laboratory samples obtained under the SSS of the real structure can improve calculations accuracy. The need for strength parameters depending on primary stresses complicate the strength criterion. The author and his co-authors used a prismatic shape sample for the assessment of the strength of the structure under the complex stress state [12]. That helped obtain strength data with regard to the required coefficient P using a standard test machine compressing the sample. The principle of multidirectional test forces formation in the sample and the sample structure have been described in [22].

3. Calculation results

To improve the strength criterion with regard to deformation characteristics by the method presented in Fig. 2, strength coefficients α and A were calculated for 50CrV (high quality) steel which is in the most rigid SSS (using the Smirnov-Alyaev terms) under biaxial tension (1< P <2). The SSS with P =1.85 was used.

(5)

(6)

The state at P = 1,85 corresponds to the type of the SSS of the experimental model of the pressure vessel's choke part whose destruction area is on its external surface in the area adjacent to the weld of the choke (Fig. 3-b) [19]. In [19], the experimental model of the choke part consisted of a spherical frame and a welded choke (148 mm in internal diameter, and 216 mm in external diameter) made from the same material. The model was loaded with internal pressure in a quasi-static way. The destruction pressure of the model was $p_{pf} = 77.7$ MPa. As a result of the model destruction, a thorough crack cutting the choke wall along the meridian line formed. The crack is maximum in the area adjacent to the weld of the choke on its external surface (see Fig. 3-b). The view of the fracture surface corresponded to the quasi-brittle nature of destruction [19].



Fig. 3. Distribution of the calculated values of coefficient *P* (a) at the moment of destruction along the cross-section of the choke part (b)

The calculated value of P at the moment of destruction of the pressure vessel's choke model was determined by numerical analysisin MSC Patran and MSC Nastran. The numerical solution was based on the experimental results obtained when testing the model before destruction with regard to the elastoplastic properties of the deformed material. The mathematical elastoplastic deformation model described by Prandl-Reiss equations [20, 21] was used.

The comparison of the calculated value $p_{pc} = 75$ MPa and the real destruction pressure $p_{pf} = 77.7$ MPa shows that the calculation error does not exceed 5%.

With regard to the SSS characteristics at the moment of destruction, P in the FE-network along the cross-section of the choke part and in the area of destruction of the choke (on the external surface in the weld adjacent zone) was calculated using (3). Fig. 3-a shows the distibution of the calculated values of P along the cross-section of the choke part. In the area of destruction, the maximum value of P was P = 1.85.

Model development is the first implementation stage for the method which can improve the accuracy of the strength criterion. This part of the article is a methodological description of the stage.

4. Results of experiments and calculations

To determine the conventional values of mechanical characteristics of 50CrV (high quality) steel, standard round samples were tested for tension. Static machining of five samples identified that 50CrV (high quality) steel has strength limit σ_t = 1270 MPa and relative extension δ = 7.5 %.

According to the method (see Fig. 1), to determine the values of α and *A* introduced by equation (5), it is necessary to destroy two structural samples of different size and value of $\sigma_1^{1 \ lim}$, $\sigma_i^{1 \ lim}$ and $\sigma_1^{2 \ lim}$, $\sigma_i^{2 \ lim}$ at the moment of destruction. The samples have to have equal (or close) values of *P* in their working zones. Sampling was described in [4, 23]. Two series of samples (series 1 and series 2) with three samples in each series were produced. Their sizes had to ensure P = 1.85 in the working zone [23].

Prismatic samples of series 1 and series 2 were tested using Instron 5989 Testing System. The load diagrams presented in Fig. 4 show averaged values of force characteristics of three loaded samples in each series. The relative mean square deviation of these values did not exceed 5%.



Fig. 4. Averaged load diagrams for prismatic samples series 1 (a) and series 2 (b): point 1 – crack formation moment in the working zone of the prismatic samples

Destructive forces were $F_1 = 205$ kN, $F_2 = 235$ kN. F_1 and F_2 were used as initial values for the numerical FE analysis of the samples at the moment of destruction. The accuracy of calculated deformation models was proved by calculations and full-sized experiments [4, 23]. Values $\sigma_1^{1 \ lim}$, $\sigma_i^{1 \ lim}$ were calculated for the first prismatic sample $(P^{1 \ lim} = 1.9)$. Values $\sigma_1^{2 \ lim}$, $\sigma_i^{2 \ lim}$ were calculated for the second prismatic sample $(P^{2 \ lim} = 1.8)$. Fig. 5-a shows the results of the numerical analysis of prismatic samples series 1 at the moment of destruction (corresponds to the moment of crack formation). Fig. 5-b shows the distribution of the component of the first primary stress.

