Phase field microelasticity theory and modeling of elastically and structurally inhomogeneous solid

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The phase field microelasticity theory of a three-dimensional elastically anisotropic solid of arbitrarily inhomogeneous modulus also containing arbitrary structural inhomogeneities is proposed. The theory is based on the equation for the strain energy of the elastically and structurally inhomogeneous system presented as a functional of the phase field, which is the effective stress-free strain of the ''equivalent'' homogeneous modulus system. It is proved that the stress-free strain minimizing this functional fully determines the exact elastic equilibrium in the elastically and structurally inhomogeneous solid. The stress-free strain minimizer is obtained as a steady state solution of the time-dependent Ginzburg–Landau equation. The long-range strain-induced interaction due to the elastic and structural inhomogeneities is explicitly taken into account. Systems with voids and cracks are the special cases covered by this theory since voids and cracks are elastic inhomogeneities that have zero modulus. Other misfitting defects, such as dislocations and coherent precipitates, are also integrated into this theory. Examples of elastic equilibrium of elastically inhomogeneous solid under applied stress are considered. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1492859]

I. INTRODUCTION

Most of the material systems of engineering importance are structurally and/or elastically inhomogeneous. One common example of such systems is polycrystal. Even if each grain of the polycrystal is a perfect crystallite, the entire material is elastically inhomogeneous. This is because the components of elastic modulus tensor within each grain are transformed due to the grain mutual rotation and thus the elastic moduli of different grains become different. A multiphase coherent mixture produced by a phase transformation is another example of structurally and elastically inhomogeneous systems—as a rule, the domains of the product phase have elastic moduli that are different from those of the parent phase because they have different crystallographic structures and orientations. Systems with cracks and voids, which can be considered as ''particles'' with zero elastic modulus, represent an important class of elastically inhomogeneous materials. The advanced man-made materials, such as composites, multilayers, and graded materials, are also structurally and/or elastically inhomogeneous systems. Their artificially built-in structural and/or elastic inhomogeneities are intended to produce the superior functional performance.

In spite of the importance of elastically inhomogeneous materials, the progress in their theoretical study is hindered by serious mathematical difficulties in an analytical treatment of a three-dimensional (3D) system with an arbitrarily inhomogeneous elastic modulus under applied stress. There are very few problems that are really solved. The case of a single ellipsoidal elastic inhomogeneity is solved by Eshelby in his classical work.[1] The generalized plane strain problems of inhomogeneous materials with specific distributions of elastic moduli, such as layered,[2,3] angular,[4] and cylindrical[5] media, have recently been solved. The analytical solution for a planar crack has been obtained using dislocation pileup theory.[6] The extended stress field around a cylindrical crack in an infinite homogeneous isotropic elastic medium is calculated in Ref. 7 by using this theory, which models the crack as a pileup of Somigliana ring dislocations.

The precipitations involving inhomogeneous modulus linearly coupled with the concentration field have recently been simulated using the conjugate gradient method.[8,9] The perturbation theory with respect to a variation of the elastic modulus has been used,[10–20] where the modeling is reduced to a numerical solution of the approximated equations of the elastic equilibrium. In most cases,[10–18] these equations are the first order approximation with respect to the perturbation of the modulus. The higher-order corrections in the perturbation theory have been used.[19,20] However, for a system with a significant difference in the elastic moduli, like the system with voids and/or cracks of arbitrary configuration, use of the perturbation theory may pose a problem: the convergence in the perturbation series in this case becomes questionable. Even if this series is convergent, a required increase in the number of terms of the perturbation series may make the computational procedure prohibitively expensive.

The problem of the elastically inhomogeneous system is much more complex than that of the structurally inhomogeneous (but elastically homogeneous) system. In fact, the effect of the structural inhomogeneities in the elastically homogeneous systems has been comparatively well investigated.[21] It is now reasonably well understood how the structural inhomogeneities affect the coherent mesoscopic

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microstructures and alter the system thermodynamics.[21–31] This success has been achieved mostly due to the use of the Khachaturyan–Shatalov (KS) theory,[21] which provides the exact explicit solution for the system strain energy as a functional of the arbitrary misfit strain distribution. The misfit strain tensor, which is the stress-free strain (also called eigenstrain), adequately describes the structural inhomogeneities and their spatial distribution in the mesoscopic scale.

The phase field microelasticity (PFM) method based on the KS theory has been used for a realistic modeling of various processes, e.g., the coherent decompositions of ordered precipitates in alloys,[22–25] the solute segregations around static dislocations,[26,27] the martensitic transformations in the constrained and unconstrained single crystals,[28,29] and the low-symmetry martensitic transformation in elastically isotropic polycrystals.[29] The PFM simulation has also been successfully applied to the 3D dislocation dynamics in plastic deformation.[30,31]

The assumption of the elastic homogeneity is a limitation of the PFM theory hindering its wider application. If we remove this limitation and adequately address the problem of elastic inhomogeneity, the PFM theory would be universal in a sense that it could be applied to a mesoscale characterization of practically any engineering materials. The materials could be single crystals and polycrystals with dislocations, voids, cracks, as well as multiphase structures. So far, there was only one attempt to formulate the PFM theory of elastically inhomogeneous materials without the use of perturbation theory approximations.[32,33] However, it was made to characterize a particular (although important) case of the elastically inhomogeneous systems, viz. the systems with voids and cracks.[32,33]

In this work, we demonstrate that a further advance in the theoretical characterization of the elastically (and structurally) inhomogeneous system is still possible.[34] It is based on the formulation of the PFM equations describing the exact elastic equilibrium and the development of a computationally effective method for their numerical solution using fast Fourier transform. This advance turns out to be possible even without a serious complication of the theory and computational procedure with respect to those employed for the PFM characterizations of the elastically homogeneous systems.[21–31] In particular, the proposed approach can be used to extend the mesoscopic modeling of martensitic transformation,[28,29] dislocation dynamics,[30,31] and void/crack evolutions[32,33] under applied stress to the more realistic case of polycrystals comprised of elastically anisotropic grains.

II. EQUILIBRIUM EQUATIONS OF ELASTICITY FOR ARBITRARILY INHOMOGENEOUS SYSTEM IN TERMS OF EQUIVALENT STRESS-FREE STRAIN

A. Strain energy functional for arbitrary distribution of stress-free strain in elastically homogeneous body

To address the problem of an elastically inhomogeneous anisotropic system under applied stress, we consider first a much simpler system. It is an elastically homogeneous anisotropic system of the same macroscopic size and shape as the original elastically inhomogeneous system but with the heterogeneous misfit-generating stress-free strain. This misfit strain is described by the tensor field $\varepsilon^0_{ij}(\mathbf{r})$. The field $\varepsilon^0_{ij}(\mathbf{r})$ is assumed to be arbitrarily heterogeneous on the mesoscale but homogeneous on the macroscale. The KS theory gives the exact elastic strain and strain energy of this system as a functional of the fixed field $\varepsilon^0_{ij}(\mathbf{r})$.[21] The strain energy is also a function of the macroscopic strain $\overline{\varepsilon}_{ij}$ fixing the macroscopic shape of the body and determined by the boundary condition (clamping). For a macroscopically homogeneous body, this strain coincides with the macroscopically averaged strain

$$\overline{\varepsilon}_{ij}=\frac{1}{V}\int_V \varepsilon_{ij}(\mathbf{r})d^3r, \tag{1}$$

where V is the system volume.

