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Three-dimensional phase field microelasticity theory and modeling of multiple cracks and voids

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It is proved that the stress-free strain distribution minimizing the strain energy of the homogeneous modulus body fully determines the elasticity of the discontinuous body. This result is used as a basis for the proposed three-dimensional phase field microelasticity theory and model of a discontinuous body with cracks and voids in elastically anisotropic crystal under applied stress. The elastic equilibrium and spontaneous evolution of these defects are described by the Ginzburg–Landau kinetic equation. Examples of computations of elastic equilibrium and evolutions of systems with cracks and/or voids are considered.
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The analytical treatment of a system with a group of cracks and/or voids under applied stress poses serious mathematical difficulties. There are very few problems that are really solved.[1–3] These solutions are obtained only for simple geometrical configurations and simple loading conditions (review of recent results in the mechanics of cracks can be, for example, found in Refs. 4–6). The pure analytical approach to a characterization of a discontinuous body is hardly possible because of mathematical complexity of the problem: the real material is usually elastically anisotropic and is often a polycrystal, the cracks and/or voids elastically interact with each other and with dislocations and precipitates and usually form a complex evolving three-dimensional (3D) pattern. It is obvious that the only feasible option to address this complex multi-body problem is a use of computational methods.

The success of recent 3D computer simulations of the stress-accommodating development of complex mesoscale structures in phase transformations and dislocation plasticity in single and polycrystals[7–10] indicates that a development of a similar phase field microelasticity (PFM) theory for a multi-crack and/or multi-void system, which is important for the fracture mechanics, may also be equally successful. The computational results presented in this letter demonstrate that such an advance is possible.

In this study, the problem of cracks and voids under applied stress $\sigma_{ij}^{\mathrm{appl}}$ is reduced to the equivalent problem of the continuous elastically homogeneous body with macroscopically homogeneous but mesoscopically heterogeneous misfit-generating stress-free strain, $\epsilon_{ij}^{o}(\mathbf{r})$. The Khachaturyan–Shatalov (KS) theory[11] gives the exact solution for the strain energy functional, E^{el}, and the stress distribution, $\sigma_{ij}(\mathbf{r})$, of the latter system. The stress is

$$\sigma_{ij}(\mathbf{r})=C_{ijkl}\left[\fint\frac{d^3k}{(2\pi)^3}n_k\Omega_{lm}(\mathbf{n})\tilde{\sigma}_{mn}^{o}(\mathbf{k})n_n e^{i\mathbf{k}\cdot\mathbf{r}}-\epsilon_{kl}^{o}(\mathbf{r})+\overline{\epsilon_{kl}^{o}}\right]+\sigma_{ij}^{\mathrm{appl}},\tag{1}$$

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 $\mathbf{k}=0$, $\mathbf{n}=\mathbf{k}/k$, $\Omega_{ij}(\mathbf{n})$ is the Green function tensor inverse to the tensor $\Omega_{ij}^{-1}(\mathbf{n})=C_{ikjl}n_k n_l$, C_{ijkl} is the elastic modulus, $\tilde{\sigma}_{ij}^{o}(\mathbf{k})=C_{ijkl}\tilde{\epsilon}_{kl}^{o}(\mathbf{k})$, the superscript * indicates the complex conjugate, $\tilde{\epsilon}_{ij}^{o}(\mathbf{k})=\int_V\epsilon_{ij}^{o}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d^3r$, and $\overline{\epsilon_{ij}^{o}}=1/V\int_V\epsilon_{ij}^{o}(\mathbf{r})d^3r$.

