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Extreme Strain Fluctuations in Polycrystalline Materials

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Abstract—The stochastic structure of polycrystalline materials causes a high inhomogeneity of the kinematic and force fields in grains of materials and large fluctuations of these fields. The inhomogeneity and fluctuations are insignificant in some cases, but they become crucial in the study of various critical phenomena whose occurrence strongly depends on the type of material microstructure. Fluctuations mainly arise due to the elastic interaction of grains, which has a long-range effect. Therefore, it is necessary to account for the interaction of a large number of grains, which is difficult to do using conventional methods (direct computer modeling and others). In the present paper, inhomogeneous mesostrain fluctuations in grains of polycrystalline materials were estimated using a field-theoretical approach to a boundary-value problem of microheterogeneous material deformation. Particular attention is paid to the calculation of extreme fluctuations that are important for some critical phenomena, such as, e.g., crack initiation under gigacycle fatigue when the macrostress amplitude and the mean stresses in grains are much lower than the quantities included in any macroscopic damage or fatigue criteria. The maximum mesostrains in grains can exceed several times the macrostrains. Extreme fluctuations in a grain are generated in grain clusters of specific configuration. The applied approach makes it possible to predict patterns of such clusters. Extreme fluctuations in the bulk grains of a polycrystalline body are much higher than in the surface grains, due to which the behavior of the material surface layers and bulk volumes is different. Quantitative data are given for the case of uniaxial tension of polycrystalline zinc.

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1. INTRODUCTION

Polycrystalline materials are heterogeneous on the mesoscale and have a stochastic microstructure. Their mechanical and other parameters are highly oscillating functions of coordinates. Mesostrain and mesostress fields are random functions. These fields can be studied either as random coordinate functions in a certain macroscopic polycrystalline specimen or as random variables at a point for the ensemble of polycrystalline microstructural configurations. These approaches are equivalent in the context of the ergodic hypothesis. In the present paper, we employ the statistical ensemble method, which includes the solution of a boundary-value problem for strain fields at a point for every structural realization from the ensemble and the study of statistical characteristics of the derived data array. A conventional solution of the problem, which treats polycrystals as heterogeneous composite solids, faces the two major problems: a huge number of homogeneity ranges (grains), whose geometry should be described explicitly, and the stochastic behavior of material functions, which randomly change in transition from one homogeneity range to another or in transition to the next microstructural realization from the ensemble. To solve boundary-value problems for a large number of realizations, regardless of the solution method, is a challenge. In the paper we employ a field-theoretical approach alternative to widely used methods of solution of boundary-value problems (finite-element method, statistical averaging, etc.) [1].

Mechanical properties of polycrystals depend on many microstructural parameters. Some dependences have a qualitative character, without rigorous quantification of the related parameters. The latter are divisible into geometrical (shape and size of crystallites), crystallographic (anisotropy of grains and spatial orientation of their axes), physical ones (energy of grain boundaries, equilibrium angles in triple joints, etc.). The first two groups of parameters are of interest in continuum mechanics.

Stochastic fields are most completely described by the construction of distribution functions or calculation of stochastic moments of all orders. For the field at a point of the polycrystal grain, distribution functions can be plotted by the previously described field-theoretical method [2]. This is a tedious procedure when calculating for the value ensemble. However, many phenomena require knowledge of not the entire distribution function but fluctuation values or extrema responsible for the onset of critical events. Here we limit ourselves to the search for extreme strains in polycrystalline solids.

Estimation of maximum strain fluctuations is very important in the problem of gigacycle fatigue. In this mode, time to failure is largely determined by the incubation period of the first crack initiation. Macrostress amplitudes are small, and macrostrains are accurately elastic. Irreversible strains, being a precursor of crack initiation, arise in only a small number of grains, in which fluctuating resultant stresses exceed critical stresses in individual sliding systems. A decisive role in high fluctuations is played by the microheterogeneity of polycrystals [3]. It is experimentally found that such fluctuations exist in clusters of specifically oriented (relative to external loads) grains [4]. In the present paper, extreme mesostrains in grains for the ensemble of all possible polycrystalline microstructural configurations are calculated using the field-theoretical method of solution of grain-boundary problems of mechanics.

A macroscopic specimen of randomly oriented single-phase polycrystal at the average grain size of about tens of micrometers and the specimen size of about tens of millimeters includes about a billon grains. A statistical ensemble of various microstructures of such a polycrystal will contain an extremely large number of possible configurations. It is essential that a boundary-value problem of deformation of a heterogeneous solid should be solved for every configuration, and extreme values should be chosen from the derived data array. Obviously, no conventional methods can solve this problem.