The strain energy presented in this form is a functional of the field $\varepsilon^0_{ij}(\mathbf{r})$[21]

$$E^{\mathrm{el}}=\frac{1}{2}\int_V C^0_{ijkl}\varepsilon^0_{ij}(\mathbf{r})\varepsilon^0_{kl}(\mathbf{r})d^3r - \overline{\varepsilon}_{ij}\int_V C^0_{ijkl}\varepsilon^0_{kl}(\mathbf{r})d^3r+\frac{V}{2}C^0_{ijkl}\overline{\varepsilon}_{ij}\overline{\varepsilon}_{kl} - \frac{1}{2}\fint\frac{d^3k}{(2\pi)^3}n_i\tilde{\sigma}^0_{ij}(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{\sigma}^0_{kl}(\mathbf{k})^*n_l, \tag{2}$$

where the integral $\fint$ in the infinite reciprocal space is evaluated as a principal value excluding a volume $(2\pi)^3/V$ around the point $\mathbf{k}=\mathbf{0}$, $\mathbf{n}=\mathbf{k}/k$ is a unit directional vector in the reciprocal space, $\Omega_{ij}(\mathbf{n})$ is the Green function tensor inverse to the tensor $\Omega^{-1}_{ij}(\mathbf{n})=C^0_{ikjl}n_kn_l$, C^0_{ijkl} is the elastic modulus, $\tilde{\sigma}^0_{ij}(\mathbf{k})=C^0_{ijkl}\tilde{\varepsilon}^0_{kl}(\mathbf{k})$, the superscript asterisk indicates the complex conjugate, and $\tilde{\varepsilon}^0_{ij}(\mathbf{k})$ is the Fourier transform of the field $\varepsilon^0_{ij}(\mathbf{r})$, $\tilde{\varepsilon}^0_{ij}(\mathbf{k})=\int_v\varepsilon^0_{ij}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d^3r$. The strain energy in the form T (2) is convenient when the body is under a strain-controlled boundary condition. The strain energy functional for a stress-controlled boundary condition is given by Eq. (A3) in the Appendix.

The KS theory determines the equilibrium strain $\varepsilon_{ij}(\mathbf{r})$ at a point $\mathbf{r}$ through the misfit strain field $\varepsilon^0_{ij}(\mathbf{r})$ as[21]

$$\varepsilon_{ij}(\mathbf{r})=\overline{\varepsilon}_{ij}+\frac{1}{2}\fint\frac{d^3k}{(2\pi)^3}[n_i\Omega_{jk}(\mathbf{n})+n_j\Omega_{ik}(\mathbf{n})]\times\tilde{\sigma}^0_{kl}(\mathbf{k})n_le^{i\mathbf{k}\cdot\mathbf{r}}. \tag{3}$$

The energy functional (2) and strain (3) are valid for a macroscopically homogeneous system, which means that the typical size of the macroscopic system is significantly greater than the typical size of the mesoscopic structural heterogeneities characterized by the misfit strain $\varepsilon^0_{ij}(\mathbf{r})$.

B. Equilibrium equation of elasticity for an elastically and structurally inhomogeneous system

Let us consider a general case of the elastically anisotropic and elastically inhomogeneous body, which also is structurally inhomogeneous. The elastic modulus of such a body is coordinate dependent, $C_{ijkl}(\mathbf{r})$. The structural inhomogeneities are described by the fixed crystal lattice misfit

strain (stress-free strain or eigenstrain), $\varepsilon_{ij}^{*}(\mathbf{r})$, arbitrarily distributed in the body (note that there is no confusion between the superscript* in $\varepsilon_{ij}^{*}(\mathbf{r})$ and that in $\tilde{\sigma}_{ij}^{o}(\mathbf{k})^{*}$ indicating the complex conjugate). The misfit strain $\varepsilon_{ij}^{*}(\mathbf{r})$ can be generated by a fixed distribution of crystal lattice defects, such as coherent new phase inclusions, concentration heterogeneities, dislocations, etc. The system can be either a single crystal or polycrystal. This is the most general formulation of the problem. It is applicable to a majority of technologically important materials.

The coordinate-dependent modulus $C_{ijkl}(\mathbf{r})$ can always be presented as a sum

$$C_{ijkl}(\mathbf{r}) = C_{ijkl}^{0} - \Delta C_{ijkl}(\mathbf{r}), \tag{4}$$

where $\Delta C_{ijkl}(\mathbf{r})$ is the modulus variation from the reference value C_{ijkl}^{0}, which characterizes the elastic inhomogeneities. If the body is constrained so that its macroscopic deformation is fixed and determined by the value $\bar{\varepsilon}_{ij}$, this constraint generates the strain field $\varepsilon_{ij}(\mathbf{r})$, which is heterogeneous due to both the elastic inhomogeneities $\Delta C_{ijkl}(\mathbf{r})$ and the structural inhomogeneities $\varepsilon_{ij}^{*}(\mathbf{r})$. The stress is related to the strain $\varepsilon_{ij}(\mathbf{r})$ by Hooke's law

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}(\mathbf{r})[\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{*}(\mathbf{r})]. \tag{5}$$

The stress satisfies the following equilibrium equation at every point $\mathbf{r}$,

$$\frac{\partial \sigma_{ij}(\mathbf{r})}{\partial r_j} = 0. \tag{6}$$

Using the modulus definition (4) and the stress (5), the elastic equilibrium equation (6) can be rewritten as

$$C_{ijkl}^{0}\frac{\partial \varepsilon_{kl}(\mathbf{r})}{\partial r_j} = \frac{\partial}{\partial r_j}\{C_{ijkl}^{0}\varepsilon_{kl}^{*}(\mathbf{r}) + \Delta C_{ijkl}(\mathbf{r})[\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{*}(\mathbf{r})]\}. \tag{7}$$

The strain $\varepsilon_{ij}(\mathbf{r})$ can be expressed as a sum of the homogeneous part $\bar{\varepsilon}_{ij}$ determined by the external constraint and the heterogeneous part

$$\varepsilon_{ij}(\mathbf{r}) = \bar{\varepsilon}_{ij} + e_{ij}(\mathbf{r}), \tag{8}$$

where the heterogeneous strain $e_{ij}(\mathbf{r})$ is determined by the displacement $\mathbf{v}(\mathbf{r})$

$$e_{ij}(\mathbf{r}) = \frac{1}{2}\left[\frac{\partial v_i(\mathbf{r})}{\partial r_j} + \frac{\partial v_j(\mathbf{r})}{\partial r_i}\right]. \tag{9}$$

For a macroscopically homogeneous clamped system, the total displacement at the external boundary is $\bar{\varepsilon}_{ij} r_j^{s}$, which is determined by the homogeneous strain $\bar{\varepsilon}_{ij}$ and the surface coordinate vector $\mathbf{r}^{s}$ at the external boundary. The displacement $\mathbf{v}(\mathbf{r})$ associated with the heterogeneous strain $e_{ij}(\mathbf{r})$ is assumed to vanish at the external boundary of the body. The macroscopically homogeneous system, for which the above assumption is valid, is a system whose typical size Λ is significantly greater than the typical mesoscopic length λ over which the elastic modulus $C_{ijkl}(\mathbf{r})$ considerably changes. This approximation is asymptotically correct with an accuracy of $\lambda/\Lambda \ll 1$. Indeed, according to Saint Venant's principle, this approximation produces inaccuracy in the strain field only within the surface layer at the external boundary of the body. The thickness of this layer is commensurate with a typical size of the elastic inhomogeneity $\Delta C_{ijkl}(\mathbf{r})$. Therefore, the error introduced by the approximate boundary condition $\mathbf{v}(\mathbf{r}^{s}) = 0$ is asymptotically small for a macroscopically large and a macroscopically homogeneous system where $\lambda/\Lambda \to 0$.

