FIELD THEORY EVALUATION OF THE STRESS STATES OF GRAINS IN ELASTICALLY DEFORMED POLYCRYSTALS

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Most of inorganic structural materials (metallic alloys, ceramics, minerals etc.) are polycrystalline aggregates, consisted of macroscopically large quantity of single-crystal grains (crystallites). The mechanical behavior of the specimen of polycrystalline material is governed by the physical and mechanical processes in the grains and interaction of the grains. Thus the deformation of polycrystalline material is a cooperative phenomenon typical for condensed matter physics and mechanics of heterogeneous materials. The passing of these processes depend on many parameters, including stress states of individual grains and its evolution during macrodeformation.

In this paper we note a mathematical analogy between the equations of the mechanics of heterogeneous polycrystalline materials and the equations of quantum theory of particles scattering. This analogy allows to apply the methods of quantum field theory to solution of the equations of solid mechanics for heterogeneous media. It is considered the application of Corringa-Kohn-Rostoker method [1], used in quantum theory for calculating wave function $\psi(\vec{r})$ of electrons in metallic alloys from equation

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int_V d\vec{r}_1 G(\vec{r}-\vec{r}_1)\left[\sum_{i=1}^{N} w_i(\vec{r}_1)\right]\psi(\vec{r}_1)\,, \tag{1}$$

where w_i - potential of electron interaction with *i*-th impurity atom, *G*- Green's function of Schrödinger equation, to elasticity of polycrystals. The strains $\varepsilon_{ij}(\vec{r})$ in polycrystals are governed by equation (integral form of elastic boundary value problem)

$$\varepsilon_{ij}(\vec{r}) = \varepsilon^*_{ij} + \int_V d\vec{r}_1 g_{ijkl}(\vec{r}-\vec{r}_1)\left[\sum_{\xi=1}^{N} \lambda_\xi(\vec{r}_1)\left(C^{(\xi)}_{klmn}(\vec{r}_1) - \langle C_{klmn}\rangle\right)\right]\varepsilon_{mn}(\vec{r}_1)\,, \tag{2}$$

where $C^{(\xi)}_{klmn}$ - elastic moduli tensor of ξ-th crystallite, g_{ijkl} - Green's tensor, λ_ξ - indicator of ξ-th crystallite (equal to 1 within crystallite ad zero otherwise), $\langle C_{klmn}\rangle$ - averaged moduli tensor of the medium. Equations (1) and (2) are mathematically fully equivalent, so we can use the methods of solving (1) to solve (2). This approach allowed, for instance, to calculate probability density function for stresses in grains under arbitrary macrodeformation of polycrystal. Figure 1 represents this probability distribution for normal stresses under macroshear for polycrystalline zinc [2]. Application of the method to classical problem of homogenization gives new formulae for the effective moduli of disordered polycrystalline medium [3]. The effective moduli of multiphase polycrystal with grains moduli $C^{(\eta)}_{klmn}$ (v_η - is volume share of grains of η-th type) represented as

$$C^*_{ijmn} = \sum_{\eta=1}^{n} v_\eta \langle C^{(\eta)}_{ijkl}(\vec{r}_\eta)\left[I_{klmn} - A^{(\eta)}_{klmn}\right]^{-1}\rangle_\eta \ ,$$

which differs from Foigt approximation of non-interacting grains by renormalization factors $A^{(\eta)}_{klmn}$. It resembles the situation in condensed matter physics, when the system of strongly interacting particles can be replaced by non-interacting quasiparticles but with renormalized masses [4].

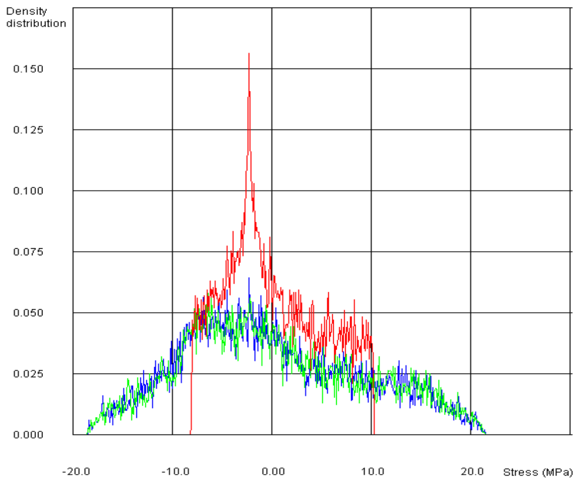

Fig. 1. Probability distribution of normal stresses in grains under macroshear.

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