NUMERICAL ANALYSIS OF THE TEXTURE AND ACOUSTOELASTIC PROPERTIES OF A PRESTRESSED POLYCRYSTALLINE AGGREGATE

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Summary A bulk sample made of an uniaxially rolled polycrystalline aggregate (e.g., steel) is assumed to be subjected to plane stress which causes changes in acoustoelastic properties and texture of the bulk sample. The principal directions of the stress are coincident with the axes of the orthorhombic symmetry of the bulk sample. The dependences of the changes on the plane stress are analysed numerically.

EXTENDED SUMMARY

Some forming processes (e. g., rolling, drawing, forging) of polycrystalline aggregates (e.g., steel) are accompanied by plastic deformation which leaves the crystallites (grains) in certain preferred orientations called the texture as well as induce residual stress in the material and changes in the polycrystal acoustioelastic properties. The purpose of the work is to propose a numerical method of evaluating the texture, stress and changes in the acoustioelastic properties, the method being based on the observation and theoretical predictions that the speeds at which elastic waves propagate through a textured and prestressed body depend on the directions of the wave propagation and polarization as well as on the texture of the body and the state of the background (i. e., applied or residual) stress to which the body is subjected. For the sake of brevity, we confine ourselves to present the preliminaries of the method.

The propagation of ultrasonic plane waves in a solid bulk sample is considered for the case when the sample material is of the form of a polycrystalline aggregate (e.g., steel) made of Fe crystallites of the highest cubic symmetry. The crystallite orientation distribution is assumed to imply the orthorhombic symmetry of the macroscopic (effective) acoustoelastic properties of the polycrystalline aggregate. Suppose an Euler orthogonal reference system $0x_1x_2x_3$ with the axes $0x_1$, $0x_2$ and $0x_3$ is suitably chosen for the sample; for example, in the case of a rolled plate, $0x_1$ could coincide with the rolling direction, the axes $0x_2$ and $0x_3$ being transverse to the rolling direction and normal to the rolling plane, respectively. Then the axes $0x_1$, $0x_2$ and $0x_3$ are also coincident with the axes of the orthorhombic symmetry. The other orthogonal reference system $0X_1X_2X_3$ is supposed to be chosen for a single cubic crystallite, the axes being chosen in the crystallographic directions [100], [010] and [001], respectively. The unit vectors along the directions of the axes $0x_1$, $0x_2$ and $0x_3$ as well as along the directions of the axes $0X_1$, $0X_2$ and $0X_3$ are denoted by $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ as well as by $\mathbf{E}_1$, $\mathbf{E}_2$, and $\mathbf{E}_3$, respectively. Henceforth, all equations, relations and formulae are written with locating the vector and tensor quantities as well as the orientations and coordinates to the $0x_1x_2x_3$ reference system. Then the position vector $\mathbf{x}$ can be writen as $\mathbf{x}=(x_1, x_2, x_3)$ where $x_i=\mathbf{x}\cdot\mathbf{e}_i$, $i=1, 2, 3$. In the subsequent considerations, the orientation of a single crystallite within the polycrystalline sample is defined by giving the values of three Eulerian angles, θ, φ, and ϕ, of the axes $0X_1$, $0X_2$ and $0X_3$ relative to the sample axes, $0x_1$, $0x_2$ and $0x_3$. The notations θ ($\theta=cos^{-1}(\mathbf{E}_3\cdot\mathbf{e}_3) \doteq cos^{-1}\xi$), φ, and ϕ stand for the angle of nutation, precession and proper rotation, respectively, where $0\leq\theta\leq\pi$, $0\leq\varphi\leq 2\pi$, $0\leq\phi\leq 2\pi$.

Since it is not possible to measure the phase velocity of an acoustic wave at a point $\mathbf{x}$, such terms as the *local* texture and acoustoelastic properties of the sample material revealed by or deduced from the *local* measurements of ultrasosonic phase velocity do not mean the texture, and properties in a point $\mathbf{x}$ in the sample under study but mean the texture and properties at every point of the sample material filling a subdomain (mesodomain) centered at the point $\mathbf{x}$ and having at least the *smallest size* at which performing the ultrasosonic measurements is still possible. On the other hand, the subdomain is assumed to be enough large to contain a statistical ensemble of crystallites.

The texture of a subdomain may be characterized by the probability density function of the crystallite orientation, $p(\theta,\varphi,\phi)$. Then $p(\theta,\varphi,\phi)\,d\theta\,d\varphi\,d\phi$ expresses the probability that a crystallite in the subdomain of the sample has an orientation described by the Euler angles θ, φ, and ϕ, lying in the intervals $<\theta,\theta+d\theta)>$, $<\varphi,\varphi+d\varphi>$ and $<\phi,\phi+d\phi>$, respectively. Therefore, we treat the texture $p(\theta,\varphi,\phi)$, elastic stiffness moduli $C(\mathbf{x})_{ijkl}$ and the density ρ as quantities independent of $\mathbf{x}$ within the mesodomain of the *smallest size*, corresponding to the intermediary scale and being defined by the size conditions of performing the ultrasonic measurements. The analysis presented here concerns always the subdomain involved in the definition of the considered local value of the phase velocity. To analyse the acoustoelastic response, the effective modulus concept [1] is applied to a subdomain of the bulk sample.