Substituting Eqs. (8) and (9) into the left-hand side of the equilibrium equation (7) yields

$$C_{ijkl}^{0}\frac{\partial^2 \nu_k(\mathbf{r})}{\partial r_j \partial r_l} = \frac{\partial}{\partial r_j}\{C_{ijkl}^{0}\varepsilon_{kl}^{*}(\mathbf{r}) + \Delta C_{ijkl}(\mathbf{r})[\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{*}(\mathbf{r})]\}. \tag{10}$$

Let us assume that the external surface of the body is covered by an infinitesimally thin layer whose elastic modulus is C_{ijkl}^{0}. The introduction of this infinitesimally thin layer does not affect the elastic equilibrium in the system, however it simplifies the boundary condition giving $\Delta C_{ijkl}(\mathbf{r}^{s}) = 0$. Let us also assume that the structural inhomogeneities do not locate on the system surface, which gives the boundary condition $\varepsilon_{ij}^{*}(\mathbf{r}^{s}) = 0$. Using the Fourier transform of Eq. (10) and the boundary conditions $\mathbf{v}(\mathbf{r}^{s}) = 0$, $\Delta C_{ijkl}(\mathbf{r}^{s}) = 0$, and $\varepsilon_{ij}^{*}(\mathbf{r}^{s}) = 0$ transforms the equilibrium equation (10) into the integral form

$$\nu_i(\mathbf{r}) = \oint\!\!\!\!\!\!- \frac{d^3k}{(2\pi)^3}\left\{ -i\frac{1}{k}\Omega_{ij}(\mathbf{n})\{C_{jklm}^{0}\varepsilon_{lm}^{*}(\mathbf{r}) + \Delta C_{jklm}(\mathbf{r})[\varepsilon_{lm}(\mathbf{r}) - \varepsilon_{lm}^{*}(\mathbf{r})]\}_{\mathbf{k}} n_k \right\} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{11}$$

where $\{C_{ijkl}^{0}\varepsilon_{kl}^{*}(\mathbf{r}) + \Delta C_{ijkl}(\mathbf{r})[\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{*}(\mathbf{r})]\}_{\mathbf{k}}$ is the Fourier transform of the corresponding function in the braces.

Using Eqs. (9) and (11), the strain, (8) can be expressed as

$$\varepsilon_{ij}(\mathbf{r}) = \bar{\varepsilon}_{ij} + \frac{1}{2}\oint\!\!\!\!\!\!- \frac{d^3k}{(2\pi)^3}[n_i\Omega_{jk}(\mathbf{n}) + n_j\Omega_{ik}(\mathbf{n})] \times \{C_{klmn}^{0}\varepsilon_{mn}^{*}(\mathbf{r}) + \Delta C_{klmn}(\mathbf{r})[\varepsilon_{mn}(\mathbf{r}) - \varepsilon_{mn}^{*}(\mathbf{r})]\}_{\mathbf{k}} n_l e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{12}$$

Equation (12) is an integral equation for the equilibrium strain $\varepsilon_{ij}(\mathbf{r})$ in the elastically and structurally inhomogeneous system characterized by the elastic inhomogeneities $\Delta C_{ijkl}(\mathbf{r})$ and the structural inhomogeneities $\varepsilon_{ij}^{*}(\mathbf{r})$.

Now let us change variables in Eq. (12). We introduce a new variable $\varepsilon_{ij}^{0}(\mathbf{r})$ related to the variable $\varepsilon_{ij}(\mathbf{r})$ by definition

$$C_{ijkl}^{0}\varepsilon_{kl}^{0}(\mathbf{r}) = C_{ijkl}^{0}\varepsilon_{kl}^{*}(\mathbf{r}) + \Delta C_{ijkl}(\mathbf{r})[\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{*}(\mathbf{r})]. \tag{13}$$

Using $C^0_{ijkl}\varepsilon^0_{kl}(\mathbf{r})$ to replace $C^0_{ijkl}\varepsilon^*_{kl}(\mathbf{r})+\Delta C_{ijkl}(\mathbf{r})[\varepsilon_{kl}(\mathbf{r})-\varepsilon^*_{kl}(\mathbf{r})]$ in Eq. (12) yields

$$\varepsilon_{ij}(\mathbf{r})=\overline{\varepsilon}_{ij}+\frac{1}{2}\int\frac{d^3k}{(2\pi)^3}[n_i\Omega_{jk}(\mathbf{n})+n_j\Omega_{ik}(\mathbf{n})]\times C^0_{klmn}\tilde{\varepsilon}^0_{mn}(\mathbf{k})n_l e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{14}$$

Equation (14) coincides with Eq. (3) for the equilibrium strain in an elastically homogeneous body of elastic modulus C^0_{ijkl} with a misfit strain $\varepsilon^0_{ij}(\mathbf{r})$, i.e., the elastically and structurally inhomogeneous body assumes the same strain as the elastically homogenous body with the appropriate choice of the misfit strain $\varepsilon^0_{ij}(\mathbf{r})$. It is important that the elastically and structurally inhomogeneous body also assumes the same stress as the elastically homogenous body with this choice of the misfit strain $\varepsilon^0_{ij}(\mathbf{r})$. Indeed, deducting the same term $C^0_{ijkl}\varepsilon_{kl}(\mathbf{r})$ from both sides of Eq. (13) gives

$$C^0_{ijkl}[\varepsilon_{kl}(\mathbf{r})-\varepsilon^0_{kl}(\mathbf{r})]=[C^0_{ijkl}-\Delta C_{ijkl}(\mathbf{r})]\times[\varepsilon_{kl}(\mathbf{r})-\varepsilon^*_{kl}(\mathbf{r})]. \tag{15}$$

Equation (15) demonstrates that the stress in the elastically homogeneous body $\sigma_{ij}(\mathbf{r})=C^0_{ijkl}[\varepsilon_{kl}(\mathbf{r})-\varepsilon^0_{kl}(\mathbf{r})]$ is equal to the stress in the original elastically and structurally inhomogeneous body $\sigma_{ij}(\mathbf{r})=[C^0_{ijkl}-\Delta C_{ijkl}(\mathbf{r})][\varepsilon_{kl}(\mathbf{r})-\varepsilon^*_{kl}(\mathbf{r})]$. Therefore, the elastically homogeneous system with the misfit strain $\varepsilon^0_{ij}(\mathbf{r})$ is equivalent to the original elastically and structurally inhomogeneous system with the elastic inhomogeneities $\Delta C_{ijkl}(\mathbf{r})$ as well as the structural inhomogeneities $\varepsilon^*_{ij}(\mathbf{r})$.

Transforming the variable $\varepsilon_{ij}(\mathbf{r})$ in the equilibrium equation (12) for the elastically and structurally inhomogeneous system to the variable $\varepsilon^0_{ij}(\mathbf{r})$ defined by Eq. (13) formulates the original equilibrium equation in terms of the virtual misfit strain $\varepsilon^0_{ij}(\mathbf{r})$:

$$\Delta S_{ijkl}(\mathbf{r})C^0_{klmn}[\varepsilon^0_{mn}(\mathbf{r})-\varepsilon^*_{mn}(\mathbf{r})]+\varepsilon^*_{ij}(\mathbf{r})=\overline{\varepsilon}_{ij}+\frac{1}{2}\int\frac{d^3k}{(2\pi)^3}[n_i\Omega_{jk}(\mathbf{n})+n_j\Omega_{ik}(\mathbf{n})]\times C^0_{klmn}\tilde{\varepsilon}^0_{mn}(\mathbf{k})n_l e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{16}$$

where $\Delta S_{ijkl}(\mathbf{r})=\Delta C^{-1}_{ijkl}(\mathbf{r})$. Equation (16) is, in fact, an integral equation for the determination of $\varepsilon^0_{ij}(\mathbf{r})$. It is the equilibrium equation of elasticity for the elastically and structurally inhomogeneous system. A similar type of equilibrium equation, in which a difference in the elastic modulus is emulated by virtual stress-free strain field, has been obtained in Ref. 2, where it was employed for solving a problem of the multilayer of parallel misfitting lamellae with different elastic moduli.