2. FIELD-THEORETICAL METHOD OF STRAIN CALCULATION IN POLYCRYSTALLINE (MICROHETEROGENEOUS) SOLIDS

A conventional method for determining strain fields in heterogeneous solids is the solution of a boundary-value problem in the differential form or the equivalent variational formulation (finite-element method, etc.). Material properties and mechanical fields in polycrystals are discontinuous functions of coordinates. Therefore, their derivatives entering the equations of boundary-value problems should be studied separately for each grain, and the conjugation condition should be introduced at grain boundaries. At a large number of grains, this presents considerable calculational difficulties. In the case of polycrystalline solids, direct computer modeling by conventional methods is also a problem due to a large number of structural elements, i.e. grains. The restriction of the model to several thousands of grains (the limitation of modern computers) raises many questions about statistical sufficiency, mathematical generation of microstructural geometry, the influence of boundary conditions, etc. Many of these difficulties are surmounted in transition from the differential form of the boundary-value problem to the integral one (note that the transition from the differential equations to equivalent integral ones is the main method in quantum field theory). The integral form finds wide application in dislocation theory. Let us perform such a transition for the boundary-value problem of linear elasticity of a polycrystalline solid based on the scheme described by de Wit [5].

Within the continuum model, a polycrystalline solid presents a multiply-connected domain of volume V with external area S consisted of subdomains (crystallites) with volumes ω_ξ and boundaries S_ξ, which are intergranular (phase) boundaries:

$$V = \sum_{\xi=1}^{N} \omega_\xi,$$

the subscript ξ numbers crystallites, and N is the total number of crystallites in the solid (a macroscopically large number).

The elastic modulus tensor of the polycrystalline medium has the form

$$C_{ijmn}(\mathbf{r}) = \sum_{\xi=1}^{N} \lambda_\xi(\mathbf{r}) C^{(\xi)}_{ijmn}(\mathbf{r}), \qquad (1)$$

where $\lambda_\xi(\mathbf{r})$ is the indicator function of the ξth crystallite with the modulus tensor $C^{(\xi)}_{ijmn}(\mathbf{r})$:

$$\lambda_\xi(\mathbf{r}) = \begin{cases} 1, & \text{if } \mathbf{r} \in \omega_\xi, \\ 0, & \text{otherwise.} \end{cases}$$

The tensor $C_{ijmn}(\mathbf{r})$ is constant within any domain ω_ξ and changes in a stepwise manner in transition across boundaries S_ξ due to the variation of crystal lattice orientation of the crystallite in space.

The boundary-value problem of the elasticity theory for a heterogeneous solid in displacements consists of equilibrium equations and governing relations:

$$\begin{gathered} \sigma_{ij,j}(\mathbf{r}) + f_i(\mathbf{r}) = 0, \\ \sigma_{ij}(\mathbf{r}) = C_{ijmn}(\mathbf{r}) \varepsilon_{mn}(\mathbf{r}), \\ \varepsilon_{mn}(\mathbf{r}) = [u_{m,n}(\mathbf{r}) + u_{n,m}(\mathbf{r})]/2, \end{gathered} \qquad (2)$$

where $\varepsilon_{ij}(\mathbf{r}), \sigma_{ij}(\mathbf{r}), u_i(\mathbf{r}), f_i(\mathbf{r})$ are the global tensors of strain, stress and the vectors of displacements, volume forces. Subscripts after the comma points to a differentiation with respect to the corresponding coordinate. Use boundary conditions in displacements

$$u_i(\mathbf{r})|_{\mathbf{r}\in\Gamma} = \psi_i(\mathbf{r}), \tag{3}$$

where $\psi_i(\mathbf{r})$ is the smooth coordinate function.

The structure of a polycrystalline solid is set by the tensor function of elastic moduli $C_{ijmn}(\mathbf{r})$, which is a piecewise constant coordinate function. We decompose the global tensor of elastic moduli into the averaged and fluctuating parts: $C_{klmn}(\mathbf{r}) = \langle C_{klmn}\rangle + C'_{klmn}(\mathbf{r})$, and study the two boundary-value problems: for the displacement vector $u_i(\mathbf{r})$ of a heterogeneous solid (the initial problem)

$$\langle C_{ijkl}\rangle u_{k,jl}(\mathbf{r}) + [C'_{ijkl}u_{k,l}(\mathbf{r})]_{,j} + f_i(\mathbf{r}) = 0 \tag{4}$$

and for the displacement vector $u^*_i(\mathbf{r})$ of a homogeneous solid with the averaged elastic modulus tensor

$$\langle C_{ijkl}\rangle u^*_{k,jl}(\mathbf{r}) + f_i(\mathbf{r}) = 0 \tag{5}$$

subject to the boundary conditions $u^*_i(\mathbf{r})|_{\mathbf{r}\in\Gamma} = \varphi_i(\mathbf{r})$.