Taking the first variational derivative of E^{el} with respect to $\epsilon_{ij}^{o}(\mathbf{r})$ results in a relation

$$\frac{\delta E^{\mathrm{el}}}{\delta\epsilon_{ij}^{o}(\mathbf{r})}=-\sigma_{ij}(\mathbf{r}),\tag{2}$$

where $\sigma_{ij}(\mathbf{r})$ is given by Eq. (1). Below we consider $\epsilon_{ij}^{o}(\mathbf{r})$, which does not vanish only within arbitrary-shaped preselected regions (domains) in the continuous body. If $\epsilon_{ij}^{o}(\mathbf{r})=\epsilon_{ij}^{oo}(\mathbf{r})$ where $\epsilon_{ij}^{oo}(\mathbf{r})$ is the minimizer of the energy E^{el}, the minimum condition for E^{el} is

$$\left.\frac{\delta E^{\mathrm{el}}}{\delta\epsilon_{ij}^{o}(\mathbf{r})}\right|_{\epsilon_{ij}^{o}(\mathbf{r})=\epsilon_{ij}^{oo}(\mathbf{r})}=0.\tag{3}$$

Since we consider here a situation where the stress-free strain $\epsilon_{ij}^{o}(\mathbf{r})$ assumes nonzero values only within the domains, the condition (3) is valid only for points $\mathbf{r}=\mathbf{r}_d$ located within the domains. Comparing Eq. (3) with Eq. (2) proves that when the strain energy of the continuous body reaches its minimum value at $\epsilon_{ij}^{o}(\mathbf{r})=\epsilon_{ij}^{oo}(\mathbf{r})$, the stress within the domains vanishes, i.e., $\sigma_{ij}(\mathbf{r}_d)=0$. The latter together with the equation for the stress (1) gives the equilibrium equation

$$C_{ijkl}\left[\fint\frac{d^3k}{(2\pi)^3}n_k\Omega_{lm}(\mathbf{n})\tilde{\sigma}_{mn}^{oo}(\mathbf{k})n_n e^{i\mathbf{k}\cdot\mathbf{r}_d}-\epsilon_{kl}^{oo}(\mathbf{r}_d)+\overline{\epsilon_{kl}^{oo}}\right]+\sigma_{ij}^{\mathrm{appl}}=0.\tag{4}$$

It should be noticed that, although the stress vanishes inside the domains at $\epsilon_{ij}^{o}(\mathbf{r})=\epsilon_{ij}^{oo}(\mathbf{r})$, it does not vanish outside them.

Since the stress-free strain $\epsilon_{ij}^{oo}(\mathbf{r}_d)$ in the continuous body does not produce stress inside the domains, these stress-free domains containing the misfit-generating strain

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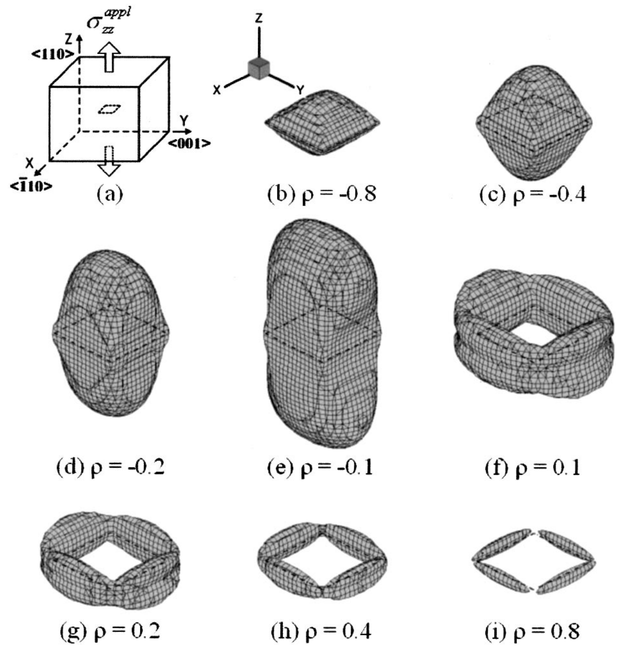

FIG. 1. The calculated 3D stress field of a square crack under normal tensile stress in the elastically anisotropic body. (a) Schematic illustration of the system and crystallographic orientation; isosurfaces of the disturbed stress field $\rho=(\sigma_{zz}-\sigma_{zz}^{\mathrm{appl}})/\sigma_{zz}^{\mathrm{appl}}$ at different values: (b) -0.8, (c) -0.4, (d) -0.2, (e) -0.1, (f) 0.1, (g) 0.2, (h) 0.4, and (i) 0.8, respectively.