Finding the misfit strain $\varepsilon^0_{ij}(\mathbf{r})$ in the equivalent elastically homogeneous system fully solves the elasticity problem of the elastically and structurally inhomogeneous system—the equilibrium strain is given by Eq. (14) through the field $\varepsilon^0_{ij}(\mathbf{r})$, and the stress is determined by Eq. (5).

III. VARIATIONAL PRINCIPLE AND ITS APPLICATION FOR DETERMINATION OF ELASTIC EQUILIBRIUM OF ARBITRARILY INHOMOGENEOUS SYSTEM

A. Strain energy functional for elastically and structurally inhomogeneous body

The strain energy of the elastically and structurally inhomogeneous system can be obtained through the strain energy of the elastically homogeneous system. Indeed, the strain energy of the equivalent elastically homogeneous system is determined by

$$E^{\text{hom}}=\frac{1}{2}\int_V C^0_{ijkl}[\varepsilon_{ij}(\mathbf{r})-\varepsilon^0_{ij}(\mathbf{r})][\varepsilon_{kl}(\mathbf{r})-\varepsilon^0_{kl}(\mathbf{r})]d^3r, \tag{17}$$

while the strain energy of the original elastically and structurally inhomogeneous system is

$$E^{\text{inhom}}=\frac{1}{2}\int_V[C^0_{ijkl}-\Delta C_{ijkl}(\mathbf{r})][\varepsilon_{ij}(\mathbf{r})-\varepsilon^*_{ij}(\mathbf{r})]\times[\varepsilon_{kl}(\mathbf{r})-\varepsilon^*_{kl}(\mathbf{r})]d^3r. \tag{18}$$

Using Eq. (13) , the energy difference is

$$\Delta E=E^{\text{inhom}}-E^{\text{hom}}=\frac{1}{2}\int_V[C^0_{ijmn}\Delta S_{mnpq}(\mathbf{r})C^0_{pqkl}-C^0_{ijkl}]\times[\varepsilon^0_{ij}(\mathbf{r})-\varepsilon^*_{ij}(\mathbf{r})][\varepsilon^0_{kl}(\mathbf{r})-\varepsilon^*_{kl}(\mathbf{r})]d^3r. \tag{19}$$

Substituting Eq. (2) for E^{hom} into Eq. (19) yields the strain energy of the elastically and structurally inhomogeneous system as a functional of $\varepsilon^0_{ij}(\mathbf{r})$,

$$\begin{aligned}E^{\text{inhom}}=&\frac{1}{2}\int_V[C^0_{ijmn}\Delta S_{mnpq}(\mathbf{r})C^0_{pqkl}-C^0_{ijkl}]\times[\varepsilon^0_{ij}(\mathbf{r})-\varepsilon^*_{ij}(\mathbf{r})][\varepsilon^0_{kl}(\mathbf{r})-\varepsilon^*_{kl}(\mathbf{r})]d^3r\\&+\frac{1}{2}\int_V C^0_{ijkl}\varepsilon^0_{ij}(\mathbf{r})\varepsilon^0_{kl}(\mathbf{r})d^3r\\&-\overline{\varepsilon}_{ij}\int_V C^0_{ijkl}\varepsilon^0_{kl}(\mathbf{r})d^3r+\frac{V}{2}C^0_{ijkl}\overline{\varepsilon}_{ij}\overline{\varepsilon}_{kl}\\&-\frac{1}{2}\int\frac{d^3k}{(2\pi)^3}n_i\tilde{\sigma}^0_{ij}(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{\sigma}^0_{kl}(\mathbf{k})^*n_l.\end{aligned} \tag{20}$$

B. Variational approach for determining the equivalent stress-free strain

The strain energy functional (20) meets the variational principle: its minimum is reached when the minimizing function $\varepsilon^0_{ij}(\mathbf{r})$ satisfies the equilibrium equation (16). Indeed, the minimum condition of the functional (20) with respect to the function $\varepsilon^0_{ij}(\mathbf{r})$ is

$$\frac{\delta E^{\text{inhom}}}{\delta\varepsilon^0_{ij}(\mathbf{r})}=0. \tag{21}$$

Taking the variational derivative of the functional (20) with respect to $\varepsilon^0_{ij}(\mathbf{r})$ and using it in (21) gives the equilibrium equation (16).

The foregoing consideration proves the following variational principle:

The misfit strain minimizing the strain energy functional (20) determines the equilibrium strain and stress of the elastically and structurally inhomogeneous body in accordance with Eqs. (14) and (5), respectively.

The above statement indicates that finding the minimizer $\varepsilon^0_{ij}(\mathbf{r})=\varepsilon^0_{ij}(\mathbf{r})$ for the equivalent elastically homogeneous system fully solves the elasticity problem of the arbitrarily elastically and structurally inhomogeneous system. Therefore, the function $\varepsilon^0_{ij}(\mathbf{r})$ entering the functional (20) can be considered as a relaxation parameter (a phase field). This circumstance allows us to formulate the variational approach to the computationally efficient modeling of the arbitrarily inhomogeneous modulus system with arbitrary structural inhomogeneities, where the multiple cracks and voids are its particular cases.[32,33]

The energy minimizer $\varepsilon^{00}_{ij}(\mathbf{r})$ could be found through a solution of the PFM kinetic equation for $\varepsilon^0_{ij}(\mathbf{r})$, which is the time-dependent Ginzburg–Landau (TDGL) type equation. The TDGL equation in this case is

$$\frac{\partial \varepsilon^0_{ij}(\mathbf{r},t)}{\partial t}=-L_{ijkl}\frac{\delta E^{\text{inhom}}}{\delta \varepsilon^0_{kl}(\mathbf{r},t)}, \tag{22}$$

where L_{ijkl} is the kinetic coefficient, t is ''time,'' and E^{inhom} is given by Eq. (20). A specific choice of the tensor L_{ijkl} is of no importance as long as it is positively defined: since Eq. (22) is linear, it has a solution and this solution determines the minimum of the energy E^{inhom}. The simplest choice of L_{ijkl} is $L_{ijkl}=L\delta_{ik}\delta_{jl}$. Incorporating Eq. (20) into Eq. (22) gives the explicit form of the TDGL equation

$$\begin{aligned}\frac{\partial \varepsilon^0_{ij}(\mathbf{r},t)}{\partial t}=L C^0_{ijkl}\Bigg\{&\frac{1}{2}\oint\!\!\oint\frac{d^3k}{(2\pi)^3}[n_k\Omega_{lm}(\mathbf{n})\\&+n_l\Omega_{km}(\mathbf{n})]\tilde{\sigma}^0_{mn}(\mathbf{k})n_n e^{i\mathbf{k}\cdot\mathbf{r}}\\&-\Delta S_{klmn}(\mathbf{r})C^0_{mnpq}[\varepsilon^0_{pq}(\mathbf{r})-\varepsilon^*_{pq}(\mathbf{r})]-\varepsilon^*_{kl}(\mathbf{r})\\&+\overline{\varepsilon}^0_{kl}+S^0_{klmn}\sigma^{ex}_{mn}\Bigg\},\end{aligned} \tag{23}$$

where $\overline{\varepsilon}^0_{ij}=(1/V)\int_V\varepsilon^0_{ij}(\mathbf{r})d^3r$, and the tensor S^0_{ijkl} is the elastic compliance tensor inverse to the elastic modulus, $S^0_{ijkl}=C^{0\,-1}_{ijkl}$. The TDGL equation (23) is applicable to both the strain-controlled and stress-controlled boundary conditions specified by the external stress σ^{ex}_{ij}, which is