Introduce Green's function for Eq. (5)

$$\langle C_{ijkl}\rangle G_{km,jl}(\mathbf{r}) + \delta_{im}\delta(\mathbf{r}) = 0, \tag{6}$$

and, using Green's theorem, transform Eq. (5) into the integrodifferential one:

$$u^*_m(\mathbf{r}) = \int_V \mathrm{d}^3\mathbf{r}' f_i(\mathbf{r}')G_{im}(\mathbf{r}-\mathbf{r}') + \oint_V \mathrm{d}^3 S'_j \langle C_{ijkl}\rangle$$
$$\times [u^*_{k,l}(\mathbf{r}')G_{im}(\mathbf{r}-\mathbf{r}') - u^*_i(\mathbf{r}')G_{km,l}(\mathbf{r}-\mathbf{r}')]. \tag{7}$$

A similar transformation is performed for Eq. (4), with the last two terms taken as a new vector of volume forces:

$$u_m(\mathbf{r}) = \int_V \mathrm{d}^3\mathbf{r}'[C'_{ijkl}(\mathbf{r}')u_{k,l}(\mathbf{r}')]_{,j} G_{im}(\mathbf{r}-\mathbf{r}')$$
$$+ \int_V \mathrm{d}^3\mathbf{r}' f_i(\mathbf{r}')G_{im}(\mathbf{r}-\mathbf{r}') + \oint_S \mathrm{d}S'_j \langle C_{ijkl}\rangle$$
$$\times [u_{k,l}(\mathbf{r}')G_{im}(\mathbf{r}-\mathbf{r}') - u_i(\mathbf{r}')G_{km,l}(\mathbf{r}-\mathbf{r}')]. \tag{8}$$

With the same boundary conditions $\varphi_i(\mathbf{r}) = \psi_i(\mathbf{r})$ for both problems, the right-hand side of (7) and the second line in (8) coincide. A subtraction of Eq. (7) from (8) gives

$$u_m(\mathbf{r}) = u^*_m(\mathbf{r})$$
$$+ \int_V \mathrm{d}^3\mathbf{r}'[C'_{ijkl}(\mathbf{r}')u_{k,l}(\mathbf{r}')]_{,j}(\mathbf{r}')G_{im}(\mathbf{r}-\mathbf{r}'). \tag{9}$$

A differentiation in (9) with respect to x_n and integration by parts gives the equation for displacement gradient

$$u_{m,n}(\mathbf{r}) = u^*_{m,n}(\mathbf{r})$$
$$+ \int_V \mathrm{d}^3\mathbf{r}'[C'_{ijkl}(\mathbf{r}')u_{k,l}(\mathbf{r}')G_{im,n}(\mathbf{r}-\mathbf{r}')]_{,j}$$
$$+ \int_V \mathrm{d}^3\mathbf{r}' C'_{ijkl}(\mathbf{r}')u_{k,l}(\mathbf{r}')G_{im,nj}(\mathbf{r}-\mathbf{r}'). \tag{10}$$

The first integral in (10) is transformed into the surface one:

$$\oint_S \mathrm{d}S'_j C'_{ijkl}(\mathbf{r}')u_{k,l}(\mathbf{r}')G_{im,n}(\mathbf{r}-\mathbf{r}').$$

For a polycrystalline solid, a product of the function $C'_{ijkl}(\mathbf{r}')$ highly oscillating near zero by the smooth function $u_{k,l}(\mathbf{r}')G_{im,n}(\mathbf{r}-\mathbf{r}')$ is under the integral sign. Therefore, for a large polycrystalline solid this integral vanishes in any macroscopic region of the surface and for the whole solid. Then, we symmetrize over the indices *m* and *n* and derive the desired integral equation for the global strain tensor in the polycrystalline solid:

$$\varepsilon_{ij}(\mathbf{r}) = \varepsilon^*_{ij}(\mathbf{r}') + \int_V \mathrm{d}\mathbf{r}'_1 g_{ijkl}(\mathbf{r}-\mathbf{r}_1)C'_{klmn}(\mathbf{r}_1)\varepsilon_{mn}(\mathbf{r}_1), \tag{11}$$

where $g_{ijkl} \equiv 1/2(G_{ik,jl} + G_{jk,il})$ is Green's tensor of a homogeneous medium.

For a polycrystalline solid, Eq. (11) is explicit. Its distinctive feature is a separation of the influence of boundary conditions (which is studied as an individual problem for $\varepsilon^*_{ij}(\mathbf{r})$ of a homogeneous solid) and of heterogeneities (the volume integral dependent of polycrystalline structure rather than boundary conditions). Such a conclusion can be made only for polycrystalline or granular solids with highly oscillating material constants in the presence of a very large number of grains. This feature will be used below. The solution $\varepsilon^*_{ij}(\mathbf{r})$ for the homogeneous solid is thought to be known, though it can be inhomogeneous. Given homogeneous boundary conditions,

$$u^*_i(\mathbf{r})|_{\mathbf{r}\in\Gamma} = \varepsilon^*_{ij}x_j,$$

where $\varepsilon^*_{ij} = \text{const}$ and $\varepsilon^*_{ij}(\mathbf{r}) = \langle\varepsilon_{ij}\rangle$. These boundary conditions alone are thereafter used.