$\epsilon_{ij}^{oo}(\mathbf{r}_d)$ can be removed from the body without disturbing the elastic equilibrium in the system or affecting its total strain energy. The removal of the domains leaves *cracks/voids* in the body, their shapes and locations coinciding with those of the domains [a crack is characterized by the laminar domain (slit) of thickness equal to the interplanar distance]. This reduces the crack/void problem to a much simpler and previously resolved[11] problem of an elastically homogeneous continuous body with distributed misfit-generating strain.

The foregoing consideration proves the variation principle theorem: *the elastic strain and strain energy of a continuous homogeneous modulus system with distributed misfitting strain is the elastic strain and strain energy of the discontinuous system with cracks and/or voids if the misfitting strain minimizes the strain energy of the homogeneous modulus system*.

According to this theorem, $\epsilon_{ij}^{o}(\mathbf{r})=\epsilon_{ij}^{oo}(\mathbf{r})$ fully describes the elastic equilibrium and $\epsilon_{ij}^{o}(\mathbf{r})$ is a variational relaxing parameter. Therefore, we can formulate the PFM equation for $\epsilon_{ij}^{o}(\mathbf{r})$ in a situation of domains of fixed shapes and locations (corresponding to fixed cracks/voids)

$$\frac{\partial\epsilon_{ij}^{o}(\mathbf{r},t)}{\partial t}=-L_{ijkl}\frac{\delta E^{\mathrm{el}}}{\delta\epsilon_{kl}^{o}(\mathbf{r},t)} \tag{5}$$

where L_{ijkl} is the kinetic coefficient, and t is "time." The numerical solution of this equation gives a computationally efficient way of finding the solution for the corresponding fixed multi-crack/multi-void system. Numerical solutions of Eq. (5) coincide with those very few solutions obtained analytically (e.g., a two-dimensional crack and a cylindrical hole).[12] An example of the solution of Eq. (5) is shown in Fig. 1. It gives the stress field of a square crack in the 3D elastically anisotropic body ($C_{11}/C_{44}=2.16$ and $C_{12}/C_{44}=1.30$ in cubic crystal).

A similar PFM equation can also be formulated and used to characterize a multi-crack system that spontaneously evolves under applied stress. The effective stress-free strain $\epsilon_{ij}^{o}(\mathbf{r})$ in this case has a form of invariant plane strain[12]

$$\epsilon_{ij}^{o}(\mathbf{r})=\sum_{\alpha=1}^{p}h_i(\alpha,\mathbf{r})H_j(\alpha), \tag{6}$$

where the reciprocal lattice vectors $\mathbf{H}(\alpha)$ characterize several possible cleavage planes $(\alpha=1,2,...,p)$. The crack-opening vector $\mathbf{h}(\alpha,\mathbf{r})$ describes the displacement discontinuities across crack cleavage plane of the type α. They can be considered as nonconserved long-range order parameters. They can describe the most general case of mixed-mode cracks of arbitrary configuration. The strain energy E^{el} of the system with $\epsilon_{ij}^{o}(\mathbf{r})$ given by Eq. (6) is given by the KS theory.[11]

To describe the effect of cohesive forces resisting crack opening, we have to supplement the strain energy by the "coarse-grained" Landau energy[12]

$$E^{\mathrm{ch}}=\sum_{\alpha=1}^{p}\int_V f^{\mathrm{ch}}[\mathbf{h}(\alpha,\mathbf{r})]d^3r. \tag{7}$$

The energy $f^{\mathrm{ch}}[\mathbf{h}(\alpha)]$ describes the effect of a continuous breaking of atomic bonds along the cleavage plane during a process of the crack opening.

The gradient energy in the case of cracks describing the effect of crack surface curvature can be presented as[12]

$$E^{\mathrm{grad}}=\sum_{\alpha=1}^{p}\int_V\frac{1}{2}D_{ijkl}(\alpha)[\mathbf{H}(\alpha)\times\nabla]_i h_j(\alpha,\mathbf{r})\times[\mathbf{H}(\alpha)\times\nabla]_k h_l(\alpha,\mathbf{r})d^3r. \tag{8}$$

The gradient energy vanishes at the flat crack surfaces parallel to the cleavage planes, but gives a considerable contribution near the crack tip.