$$\sigma^{ex}_{ij}=C^0_{ijkl}(\overline{\varepsilon}_{kl}-\overline{\varepsilon}^0_{kl}) \tag{24}$$

for the strain-controlled boundary condition, while in the case of stress-controlled boundary condition $\sigma^{\text{ex}}_{ij}=\sigma^{\text{appl}}_{ij}$. Once the field $\varepsilon^0_{ij}(\mathbf{r},t)$ reaches the saturation and becomes equal to the energy minimizer function $\varepsilon^{00}_{ij}(\mathbf{r})$, the driving force $\delta E^{\text{inhom}}/\delta\varepsilon^0_{ij}(\mathbf{r},t)$ vanishes and, as follows from Eq. (22), the field $\varepsilon^0_{ij}(\mathbf{r},t)$ stops evolving. Knowing the minimizer $\varepsilon^{00}_{ij}(\mathbf{r})$, we can calculate the equilibrium strain, stress, and strain energy of the elastically and structurally inhomogeneous system by using Eqs. (14), (5), and (20), respectively.

The cracks and voids are special cases of elastic inhomogeneities with zero modulus, $C_{ijkl}(\mathbf{r})=0$. Assuming $\Delta C_{ijkl}(\mathbf{r})=C^0_{ijkl}$, which results in $C_{ijkl}(\mathbf{r})=0$, reduces Eq. (23) to the TDGL equation characterizing cracks and voids.[32,33]

C. Examples of PFM computation of elastic equilibrium of elastically inhomogeneous body

To test the proposed PFM method, we consider a large elastically inhomogeneous body consisting of periodically repeated and coherently adjacent identical regions. Each region, which is a motif of this periodical structure and is a computational cell, contains a group of elastic inhomogeneities of the same configuration. The entire body consisting of a large number of such blocks can be considered as a macroscopically homogeneous system, to which the PFM theory is applicable. If the typical distance characterizing the distribution of elastic inhomogeneities is much smaller than the size of a computational cell, a solution for the elastic field generated by the group of elastic inhomogeneities in this cell is asymptotically close to the corresponding solution for the same group of elastic inhomogeneities in the infinite body.

As has been shown in the previous sections, the macroscopically homogeneous body with arbitrarily distributed elastic and structural inhomogeneities can be described by the PFM theory applied to the equivalent elastically homogeneous body with the distributed misfit strain $\varepsilon^0_{ij}(\mathbf{r})$. The energy minimizer $\varepsilon^{00}_{ij}(\mathbf{r})$ is a steady state solution of the TDGL equation (23). To find it, we will numerically solve Eq. (23). The strain, stress, and strain energy are expressed through the minimizer $\varepsilon^{00}_{ij}(\mathbf{r})$ by Eqs. (14), (5), and (20), respectively, with $\varepsilon^{00}_{ij}(\mathbf{r})$ replacing $\varepsilon^0_{ij}(\mathbf{r})$. In solving Eq. (23) numerically, we use the fast Fourier transform technique.

The PFM theory of an elastically inhomogeneous system proposed in this paper is formulated for an arbitrary pattern of elastic and structural inhomogeneities in an elastically anisotropic body. To verify the accuracy of the proposed PFM approach, we have to compare the PFM calculation results with the analytical results obtained for the same system. Unfortunately, analytical solutions are known only for very few simple systems. Below we apply our computational method to one of them, for which an analytical solution has been obtained. This is the case of a cylindrical inhomogeneity in an elastically isotropic solid. We also apply our PFM calculations for more complicated systems, such as polycrystals comprised of elastically anisotropic grains under applied stress. We investigate only the effects of the elastic inhomogeneities on the elastic equilibrium while assuming $\varepsilon^*_{ij}(\mathbf{r})=0$ everywhere (no structural inhomogeneities). A PFM calculation of more complex systems practically takes the same computational time as that for the simple ones for given system size.

1. Cylindrical inhomogeneity in isotropic crystal

The uniaxial tensile stress is assumed to be perpendicular to the cylinder axis as shown in Fig. 1(a). This system has

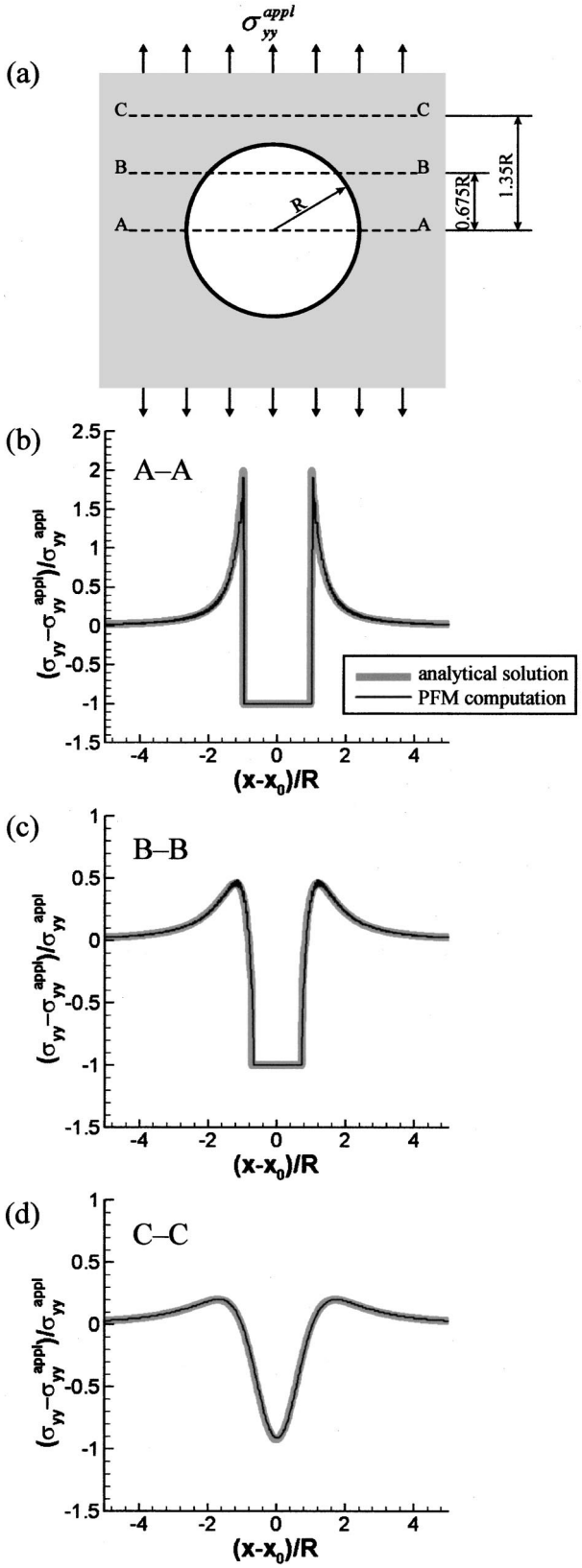

FIG. 1. A cylindrical hole under tension in the y direction in the elastically isotropic body ($\nu=0.3$). (a) Schematic illustration of a cross section of the system perpendicular to the cylinder axis (z axis); the PFM computational solutions (thin black lines) and the corresponding analytical solutions (thick gray lines) for $(\sigma_{yy}-\sigma_{yy}^{appl})/\sigma_{yy}^{appl}$along three different cross sections: (b) A-A; (c) B-B; and (d) C-C, respectively, as indicated in (a).

the exact analytical solution. In the computation, we used a computational cell of 1024×1024. The cylinder diameter is 80 grid increments. Although the PFM theory is formulated for materials of arbitrary elastic anisotropy, we consider here an elastically isotropic system with Poisson's ratio $\nu=0.3$ since the corresponding analytical solution has a comparatively simple form for the isotropic case. We first consider the cylindrical inhomogeneity that is a hole $[C_{ijkl}(\mathbf{r})=0]$. The computational results are shown in Figs. 1(b)–1(d) as plots of the disturbed stress field, $(\sigma_{yy}-\sigma_{yy}^{appl})/\sigma_{yy}^{appl}$, along three typical cross sections of the system as indicated in Fig. 1(a). To make a visual quantitative comparison of the stress field distribution obtained from the proposed PFM method and analytical solution, we used the thick gray lines to describe the analytically calculated values and thin black lines to describe the values calculated by a numerical solution of Eq. (23). This comparison shows an excellent agreement between analytical and numerical solutions.