To study deformation in individual grains, the global strain tensor is presented in the form of the superposition of local tensors with the use of the indicator functions:

$$\varepsilon_{ij}(\mathbf{r}) = \sum_{\xi=1}^{N} \lambda_\xi(\mathbf{r})\varepsilon^{(\xi)}_{ij}(\mathbf{r}), \tag{12}$$

and, together with (1), is inserted into (11). As a result, we derive the system of integral equations for local fields $\varepsilon^{(\xi)}_{ij}(\mathbf{r})$:

$$\varepsilon^{(\xi)}_{ij}(\mathbf{r}_\xi) = \varepsilon^*_{ij} + \int_{\omega_\xi} \mathrm{d}\mathbf{r}'_\xi g_{ijkl}(\mathbf{r}_\xi - \mathbf{r}'_\xi)C'^{(\xi)}_{klmn}(\mathbf{r}'_\xi)\varepsilon^{(\xi)}_{mn}(\mathbf{r}'_\xi)$$
$$+ \sum_{\eta\neq\xi}\int_{\omega_\eta} \mathrm{d}\mathbf{r}'_\eta g_{ijkl}(\mathbf{r}_\xi - \mathbf{r}'_\eta)C'^{(\eta)}_{klmn}(\mathbf{r}'_\eta)\varepsilon^{(\eta)}_{mn}(\mathbf{r}'_\eta). \tag{13}$$

In the field-theoretical terminology [1], Eq. (13) means that strain at any point is a superposition of external field ε^*_{ij}, interaction with strains at the other points of this grain (the second term in the right-hand part) and with strains in the rest polycrystal grains (terms under the

summation sign). In so doing, contributions from the interactions are additive.

3. FLUCTUATION EXTREMUM SEARCH ALGORITHM FOR THE ENSEMBLE OF POLYCRYSTALLINE MICROSTRUCTURES

To find strain extrema at any grain, we take a point in it and solve a set of boundary-value problems for the ensemble of all polycrystalline configurations. Then we choose the extreme value from the derived results and repeat the calculation for other points. The ensemble contains an infinite number of possible configurations. If an infinite set is replaced by a discrete one, statistical sampling should be extremely large to achieve statistical sufficiency. At such realization, this algorithm is impossible. Additivity, reducing the necessary sample size by many orders of magnitude, allows solving the problem.

Let us choose an approximation method for system (13). For local fields, we use a piecewise constant approximation. For this purpose, each grain is divided into a large number of subgrains and local intragranular fields are presented as the superposition of subgrain fields, each of which is thought to be constant within the subgrain, with the use of indicator functions of subgrains (Latin subscripts number subgrains):

$$\varepsilon_{ij}^{(\xi)}(\mathbf{r}_\xi) = \sum_{a=1}^{n} \lambda_a(\mathbf{r}_\xi)\varepsilon_{ij}^{(a)(\xi)}, \tag{14}$$

where n is the number of subgrains in a grain, and the grain volume is the sum of subgrain volumes. After this, the system of integral Eqs. (13) for local fields is transformed into the system of linear algebraic equations for sublocal fields:

$$\left[I_{ijmn} - B_{ijmn}^{(aa)(\xi)} \right] \varepsilon_{mn}^{(a)(\xi)} = \varepsilon_{ij}^{*} + \sum_{b\neq a}^{n} B_{ijmn}^{(ab)(\xi)}\varepsilon_{mn}^{(b)(\xi)} + \sum_{\eta\neq\xi}\sum_{e=1}^{n} B_{ijmn}^{(ae)(\eta)}\varepsilon_{mn}^{(e)(\eta)}, \tag{15}$$

where I_{ijmn} is the unit tensor, and the factors

$$B_{ijmn}^{(ab)(\xi)} \equiv \int\limits_{\omega_b} \mathrm{d}\mathbf{r}_b' g_{ijkl}(\mathbf{r}_a - \mathbf{r}_b') \cdot C_{klmn}'^{(\xi)}, \quad B_{ijmn}^{(ae)(\eta)} \equiv \int\limits_{\omega_b} \mathrm{d}\mathbf{r}_b' g_{ijkl}(\mathbf{r}_a - \mathbf{r}_b') \cdot C_{klmn}'^{(\eta)} \tag{16}$$

describe the interaction of subgrains in the grain and in different grains, respectively, and are numerically found for a given polycrystalline microstructure.

System (15) is solved by a method of perturbation theory [6]. All terms under the summation signs in the right-hand part of (15) are taken as perturbation. The solution is presented as a sum of various-order corrections to perturbation. It was previously shown [6] that the correction values decrease rapidly as their order increases. Here we restrict ourselves to the first order of perturbation theory. The desired solution is written in the form

$$\varepsilon_{ij}^{(a,b,e)(\xi,\eta)}(\mathbf{r}) \approx \varepsilon_{ij}^{(0)(a,b,e)(\xi,\eta)}(\mathbf{r}) + \varepsilon_{ij}^{(1)(a,b,e)(\xi,\eta)}(\mathbf{r}), \tag{17}$$