The subsequent considerations are concerned with a statistical ensemble of identical bulk samples made of the examined polycrystalline aggregate, the samples being subjected to the background plane stress, $\sigma^0(\mathbf{x})_{ij}$ $(i,j=1,2,3)$. The principal directions of the plane stress, $\sigma^0(\mathbf{x})_{11}$, $\sigma^0(\mathbf{x})_{22}=constant\cdot\sigma^0(\mathbf{x})_{11}$, $\sigma^0(\mathbf{x})_{11}\leq 750MPa$, coincide with the symmetry axes $0x_1$ and $0x_2$. It is considered the case when each sample is acted on by an ultrasonic transducer oscillating with the ultrasonic angular frequency ω in such a way that the the assembly averaged displacement response, $\langle \mathbf{u}(\mathbf{x},t)\rangle$, of the polycrystalline aggregate to this dynamic loading is of the form of one of nine different plane displacement ultrasonic waves, $\langle \mathbf{u}(\mathbf{x},t)\rangle = \mathbf{p}\, u_0\, exp\,[ik_{np}(\mathbf{n}\cdot\mathbf{x} - V_{np}t)] = \mathbf{p}\, u_0\, exp\,[i(k_{np}\mathbf{n}\cdot\mathbf{x} - \omega t)]$ with phase velocities $V_{np},\ n,\, p = 1,\, 2,\, 3.$ n and p denote the directions of the propagation $\mathbf{n}$ ($|\mathbf{n}| = 1,\ \mathbf{n} = \mathbf{e}_1,\ \mathbf{e}_2,\ \mathbf{e}_3$) and polarization $\mathbf{p}$ ($|\mathbf{n}| = 1,\ \mathbf{p} = \mathbf{e}_1,\ \mathbf{e}_2,\ \mathbf{e}_3$) of each mode being coincident with one of the axes $0x_1$, $0x_2$ and $0x_3$ of the reference system $0x_1x_2x_3$. u_0 denotes the amplitude of the wave $\langle \mathbf{u}(\mathbf{x},t)\rangle$, k_{np} stands for the wave number and $k_{np} = \omega/V_{np}$. In every heterogeneous elastic body, the ultrasonic velocities depend on the effective density and the tensor of the so-called effective dynamic moduli of stiffness as well as on the frequency. In the limit, as the wavelength increases to infinity (or the frequency diminishes to zero), the dynamic effective moduli in these relations may be replaced by the static effective moduli. Such an approximation, which was used in numerous papers, will also be employed from now in this work where the effective moduli C^{eff}_{ijkl} will be taken to be the static effective ones. For the reason explained in [2,p.385], we employ the Voigt [3] averaging procedure as a suitable one for evaluating $C^{eff}_{ijkl} = \langle C(\mathbf{x}_s)_{ijkl}\rangle$ for a subdomain Ω_s centered at $\mathbf{x}_s$. We arrive at the following equations for C^{eff}_{ijkl}:

$$C^{eff}_{ijkl} = \langle C(\mathbf{x}_s)_{ijkl}\rangle,\quad \langle C(\mathbf{x}_s)_{ijkl}\rangle \doteq \int_{-1}^{1} d\xi \int_{0}^{2\pi} d\varphi \int_{0}^{2\pi} d\phi\, C(\mathbf{x}_s)_{ijkl}\, p\,(\xi,\varphi,\phi),\quad i,j,k,l,m,n,p,q = 1,\ 2,\ 3,$$

$$C(\mathbf{x}_s)_{ijkl} = t(\xi,\varphi,\phi)_{mi}\, t(\xi,\varphi,\phi)_{nj}\, t(\xi,\varphi,\phi)_{pk}\, t(\xi,\varphi,\phi)_{ql}\, c_{mnpq},\quad X_i = t(\xi,\varphi,\phi)_{ij}\, x_j \text{ where } \xi \doteq cos\theta.$$

where c_{mnpq} denote the elastic stiffness moduli of a single crystallite (for example, c_{11}, c_{12} and c_{44} in the case of cubic crystallite) and $t(\xi,\varphi,\phi)_{im}$ stands for the components of the transformation matrix $\mathbf{t}(\xi,\varphi,\phi)$ relating x_i to X_i. Now we substitute the plane wave solution $\langle \mathbf{u}(\mathbf{x},t)\rangle$ successively in the form of each of the nine modes with phase velocities $V_{ij}, i,\ j = 1,\ 2,\ 3$, into the following equations of the considered wave motion:

$$(\tilde{C}_{ijkl} + \tilde{\sigma}^0_{jl}\delta_{ik})\,\frac{\partial^2\langle u(\mathbf{x},t)_k\rangle}{\partial x_j \partial x_l} = \frac{\partial^2 \langle u(\mathbf{x},t)_i\rangle}{\partial t^2};\quad \rho(\mathbf{x})^{eff} = \langle \rho(\mathbf{x})\rangle,\ \tilde{c} = \frac{c_{ij}}{\rho^{eff}},\ \tilde{C}_{ij} = \frac{C^{eff}_{ij}}{\rho^{eff}},\ \tilde{\sigma}^0_{ij} = \frac{\sigma^0_{ij}}{\rho^{eff}},\quad i,j,k,l = 1,\ 2,\ 3.$$