For further quantitative comparison, we considered the same system while the cylindrical inhomogeneity has different isotropic elastic moduli, namely $C_{ijkl}(\mathbf{r})=0.25C_{ijkl}^0$, $0.5C_{ijkl}^0$, $2C_{ijkl}^0$, and $4C_{ijkl}^0$, respectively. For each case, the disturbed stress fields, $(\sigma_{yy}-\sigma_{yy}^{appl})/\sigma_{yy}^{appl}$, calculated by solving Eq. (23) and analytically are plotted in Fig. 2 in two different cross sections of the system. This comparison also shows an excellent agreement between analytical and numerical solutions.

2. Polycrystal comprised of elastically anisotropic grains

A polycrystal comprised of elastically anisotropic grains is an elastically inhomogeneous system. To illustrate the effect of this elastic inhomogeneity on the system equilibrium under applied stress, we consider a particular case of a polycrystal of the Ni_3Al cubic phase with the axial texture along the [001] axis. The elastic constants of this phase are: $C_{11}=223.4$ GPa, $C_{12}=148.2$ GPa, and $C_{44}=125.2$ GPa.[35] Figure 3(a) shows the (001) cross section of this structure. The grains with this texture are parallel columns along the [001] cubic axis, which are perpendicular to the (001) cross section (perpendicular to the plane of the figure). The cubic axes [100] and [010] of the grains are randomly oriented and are indicated by arrow pairs in Fig. 3(a). The polycrystal is assumed to be formed by a periodical repetition of 12 grains shown in Fig. 3(a), which is our computational cell. In the computation, we used a computational cell of 1024×1024. A uniaxial stress σ_{yy}^{appl} along the vertical y axis is applied. The equilibrium stresses, σ_{yy}, σ_{xx}, and σ_{xy}, at each point of the polycrystal are determined by solving Eq. (23). Their normalized fields with respect to the applied stress σ_{yy}^{appl} are shown in Figs. 3(b)–3(d), respectively.

We also considered untextured Ni_3Al polycrystal under uniaxial stress σ_{zz}^{appl}. The 3D polycrystal used in this case is formed by a periodic repetition of a cube consisting of eight randomly oriented grains, which is our computational cell. In the computation, we used a computational cell of $128\times128\times128$. The equilibrium stress is determined by solving

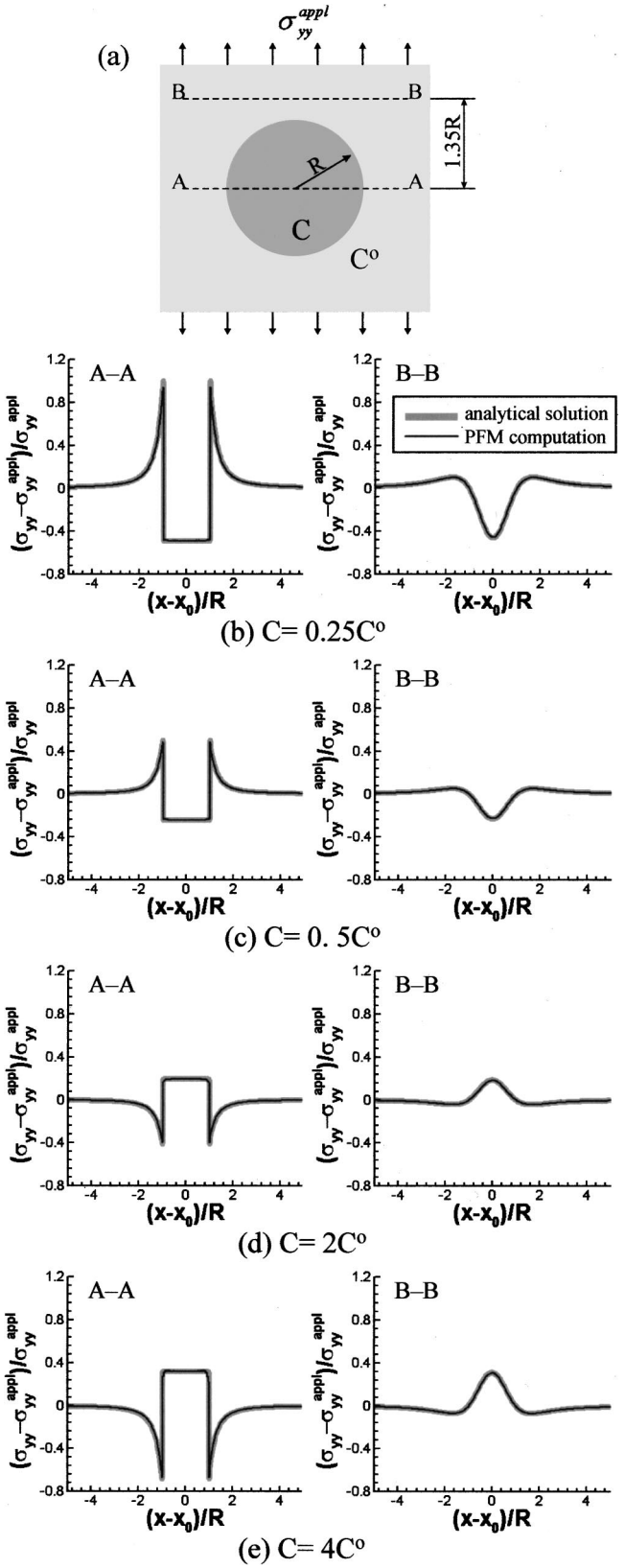

FIG. 2. A cylindrical inhomogeneity of different elastic moduli under uniaxial tension in the y direction in the elastically isotropic body ($\nu = 0.3$). The PFM computational solutions (thin black lines) and the corresponding analytical solutions (thick gray lines) for $(\sigma_{yy} - \sigma_{yy}^{appl})/\sigma_{yy}^{appl}$ along two different cross sections, A-A and B-B as indicated in (a), are plotted in (b)–(e) for each case, respectively, for quantitative comparison.

