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

Józef Lewandowski
IPPT PAN, Department of Theory of Continuous Media, PL 00-049 Warszawa, Poland

Summary. The propagation of ultrasonic waves in a polycrystalline aggregate is considered for a bulk sample made of cubic crystals (e.g., Fe) and subjected to stress, the principal directions of the stress being coincident with the axes of the orthorhombic symmetry of the macroscopic acoustoelastic properties of the sample. The dependence of the acoustoelastic properties and texture of the bulk sample on the 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 induces residual stresses in the materials and leaves their crystallites (grains) in certain preferred orientations called the texture. In turn, the texture cause the symmetry of the macroscopic acoustoelastic properties of polycrystals. In the present paper, we are interesting in the situation where the forming processes caused the orthorhombic symmetry of the macroscopic acoustoelastic properties of a polycrystal and induced in that residual stresses, which have been removed after finishing the forming process. Next the stress-free bulk sample of the textured polycrystal is subjected to small applied stresses $\Delta\sigma^0_{ij} = 1\,MPa,\, i\,j = 1,\, 2,\, 3$. After approaching the equilibrium deformed configuration [1], the values of the applied stresses are increased again by the same constant and small steps $\Delta\sigma^0_{ij}$ and the material points of the bulk sample approache a new equilibrium deformed configuration. Increasing the applied stresses σ^0_{ij} by the steps $\Delta\sigma^0_{ij}$ and approaching the new equilibrium deformed configuration are repeated as many times ($N = 750$) as the applied stresses $\sigma^0_{ij} = n \cdot \Delta\sigma^0_{ij}$, $n = 1,\, 2,\, \ldots,\, N$ reache the desired limiting values $N \cdot \Delta\sigma^0_{ij}$. The purpose of the work is to propose a method (algorithm) of computing numerically the changes in the texture and acoustoelastic properties as functions of σ^0_{ij} varying in the way described above. The method is based on the observations and theoretical predictions confirming 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 stress to which the body is subjected. For the sake of brevity, we confine ourselves to present here only the preliminaries of the method applied to the case of σ^0_{ij} being plane stresses. The problem will be presented in detail and in more general form in [2].

To describe briefly the algorithm, an Euler orthogonal reference system $0x_1x_2x_3$ with the axes $0x_1$, $0x_2$ and $0x_3$ is suitably chosen for the present equilibrium configuration of the material points of the sample, the axes $0x_1$, $0x_2$ and $0x_3$ being 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 $0 \le \theta \le \pi$, $0 \le \varphi \le 2\,\pi$, $0 \le \phi \le 2\pi$. 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.

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 *local* 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 at 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) Ω centered at the point $\mathbf{x}$. Such a subdomain corresponds to the intermediary scale and has at least the *smallest size* at which performing the ultrasosonic measurements is still possible. On the other hand, the subdomain Ω is assumed to be enough large to contain a statistical ensemble of crystallites. The analysis of the acoustoelastic response of the material to a dynamic loading, which is presented below, concerns also the subdomain Ω, however the texture $p\,(\theta, \varphi, \phi)$, effective elastic stiffness moduli C^{eff}_{ijkl} and the phase velocities of ultrasonic waves are treated within the subdomain as independent of $\mathbf{x}$.

The subsequent considerations are confined to a statistical ensemble of identical bulk samples made of the examined polycrystalline aggregate, the samples being subjected to the plane stress, $\sigma^0(\mathbf{x})_{ij}$ $(i, j = 1,\, 2,\, 3)$. The principal directions of the plane stress, $\sigma^0(\mathbf{x})_{11}$, $\sigma^0(\mathbf{x})_{22}=\gamma\cdot\sigma^0(\mathbf{x})_{11}$, $\gamma=constant$, $\sigma^0(\mathbf{x})_{11}\leq 750MPa$, 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 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 the 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, $p=1,\,2,\,3$. The bracket angles $\langle...\rangle$ denote assembly averaging. The subscripts 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 $0x_3$. 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 $\omega\rightarrow 0$), the dynamic effective moduli in these relations are replaced from now by the static effective moduli C^{eff}_{ijkl}. For the reason explained in [3,p.385], we employ the Voigt [4] 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 $\mathbf{x}_s$ and in this way arrive at the following equations for evaluating C^{eff}_{ijkl}:

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

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

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, which is superimposed on an equilibrium deformed configuration of the material points of the body:

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

In this way we obtain the following equations, after a little analysis and utilizing some results of [1, 5],

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

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

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

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

where $m=1,\,2,\,...,\,6$ and $r_m(\xi,\,\varphi,\,\phi)$ are defined by Sayers [5]. 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).

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

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

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) and three linear relations between some of $\langle r_t(\xi,\,\varphi,\,\phi)\rangle$, $t=1,\,2,\,...,\,6$, are the basis of the numerical analysis of the problem being of interest for us.

References

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