and for zero- and first-order corrections we obtain the system

$$\varepsilon_{ij}^{(0)(\xi)} - B_{ijkl}^{(aa)(\xi)}\varepsilon_{kl}^{(0)(\xi)} = \varepsilon_{ij}^{*}, \quad \varepsilon_{ij}^{(1)(a)(\xi)} - B_{ijkl}^{(aa)(\xi)}\varepsilon_{mn}^{(1)(a)(\xi)} = \sum_{\eta\neq\xi} \tilde{B}_{ijkl}^{(a\eta)}\varepsilon_{kl}^{(0)(\eta)}, \tag{18}$$

where the new factor

$$\tilde{B}_{ijmn}^{(a\eta)} \equiv \int\limits_{\omega_\eta} \mathrm{d}\mathbf{r}_\eta' g_{ijkl}(\mathbf{r}_a - \mathbf{r}_\eta') \cdot C_{klmn}'^{(\eta)} \tag{19}$$

determines the intensity of interaction of a subgrain in the ξth grain with the entire ηth grain. This factor depends on the position of the subgrain in the ξth grain, on the mutual position of the ξth and ηth grains, and on the orientation of crystallographic axes of these two grains. We take integral account of the interaction of other grains with the subgrains, i.e. it is sufficient to divide only the given grain into subgrains. By reducing the subgrain volume to zero, we derive a solution at an intragranular point.

System (18) has the dimension $Nn\times Nn$. For a practical solution, we divide the sum over all grains on the right-hand side of (18) by the sum over the nearest neighbor grains (the first range of neighbors), over the grains of the second range, third range, and so on. Such a division is convenient for analyzing the mutual elastic influence in relation to distance and searching for specific grain clusters. System (18) takes the form

$$\varepsilon_{ij}^{(0)(\xi)} - B_{ijkl}^{(aa)(\xi)}\varepsilon_{kl}^{(0)(\xi)} = \varepsilon_{ij}^{*}, \quad \varepsilon_{ij}^{(1)(a)(\xi)} - B_{ijkl}^{(aa)}\varepsilon_{mn}^{(1)(a)(\xi)} = \sum_{\eta\neq\xi}^{1\mathrm{st}} \tilde{B}_{ijkl}^{(a\eta)}\varepsilon_{kl}^{(0)(\eta)} + \sum_{\eta\neq\xi}^{2\mathrm{nd}} \tilde{B}_{ijkl}^{(a\eta)}\varepsilon_{kl}^{(0)(\eta)} + \ldots. \tag{20}$$

Factors in the sums monotonously decrease with distance, though slowly enough [6]. Elastic interaction is long-range. However, it will be shown below that, due to random orientation of crystallographic axes of grains, we can limit ourselves to the sums over grains up to the third range of neighbors. Expression (20) proves that the contribution to the strain at a grain point from the interaction with other grains is additive. Therefore it is sufficient to find extreme contributions separately for all neighboring grains and then summarize the results.

Strain in any polycrystal grain depends on the parameters of this grain (shape and orientation of its crystallographic axes with respect to external load), the microstructure of neighboring grains affecting the intensity of

elastic interaction, and the grain distance to the polycrystal surface. The latter dependence is governed by a long-range pattern of elastic interaction, resulting in the interaction of the surface grains with a smaller number of neighboring grains, in contrast to the bulk ones.

4. NUMERICAL REALIZATION ON A MODEL POLYCRYSTAL

Use a zinc polycrystal as an example. Each grain of the polycrystal is a small single crystal whose properties are known. A single crystal of zinc has a crystal lattice with hexagonal close packing (hcp) and high anisotropy characterized by the ratio of the lattice constants $c/a = 1.856$ and Zener's anisotropy factor $A = (C_{11} - C_{12})^{-1} \times 2C_{44} = 0.59$. The following elastic constants are used in the crystallographic system of coordinates, in which axis X_3 is the axis of hexagonal symmetry [7]: $C_{11}^0 = 165$ GPa, $C_{12}^0 = 31$ GPa, $C_{13}^0 = 50$ GPa, $C_{33}^0 = 62$ GPa, and $C_{44}^0 = 39.6$ GPa.

Let us study a three-dimensional model polycrystal with cubic grains of equal volumes, which is schematized in Fig. 1 (a central cross section alone is illustrated) with the axes of the global coordinate system. A grain under study is in the center and darkened; the first and second ranges of neighbors are around the grain. The first range contains 26 grains (eight of them are seen); the second, 98 grains (16 of them are seen); the third (not shown), 218 grains, etc.