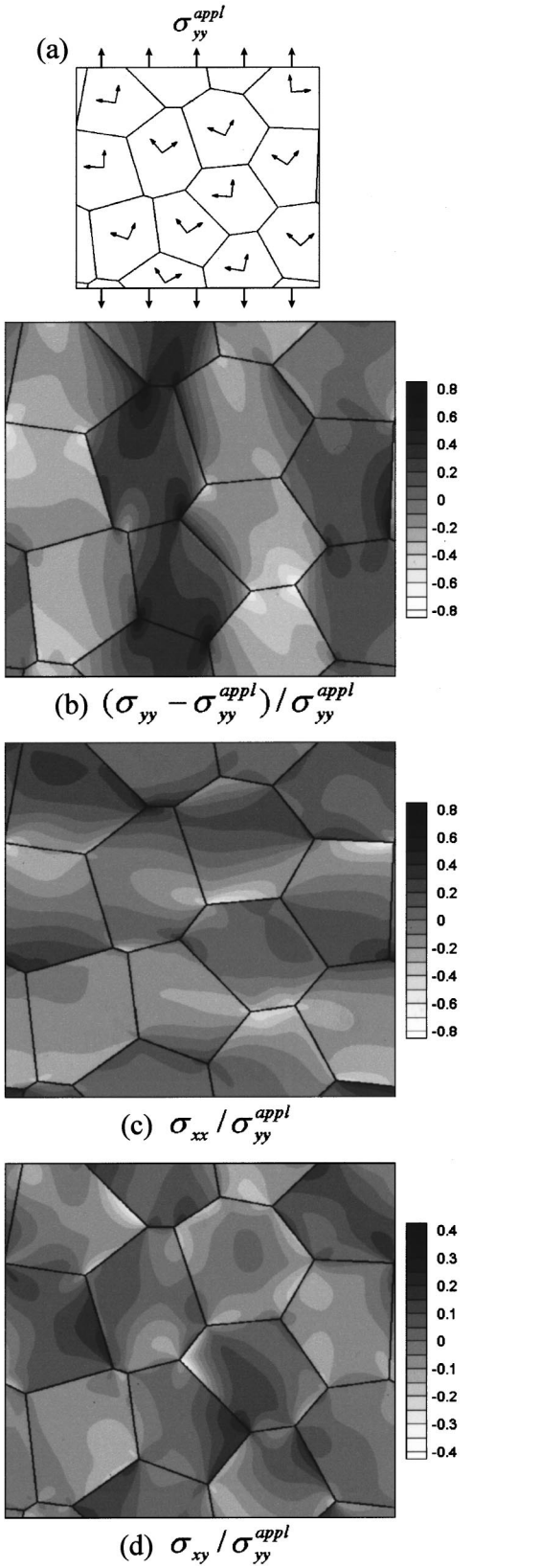

FIG. 3. A textured polycrystal comprised of anisotropic (cubic symmetry) columnar grains under uniaxial stress σ_{yy}^{appl}. (a) Cross section of the grains and their orientations. Equilibrium stress fields: (b) σ_{yy}, (c) σ_{xx}, and (d) σ_{xy}, which are normalized with respect to the applied stress σ_{yy}^{appl}.

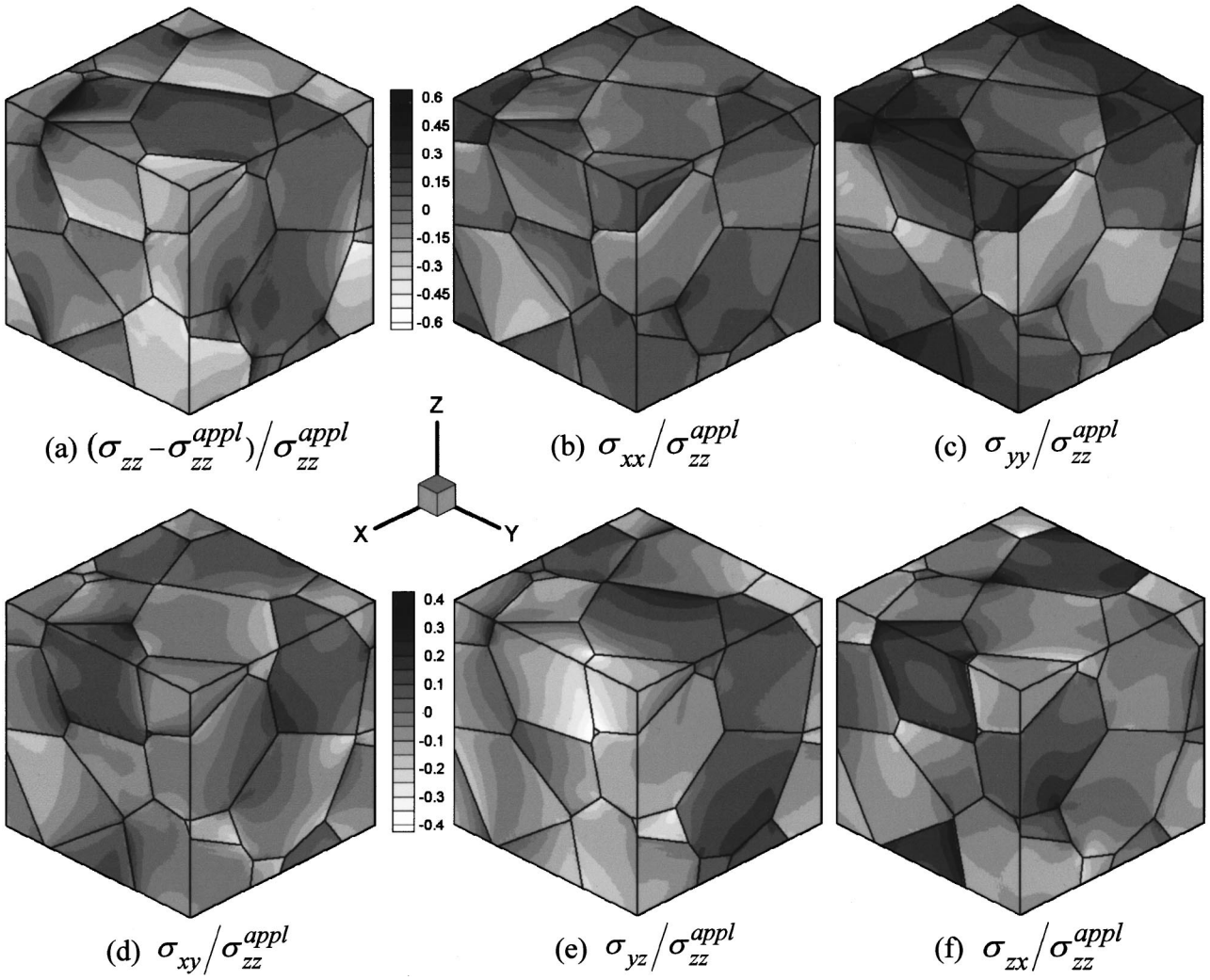

FIG. 4. A 3D polycrystal comprised of anisotropic (cubic symmetry) grains under uniaxial stress $\sigma_{zz}^{\text{appl}}$. The components of the equilibrium stress are normalized with respect to the applied stress $\sigma_{zz}^{\text{appl}}$.

Eq. (23). Its normalized components with respect to the applied stress $\sigma_{zz}^{\text{appl}}$ are shown in Figs. 4(a)–4(f), respectively.

IV. DISCUSSION

The proposed 3D PFM theory formulates a form of the exact equation of elastic equilibrium in an elastically and structurally inhomogeneous solid under external load. The solid is elastically anisotropic and both types of inhomogeneities, elastic and structural, have arbitrary geometries. It is shown that the effect of elastic inhomogeneity on the elastic strain is exactly reproduced by an appropriate choice of virtual misfit strain $\varepsilon_{ij}^{0}(\mathbf{r})$ introduced into the elastically homogeneous body of the same shape and size and under the same external load. This misfit strain is the phase field of the problem. This result proves the equivalency of a system with spatially inhomogeneous modulus and the corresponding system with elastically homogenous modulus but with the spatially inhomogeneous misfit strain $\varepsilon_{ij}^{0}(\mathbf{r})$. Using this equivalency, we found the strain energy of the elastically inhomogeneous body. It is determined by a functional (20) of this misfit strain.