In this way we obtain the following equations, after a little analysis and utilizing some results of [4, 5]],

$$\tilde{C}_{11} = \tilde{c}_{11} - 2(\tilde{c}_{11} - \tilde{c}_{12} - 2\tilde{c}_{44})\langle r_1(\xi,\ \varphi,\ \phi)\rangle = V^2_{11} - \tilde{\sigma}^0_{11},\qquad \tilde{C}_{22} = \tilde{c}_{11} - 2(\tilde{c}_{11} - \tilde{c}_{12} - 2\tilde{c}_{44})\langle r_2(\xi,\ \varphi,\ \phi)\rangle = V^2_{22} - \tilde{\sigma}^0_{22},\quad (1)$$

$$\tilde{C}_{33} = \tilde{c}_{11} - 2(\tilde{c}_{11} - \tilde{c}_{12} - 2\tilde{c}_{44})\langle r_3(\xi,\ \varphi,\ \phi)\rangle = V^2_{33},\qquad \tilde{C}_{44} = \tilde{c}_{44} + (\tilde{c}_{11} - \tilde{c}_{12} - 2\tilde{c}_{44})\langle r_4(\xi,\ \varphi,\ \phi)\rangle = V^2_{23} - \tilde{\sigma}^0_{22},\quad (2)$$

$$\tilde{C}_{55} = \tilde{c}_{44} + (\tilde{c}_{11} - \tilde{c}_{12} - 2\tilde{c}_{44})\langle r_5(\xi,\ \varphi,\ \phi)\rangle = V^2_{13} - \tilde{\sigma}^0_{11},\qquad \tilde{C}_{66} = \tilde{c}_{44} + (\tilde{c}_{11} - \tilde{c}_{12} - 2\tilde{c}_{44})\langle r_6(\xi,\ \varphi,\ \phi)\rangle = V^2_{12} - \tilde{\sigma}^0_{11}\quad (3)$$

$$\tilde{\sigma}^0_{11} = V^2_{13} - V^2_{31},\ \tilde{\sigma}^0_{22} = V^2_{23} - V^2_{32},\ \tilde{\sigma}^0_{11} - \tilde{\sigma}^0_{22} = V^2_{12} - V^2_{21},\ \langle r_m(\xi,\ \varphi,\ \phi)\rangle = \int_{-1}^{1} d\xi \int_{0}^{2\pi} d\varphi \int_{0}^{2\pi} d\phi\, r_m(\xi,\ \varphi,\ \phi)\ p(\xi,\varphi,\phi)\quad (4)$$

where $m = 1,\, 2,\, ...,\, 6$ and $r_m(\xi,\ \varphi,\ \phi)$ are defined by Sayers [4]. The bracket angles, $\langle ...\rangle$ denote assembly averaging. Accepting Jaynes' [6] principle of maximum Shannon entropy I (see Eqs. (5)) as a reliable basis for the evaluation of $p(\xi,\ \varphi,\ \phi)$, we seek $p(\xi,\varphi,\phi)$ in the form (6). In estimating $p(\xi,\ \varphi,\ \phi)$, we employ the normalization condition $\langle 1\rangle = 1$ (Eqs. 5) and only three equations from the set of Eqs. (1)-(3) since only three of the six expectation values $\langle r_t(\xi,\ \varphi,\ \phi)\rangle$, $t = 1,\, 2,\, ...,\, 6$, are linearly independent on each other and, henceforth, may be involved in the problem of determining $p(\xi,\ \varphi,\ \phi)$ by maximizing conditionally entropy I. $1 - ln\, Z$, L_1, L_3, and L_5 are the Lagrangian multipliers corresponding to the mentioned conditions. $1 - ln\, Z$ corresponds to normalization condition. Eqs. (1)-(6) are the basis for numerical analysis of the problem being of interest for us.

$$\langle 1\rangle \doteq \int_{-1}^{1} d\xi \int_{0}^{2\pi} d\varphi \int_{0}^{2\pi} d\phi\ p(\xi,\varphi,\phi) = 1,\quad I \propto -\int_{-1}^{1} d\xi \int_{0}^{2\pi} d\varphi \int_{0}^{2\pi} d\phi\ p(\xi,\varphi,\phi)\, ln\, p(\xi,\varphi,\phi).\quad (5)$$

$$p(\xi,\varphi,\phi) = (1\ Z)\, exp\,[-L_1\, r_1(\xi,\varphi,\phi) - L_3\, r_3(\xi,\varphi,\phi) - L_5\, r_5(\xi,\varphi,\phi)].\quad (6)$$

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