From (18) it follows that zero-order corrections are determined exclusively by the shape and orientation of the grain. They correspond to the neglect of intergranular interactions and account of intragranular interactions. This approximation was earlier studied [2]. The maximum zero-order corrections are derived when the crystallographic axes of the grain are symmetrically oriented relative to the load direction. We consider uniaxial tension of a polycrystal along the X_3 axis of the global coordinate system: $\langle \sigma_{33} \rangle = 33.6$ MPa, the rest $\langle \sigma_{ij} \rangle = 0$, which corresponds to the macrostrains $\langle \varepsilon_{33} \rangle = 3 \times 10^{-4}$, $\langle \varepsilon_{11} \rangle = -0.75 \times 10^{-4}$, and $\langle \varepsilon_{22} \rangle = -0.75 \times 10^{-4}$. We will search for strain extrema $\varepsilon_{33}^{(a)(\xi)}(\mathbf{r})$ at different grain points for the ensemble of all possible polycrystalline microstructures. In the given model, the ensemble of possible microstructural configurations is reduced to a set of all possible orientations of the crystallographic axes for each individual grain. In a randomly oriented polycrystal, the orientation of each grain is set by a continuous distribution of Euler angles subject to the equal probability of all orientations. Zero-order corrections $\varepsilon_{33}^{(0)(\xi)}$ are maximum when the hexagonal axis of the grain is parallel to axis X_3 of the coordinate system. Therefore, we are to search for extrema at points of a grain with such orientation. These are absolute extrema for the entire polycrystalline solid.

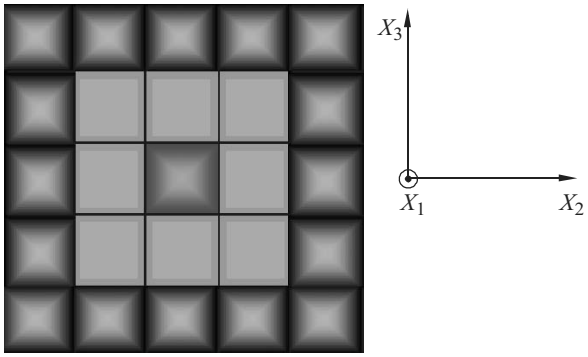

Fig. 1. Model polycrystal with cubic grains.

By problem symmetry, it is sufficient that strains be studied only at points of the vertical section through the grain center (Fig. 2).

Zero-order corrections are almost constant for all grain points within an inscribed sphere with the 90% diameter of the grain cube edge and equal $\varepsilon_{33}^{(0)}\big|_{90\%\,\text{sphere}} = 4.55 \times 10^{-4}$. In the vicinity of the edges and corners of a cubical grain, singularities typical of continuum models can arise, which makes the proposed approach (similarly to conventional ones) inapplicable. Extreme contributions from the interaction with the neighboring grains are found in the following way. For every neighboring grain an array of Euler angle triples is set using the random number generator subject to the equal probability of all orientations. The array size is 5×10^5 angle triples. For every angle triple of the array, we solve system (18) with one grain in the right-hand part of the second equation and choose the maximum (positive) and minimum (negative) corrections $\varepsilon_{33}^{(1)(a)(\xi)}(\mathbf{r})$. The procedure is re-

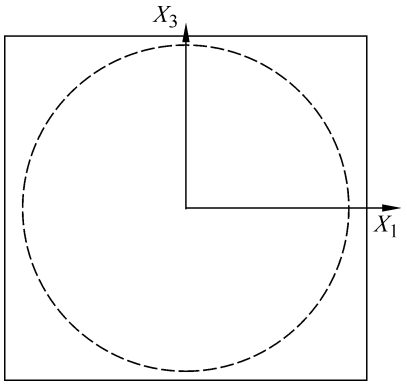

Fig. 2. Cross section of a grain.

peated for every surrounding grain. Then extreme contributions of all grains are summed, which gives the absolute extremum. Additivity of contributions from the interaction cardinally reduces the size of necessary statistical sampling. The developed algorithm also finds angles of the extreme orientation of every grain. The calculations reveal that in uniaxial macrotension at any grain point the maximum first-order corrections due to every neighboring grain are always positive, and the minimum ones are always negative, with the average value being zero. In so doing, the absolute values of these extrema are nonzero and differ strongly for different grains, even of the same range around the chosen grain. Thus, only a part of the neighboring grains provide a major contribution. Maximum strains $\varepsilon_{33}^{(a)(\xi)}(\mathbf{r}) = \varepsilon_{33}^{(0)(a)(\xi)}(\mathbf{r}) + \varepsilon_{33}^{(1)(a)(\xi)}(\mathbf{r})$ are attained at the grain periphery, i.e. at the outer surface of the inscribed sphere; at all points of this surface the maximum values are almost similar (but they are governed by different structures of the neighbors). The calculation results for a point in the grain center and at the periphery of the inscribed sphere are listed in the table. The calculations are performed with consideration for the interaction with 26 grains of the first range of neighbors, 98 grains of the second range, and 218 grains of the third range. For illustration, contributions of the grains of these ranges are given separately.

From the tabulated data it is seen that the maximum possible strain (11.3423×10^{-4}) exceeds the macrostrain (3.0×10^{-4}) by 3.78 times. It is achieved in a grain whose neighbors have a specific orientation and form a specific grain cluster in the polycrystalline microstructure. The probability of realization of such a cluster in the polycrystalline macrospecimen containing about a billion of grains can be finite. The minimum strain is similarly achieved in a grain with another type of the surroundings. In this case, the interaction with the neighboring grains generates compressive local strains in the grain despite the polycrystal tension.