It is proved that the functional (20) meets the variational principle: its minimum is reached when $\varepsilon_{ij}^{0}(\mathbf{r})\rightarrow\varepsilon_{ij}^{00}(\mathbf{r})$ where the minimizer field $\varepsilon_{ij}^{00}(\mathbf{r})$ fully determines the exact elastic equilibrium of the elastically inhomogeneous body under external load. This variational principle formulated in Sec. III B is a key element of the proposed PFM theory for elastically and structurally inhomogeneous systems.

The PFM linear kinetic equation (23) formulated in this article describes a relaxation of the elastically anisotropic system that contains arbitrary elastic and structural inhomogeneities, which may also include defects such as dislocations. The relaxation occurs by ''temporal'' evolution of the ''virtual'' misfit strain $\varepsilon_{ij}^{0}(\mathbf{r})$ driven by the minimization of the strain energy functional until the exact elastic equilibrium is reached.

The PFM kinetic equation based on this variational principle provides an effective computational tool for solving the elasticity problem of arbitrarily elastically and structurally inhomogeneous systems. The accuracy of the PFM computation, in fact, is determined by an accuracy of numerical computations since the PFM kinetic equation, whose steady

state solution describes the elastic equilibrium, is exact. To illustrate an efficiency and accuracy of the PFM method, we compared the PFM calculations of elastic inhomogeneities with the corresponding analytical solutions that exist. The results practically coincide excellently (thin black and thick gray lines, respectively, in Figs. 1 and 2).

It is important to note that the computational time for the PFM calculations does not depend on the spatial complexity of elastic and structural inhomogeneities. It depends only on the number of phase field, which is equal to six [the number of components of the misfit strain tensor $\varepsilon_{ij}^0(\mathbf{r})$]. This implies that the computational time required to determine the elastic equilibrium for the simplest elastic inhomogeneities considered in Figs. 1 and 2 is practically the same as that required for coherent composite of arbitrary spatial complexity. Examples of the PFM calculation of the elastic equilibrium for such topologically complex elastically anisotropic systems are presented in Figs. 3 and 4. These systems are axially textured and untextured polycrystals comprised of elastically coupled anisotropic grains.

The calculated stress field of mechanically loaded elastically anisotropic polycrystals shown in Figs. 3 and 4 illustrates the effect of the spatial variations of the elastic modulus caused by different orientations of grains on the stress concentration. The effect is associated with the elastic coupling between grains. As follows from Figs. 3 and 4, the coupling produces stress concentrations along grain boundaries. The stress concentration is especially significant around some grain boundary junctions and its level, in general, depends on the misalignments of neighboring grains. Location of the stress concentrations determines potentially ''weak'' areas susceptible to formation of dislocaitons and cracks.

Another interesting point is that the proposed PFM theory of elastically and structurally inhomogeneous systems is conceptually similar to the PFM theory and models of martensitic transformations,[28,29] dislocation dynamics,[30,31] and crack/void evolutions.[32,33] In fact, it is formulated in the same formalism and is as efficient as the latter. This circumstance reduces a formulation of a unified PFM theory and model describing evolution of all these defects to just an increase of the number of phase fields and introduction of the corresponding coarse-grain Landau energies.

The proposed PFM theory and model of an elastically and structurally inhomogeneous system is a computational tool for modeling technologically important systems. To illustrate a breadth of possible applications of the proposed approach, we just mention three examples of very different areas, where the theoretical characterization of a material system is impossible without utilizing the computationally effective model of an elastically inhomogeneous system. They are the swelling of irradiated materials, the effect of the elastic modulus misfit on morphology of coherent precipitates, and sintering under applied stress. These three areas are just several examples of the vast area of application of the proposed PFM theory and computational approach.

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APPENDIX

The strain of energy (2) is obtained by allowing the body to relax with respect to displacements that do not affect the macroscopic shape of the body. This is a relaxation under the constraint that the macroscopic shape of the body characterized by the macroscopic strain $\overline{\varepsilon}_{ij}$ is fixed. The strain energy in the form (2) is convenient when the body is fully clamped and thus its macroscopic deformation is determined by the strain-controlled boundary condition.

The strain energy (2) is modified if the macroscopic deformation of the body is controlled by the applied external stress $\sigma_{ij}^{\text{appl}}$. Then we have to deduct the term $V\sigma_{ij}^{\text{appl}}\overline{\varepsilon}_{ij}$ from the strain energy (2)—this term is the work done by the loading device. The result is

$$E^{\text{el}}=\frac{1}{2}\int_V C_{ijkl}^0\varepsilon_{ij}^0(\mathbf{r})\varepsilon_{kl}^0(\mathbf{r})d^3r - \overline{\varepsilon}_{ij}\int_V C_{ijkl}^0\varepsilon_{kl}^0(\mathbf{r})d^3r+\frac{V}{2}C_{ijkl}^0\overline{\varepsilon}_{ij}\overline{\varepsilon}_{kl} - \frac{1}{2}\int\frac{d^3k}{(2\pi)^3}n_i\tilde{\sigma}_{ij}^0(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{\sigma}_{kl}^0(\mathbf{k})^*n_l - V\sigma_{ij}^{\text{appl}}\overline{\varepsilon}_{ij}. \tag{A1}$$

In the situation of the stress-controlled boundary condition, we allow the body to relax at fixed $\sigma_{ij}^{\text{appl}}$ by changing its macroscopic shape. The latter is achieved by minimizing the energy (A1) with respect to $\overline{\varepsilon}_{ij}$. The energy minimizer is

$$\overline{\varepsilon}_{ij}=\overline{\varepsilon}_{ij}^0+S_{ijkl}^0\sigma_{kl}^{\text{appl}},\quad \overline{\varepsilon}_{ij}^0=\frac{1}{V}\int_V\varepsilon_{ij}^0(\mathbf{r})d^3r, \tag{A2}$$

which is the equilibrium strain achieved by the macroscopic strain relaxation. The resultant relaxed value of the strain energy (A1) at given macroscopic stress $\sigma_{ij}^{\text{appl}}$ and stress-free strain profile $\varepsilon_{ij}^0(\mathbf{r})$ is

$$E^{\text{el}}=\frac{1}{2}\int_V C_{ijkl}^0\varepsilon_{ij}^0(\mathbf{r})\varepsilon_{kl}^0(\mathbf{r})d^3r - \frac{1}{2V}C_{ijkl}^0\int_V\varepsilon_{ij}^0(\mathbf{r})d^3r\int_V\varepsilon_{kl}^0(\mathbf{r}')d^3r' - \frac{1}{2}\int\frac{d^3k}{(2\pi)^3}n_i\tilde{\sigma}_{ij}^0(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{\sigma}_{kl}^0(\mathbf{k})^*n_l - \sigma_{ij}^{\text{appl}}\int_V\varepsilon_{ij}^0(\mathbf{r})d^3r-\frac{V}{2}S_{ijkl}^0\sigma_{ij}^{\text{appl}}\sigma_{kl}^{appl}. \tag{A3}$$

The transition from energy (2) to (A1) and (A3) is similar to the transition from the Helmholtz free energy to Gibbs free energy in the classical thermodynamics.

An important particular case is the case of a body under the mixed boundary condition. This is a situation where a part of the body boundary is fixed by clamping—resulting in fixing some components of the macroscopic strain $\bar{\varepsilon}_{ij}$ while the remaining components of $\bar{\varepsilon}_{ij}$ are allowed to relax at the fixed value of the applied stress $\sigma_{ij}^{\text{appl}}$. The corresponding energy can be easily obtained from Eq. (A1) by a procedure similar to that used to obtain the energy (A3), viz. by minimizing the energy (A1) with respect to the components of $\bar{\varepsilon}_{ij}$ that are not fixed by the boundary condition.

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