The results of the numerical analysis of deformation for prismatic samples series 2 at the moment of destruction are shown in Fig. 6-a (the distribution of stress intensity) and in Fig. 6-b (the distribution of the component of the first primary stress).

The calculations and experimental results are presented in Table 1. The experimental results show that the influence of biaxial tension in the area of destruction can be significant for the samples of series 1. The limit value of the first primary stress $\sigma_1^{1 \ lim}$ corresponding to the moment of destruction is 892 MPa which is a quarter less than the value of strength limit $\sigma_t \sigma_1^{1 \ lim} = \sigma_t = 1270$ MPa determined under uniaxial tension (P = 1). The results are close to the result of experimental studies carried out by Y.A. Vilimok, K.A. Nazarov, and A.K. Evdokimov [14]. Using special test equipment, the researchers identified the same decrease (by more than a quarter) in $\sigma_1^{1 \ lim}$ under biaxial tension of X10CrNiTi18-10 steel with $P \approx 2$.



Fig. 5. Calculated distribution of stresses at the moment of destruction of samples series 1 (the view of a quarter of the sample cut by two axial planes): a – distribution of stress intensity $\sigma_i^{1 \text{ lim}}$, b – distribution of the first primary stress $\sigma_1^{1 \text{ lim}}$



Fig. 6. Calculated distribution of stresses at the moment of destruction of samples series 2 (the view of a quarter of the sample cut by two axial planes):

a – distribution of stress intensity σ_i	$_{i}^{2 lim}, b -$	distribution of	the first	primary	stress $\sigma_1^{2 lim}$
-------------------------------------------------	---------------------	-----------------	-----------	---------	---------------------------

Table 1. Calc	ulated characteristics of the SSS of the samples at the moment of destruction
	Working zono

No. of series	Working zone				
	σ_1^{lim} , MPa	σ_2^{lim} , MPa	$\sigma_i^{lim},$ MPa	Р	
1	985	743	892	1,9	
2	1050	615	917	1,8	

To calculate α and A introduced by equation (5), let us insert the calculated values of the SSS characteristics (see Table 1) into the system of equations (6)

$$\int \alpha 892 + (1 - \alpha)985 A^{1-1,9} = 1270$$

$$\left(\alpha 917 + (1 - \alpha)1050A^{1 - 1, 8} = 1270\right)$$

(7)

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Solving equations (7) by the successive approximation method, one can obtain the following values:

 $\alpha = 0.73; A = 0.40.$

(8)

Equation (5) can be used to improve the calculations of static strength of the structure made from 50CrV (high quality) steel and described by $P \approx 1.85$.

If we take into account that α and A in equation (1) do not depend on P, for 50CrV (high quality) steel strength parameters (according to the conventional terminology) α and A calculated by (4) will be $\alpha = 0.6$, A = 0.75 at any P. It contradicts the hypothesis that the strength depends on the SSS type (P). Therefore, α and A have to be adjusted. Otherwise, at given P, a rigid zone of the structure will fail (it happened to the choke part in the area adjacent to the weld where the stress intensity value was not maximum for the whole structure). If $\alpha = 0.73$ and A = 0.4, one can see that the influence of P on α and A can be significant. Thus, condition (1) has to be the approximation of the real limit state equation built for a specific (or a relatively narrow range of modifications) value of P describing the SSS type.

5. Conclusions

The proposed method for building a combined strength criterion involves using experimental data on destruction of laboratory samples whose stress state at the moment of destruction simulates the stress state of the structure. The use of these data can improve calculations accuracy for strength coefficients in the Pisarenko-Lebedev strength equation.

The calculations and experiments identified that for 50CrV (high quality) steel, the limit value of stress intensity under biaxial tension ($P \ge 1.8$) decreases by a quarter in comparison with the strength value determined under uniaxial tension (P = 1).

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