The table also shows that the contribution from the elastic interaction decreases slowly enough with distance to the interacting grains. The calculation of contributions of remote grains presents no difficulties. However, to calculate corrections to numerous grains of the fourth and farther ranges is meaningless from the following considerations. The maximum contribution of each grain corresponds to a certain orientation that has a certain finite probability of realization. The probability of simultaneous realization of certain orientations of a large number of statistically independent grains tends to zero. Therefore, the total contribution of grains of remote ranges tends to zero with the probability close to unity.

The tabulated extreme contributions correspond to specific orientations of each of the interacting grains. The mutual orientation of these grains has an interesting geometrical symmetry. Figure 3 demonstrates extreme orientations of grains of the first three ranges of neighbors, which generate the strain maximum in the grain center, in the vertical and horizontal sections of a polycrystal. A hexagon conventionally represents a plane of hexagonal elastic symmetry of single crystals of grains. The symbol ⬡ corresponds to the position of the symmetry plane in the figure plane; the symbol ↔ stands for the position perpendicular to the figure plane, and its inclination shows a rough angle between the normal to the elastic symmetry plane and axis X_3; the symbol ⬯ depicts the inclined position to the figure plane at a certain angle, but the normal to the symmetry plane is perpendicular to axis X_3.

In the extreme configuration, clusters of neighboring grains form symmetrical patterns. In hcp crystals, any direction in the transverse isotropy plane (an angle of 90° to the hexagonal symmetry axis) corresponds to the maximum of the ratio between the Young modulus in this direction and the Young modulus in the transverse direction (angle 0° to the hexagonal symmetry axis). For zinc, this ratio equals [8]

$$\frac{E_{90^\circ}}{E_{0^\circ}} = \frac{119\,047\ \text{MPa}}{34\,843\ \text{MPa}} = 3.4166.$$

Note that the absolute maximum of the Young modulus in the single crystal of zinc is 124 100 MPa, at an angle of

Extreme strains and contributions from different groups of grains

		Corrections				Total strain ε_{33}
		$\varepsilon_{33}^{(0)}$	$\varepsilon_{33}^{(1)}\|_{26}$	$\varepsilon_{33}^{(1)}\|_{98}$	$\varepsilon_{33}^{(1)}\|_{218}$	
Grain center	Maximum	4.5535×10^{-4}	2.8716×10^{-4}	1.9449×10^{-4}	1.2968×10^{-4}	10.6668×10^{-4}
	Minimum		-3.6581×10^{-4}	-2.1001×10^{-4}	-1.4382×10^{-4}	-3.6629×10^{-4}
Grain periphery	Maximum		3.6731×10^{-4}	1.8857×10^{-4}	1.2301×10^{-4}	11.3423×10^{-4}
	Minimum		-3.7850×10^{-4}	-2.1683×10^{-4}	-1.4002×10^{-4}	-2.7998×10^{-4}

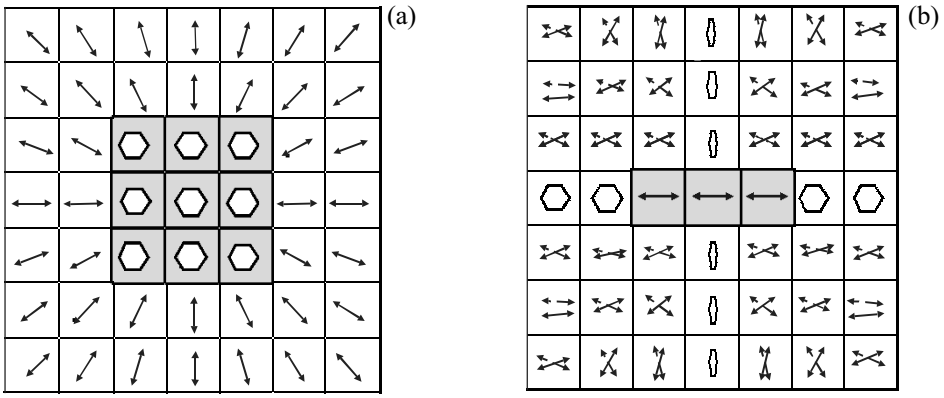

Fig. 3. Extreme orientations of the neighboring grains: horizontal (a) and vertical sections (b). Designations are given in the text.

about 70° to the hexagonal symmetry axis. However, for this direction the ratio equals

$$\frac{E_{70^\circ}}{E_{20^\circ}} = \frac{124100\ \text{MPa}}{42358\ \text{MPa}} = 2.9297.$$