The total energy functional E describing the multi-crack system is the sum of the elastic energy, "chemical" Landau energy as well as the gradient energy, i.e.,

$$E=E^{\mathrm{el}}+E^{\mathrm{ch}}+E^{\mathrm{grad}}. \tag{9}$$

The PFM equation for the evolving multi-crack system is described by Eq. (5), which is derived for a fixed crack/void system, if (i) we substitute E given by Eq. (9) for E^{el} in Eq. (5) and (ii) express $\epsilon_{ij}^{o}(\mathbf{r})$ in terms of $\mathbf{h}(\alpha,\mathbf{r})$ using Eq. (6). The resultant PFM equation is similar to that for the martensitic transformations.[7,8,12] We employed here the PFM equation for evolving crack to characterize a mode I crack. The PFM crack-opening profile is plotted in Fig. 2(a). The cohesive force results in the characteristic crack tip "beaks." We also simulated the propagation path of an inclined crack under applied stress. Figures 2(c)–2(e) show how the preexisting mixed-mode crack [Fig. 2(c)] changes its direction to propagate along other preferred cleavage planes [Figs. 2(d) and 2(e)] tending to become a mode I crack. In isotropic homogeneous amorphous material without cleavage plane preference, an advancing crack will pick up a path normal to the greatest principal tensile stress [as illustrated by the dashed line in Fig. 2(b)].

In summary, we proved a variation principle theorem that reduces the elasticity problem for a discontinuous elas-

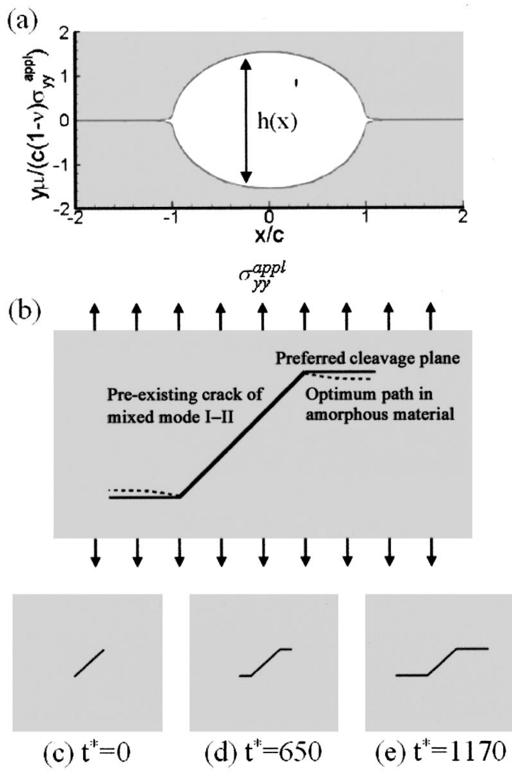

FIG. 2. Simulated mode I crack and propagation path of an inclined crack under applied stress. (a) The crack-opening profile, $h(x)$, shows the characteristic crack tip ''beaks'' due to the cohesive force. (b) Schematic illustration of the system of inclined propagating crack. (c) Preexisting crack. (d) Under stress, crack is deflected away from its original orientation of mixed mode. (e) Crack extends along the preferred cleavage plane orthogonal to the applied stress, becoming mode I crack.

tically anisotropic system with cracks/voids to the elasticity problem for the corresponding continuous elastically anisotropic system with a special stress-free strain distribution. This variation principle enables us to formulate the PFM theory to characterize the elastic equilibrium of a discontinuous elastically anisotropic body with an arbitrary system of fixed cracks and/or voids under applied stress as well as the PFM kinetic equation to describe the evolution of an arbitrary multi-crack system under the stress. The PFM theory is applicable for discontinuous systems with dislocations and misfitting coherent inclusions. The computationally effective procedure for the numerical solution of the PFM equations is developed. The formal similarity of the PFM theory of the discontinuous systems and the PFM theories of the continuous systems with the coherent phase transformation[7,8] and dislocations[9,10] opens a way to a seamless integration of all these theories into a single unified PFM theory, which could be used for the realistic 3D computational modeling of processing of single and polycrystal materials.

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