In the horizontal section, all neighboring grains are oriented so that the maximum stiffness directions (coincident with the arrows in the figure) are precisely aligned with a beam from the center of the chosen grain. A single extreme orientation exists for each grain (with accuracy to the reflection across the hexagonal axis). In the vertical section the pattern is somewhat different. Grains in outer quadrants (nine grains per each) have two equivalent orientations, which are shown by solid and dashed arrows in Fig. 3. Hexagonal symmetry axes of these grains lie in the section plane but the directions of maximum stiffness form certain fixed angles to the load direction (axis X_3). Grains in the central vertical column are perpendicular to the load direction by their hexagonal symmetry axis and random in other respects; their contribution is independent of the rotation about the vertical (relative to the figure) axis. Grains in the central horizontal column are identically oriented. We have been interested to find a flat disk-like cluster of similarly oriented nine grains immediately around the central grain (marked in grey in Fig. 3), whose plane is perpendicular to the load direction. Tensile stiffness of these nine grains is minimum in the load direction, while that of their surroundings is maximum. They form a certain weakening zone with the diameter equal to three grain diameters. An introduction of a weakening zone with the five grain diameter into the model decreases the strain in the central grain. It was experimentally found that gigacycle fatigue cracks are generated in clusters of similarly oriented grains [4]. In the vertical (aligned with loading) direction and in the two orthogonal horizontal directions the neighboring grains form chains of maximum tensile stiffness. They play the role of forces enhancing deformation of the central grain. This resembles the formation of force chains in granular media, where forces acting on the medium localize [9].

The microstructural configuration shown in Fig. 3 is a combination of well-defined orientations of the surrounding grains. In a real polycrystal, an almost correct configuration in respect to the symmetry of elastic axes of grains (though they may have a rather arbitrary geometry) can be realized in a random manner. Computational experiments show that the dependence of the contribution of one interacting grain to the strain of the other grain is a rather flat function of Euler angles near the extrema. In so doing, the dependence on the anisotropy type is much stronger than that on the grain shape. Therefore, there exist many close configurations providing almost similar contributions, and the probability of realization of such microstructures can be finite in a large polycrystal.

The amplitude of fluctuation is different for bulk and surface grains of a polycrystal. A grain on the surface interacts with a halved number of neighbors as compared to a grain deep within the specimen. As a result, maximum strains in the surface grains are 40% lower than those in the bulk grains. The fluctuation amplitude also decreases. Figure 4 plots the maximum strain in a grain as a function of the distance from its center to the specimen surface. Thus, surface grains form a special material layer. In a certain sense this is an unloading region in the polycrystalline solid. The thickness of the surface layer is approximately four average grain diameters.

The mentioned feature of surface layers of polycrystalline solids stems from their heterogeneity. For homogeneous solids, this effect vanishes. This conclusion is deduced from the equations of continuum mechanics. It neglects additional surface energy of solids related to in-

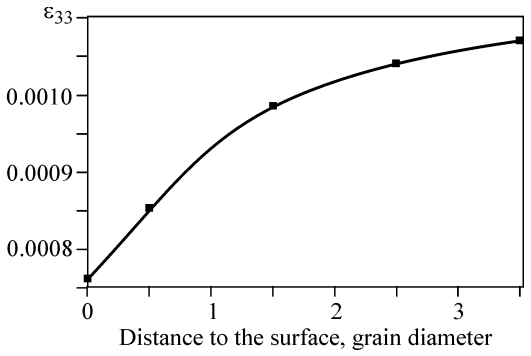

Fig. 4. Maximum strains ε_{33} as a function of the distance to the surface.

teratomic interactions, which also can be a source of surface effects. Thus, even in terms of classical continuum elasticity, the mechanical behavior of surface layers of a polycrystal differs from that for the entire volume. This complies with the concept [10] on the special role of the solid surface.

5. CONCLUSIONS

A characteristic feature of polycrystalline materials is a high inhomogeneity of kinematic and force fields in combination with a stochastic internal structure. This inhomogeneity is insufficient in some cases, but becomes crucial in the study of various critical phenomena whose occurrence is highly dependent on the type of material microstructure. The stochastic nature of heterogeneities dictates a probability-theoretical method of investigation. In many cases, a complete description of random fields, i.e. construction of distribution functions or calculation of all statistical moments can be replaced by marginal values of fields for the set of all random events. In this paper, we study extreme strains in polycrystal grains using the field-theoretical approach. In the zinc polycrystal with highly anisotropic grains, the maximum strains in a grain are 3.7 times higher than the macrostrains. This concentration is due solely to the elastic interaction of heterogeneities. Maximum strains in the bulk grains are 40% higher than those in the surface grains. This may be the reason for the displacement of damage foci from the surface into the specimen in transition from high-cycle to gigacycle fatigue.

The calculations were carried out for model polycrystals with cubic grains. The calculations for polycrystals with differently shaped grains (spherical and others) give similar results. Due to geometrical symmetry, the models clearly demonstrate patterns of the extreme microstructure of the surrounding grains generating extreme strains. A pattern depends on anisotropy of grains and the type of loading. In particular, it is theoretically predicted that maximum strains during uniaxial tension arise in the center of the cluster formed of the nearest neighbors with the same orientation, i.e. a large grain of a specific shape. In uniaxial tension, it is a disk-shaped cluster with a plane perpendicular to the load. For other loading types, clusters are of a different form.

The paper presents the calculation results on extreme strains for a macroscopically isotropic polycrystal. The method is applicable to textured polycrystals.

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