Elastoplastic phase field model for microstructure evolution

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Success has been obtained in predicting the dynamic evolution of microstructures during phase transformation or cracking propagation by using the time-dependent phase field methodology (PFM). However, most efforts of PFM were made in the elastic regime. In this letter, stress distributions around defects such as a hole and a crack in an externally loaded two-dimensional representative volume element were investigated by a proposed phase field model that took both the elastic and plastic deformations into consideration. Good agreement was found for static cases compared to the use of finite element analysis. Therefore, the proposed phase field model provides an opportunity to study the dynamic evolution of microstructures under plastic deformation. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2138358]

It is well known that microstructures of materials play a crucial role in determining the properties of materials. As a powerful computational approach to predicting mesoscale morphological and microstructure evolution in materials, the phase field method has attracted a considerable amount of research effort and has found wide application in various fields.[1,2] In a phase field model (PFM), the evolution of structural variables and chemical compositions can be described by time-dependent Ginzburg-Landau (TDGL) equations and by the Cahn-Hilliard diffusion equation, respectively. In general, the evolution of microstructures will result in the minimization of the free energy of the whole system, which may consist of the bulk chemical free energy, elastic strain energy, interfacial energy, electric and magnetic energy, and work done by applied external fields. Currently, most efforts of PFM were made in the elastic regime. However, both experimental and computational results have shown that the stresses around defects, crystal interfaces, or precipitates can significantly exceed the elastic limit. Therefore, for many applications, it is necessary to consider the contribution from plastic deformation during microstructure evolution. This is especially true when cracks are present in metals. In this situation, plastic energy could be the dominating factor controlling the initiation and propagation of a crack. In this letter, we propose to treat both elastic and plastic deformations around a void or crack as phase variables. The proposed PFM can also be applied to other microstructure analyses such as phase transformation and ordering,[3,4] defect dynamics, and pattern formation,[5] when plastic deformation is involved.

An equivalent description can be made of the displacement and strain energy of an anisotropic discontinuous body with cracks under applied stress by an anisotropic continuous noncracked body of the same macroscopic size and shape, but with the heterogeneous misfit stress-free strain. The Khachaturyan-Shatalov (KS) theory[6] gives the exact elastic strain and strain energy of a system for a given set of stress-free strains, $\varepsilon_{ij}^{0}(\mathbf{r})$. The strain energy of the system is a function of $\varepsilon_{ij}^{0}(\mathbf{r})$ and an averaged strain $\bar{\varepsilon}_{ij}$ that affects the macroscopic shape of the body. Based on KS theory,[7,8] the strain energy of a homogeneous system under a stress-controlled boundary condition can be expressed as

$$E = \frac{1}{2}\int_V C_{ijkl}\varepsilon_{ij}^{0}(\mathbf{r})\varepsilon_{kl}^{0}(\mathbf{r})d^3r - \frac{1}{2V}C_{ijkl}\int_V \varepsilon_{kl}^{0}(\mathbf{r})d^3r\int_V \varepsilon_{kl}^{0}(\mathbf{r}')d^3r' - \frac{1}{2}⨍_V \frac{d^3k}{(2\pi)^3}n_i\tilde{\sigma}_{ij}^{0}(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{\sigma}_{kl}^{0}(\mathbf{k})^{*}n_l - \sigma_{ij}^{\mathrm{appl}}\int_V \varepsilon_{ij}^{0}(\mathbf{r})d^3r - S_{ijkl}\sigma_{ij}^{\mathrm{appl}}\sigma_{kl}^{\mathrm{appl}}V/2, \qquad (1)$$

where V is the system volume; the integral $⨍$ in the infinite reciprocal space is evaluated as a principal value excluding the volume around point $\mathbf{k}=0$; $\Omega_{jk}(\mathbf{n})$ is the Green function tensor, which is the inverse of tensor $\Omega_{jk}^{-1}(\mathbf{n})=n_iC_{ijkl}n_l$; and the tensor S_{ijkl} is the elastic compliance tensor inverse to the elastic modulus C_{ijkl}; $\mathbf{n}=\mathbf{k}/k$ is a unit directional vector in the reciprocal space, $\tilde{\sigma}_{ij}^{0}(\mathbf{k})=C_{ijkl}\tilde{\varepsilon}_{kl}^{0}(\mathbf{k})$; $\tilde{\varepsilon}_{kl}^{0}(\mathbf{k})$ is the Fourier transform of the field $\varepsilon_{ij}^{0}(\mathbf{r})$, i.e., $\varepsilon ij0(\mathbf{k})=\int\varepsilon ij0(\mathbf{r})\cdot\exp(-i\mathbf{k}\cdot\mathbf{r})d3r$; *the superscript asterisk* (*) *indicates the complex conjugate; and* σ^{appl} *is the applied external stress.*

When a state of equilibrium is reached, the strain energy equation (1) approaches its minimum. According to the variational principal, the first variational derivative of the strain energy with respect to $\varepsilon_{ij}^{0}(\mathbf{r})$ will vanish in the void or crack. The total stress can be given by[8]

$$\sigma_{ij}(\mathbf{r}) = -\frac{\partial E}{\partial\varepsilon_{ij}^{0}(\mathbf{r})} = C_{ijkl}\left\{\frac{1}{2}⨍_V \frac{d^3k}{(2\pi)^3}[n_k\Omega_{lm}(\mathbf{n}) + n_l\Omega_{km}(\mathbf{n})]\tilde{\sigma}_{mn}^{0}(\mathbf{k})n_n\exp(i\mathbf{k}\cdot\mathbf{r}) - \varepsilon_{kl}^{0}(\mathbf{r}) + \bar{\varepsilon}_{kl}^{0}\right\} + \sigma_{ij}^{\mathrm{appl}}. \qquad (2)$$

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Generally, the total stress given by Eq. (2) has a nonzero value outside the voids and cracks, but it vanishes inside them. Therefore, the stress-free domains containing the misfit strain $\varepsilon_{ij}^0(\mathbf{r})$ can be removed from the body without disturbing the strain and stress outside the domains. The strain energy minimizer $\varepsilon_{ij}^0(\mathbf{r})$ of a crack can be obtained by solving the following TDGL equation:[8]

$$\frac{\partial \varepsilon_{ij}^0(\mathbf{r},t)}{\partial t} = -L_{ijkl}\frac{\delta E}{\delta \varepsilon_{kl}^0(\mathbf{r},t)}, \qquad (3)$$

where L_{ijkl} is the kinetic coefficient that characterizes the evolution rate. Equations (1)–(3) have been used to describe elastic cracks and voids.[8]

In order to include the effect of plastic deformation, we assume that the stress-free strain $\varepsilon_{ij}^0(\mathbf{r})$ contains not only the elastic strain $\varepsilon_{ij}^e(\mathbf{r})$ but also the plastic strain $\varepsilon_{ij}^p(\mathbf{r})$, namely, $\varepsilon_{ij}^0(\mathbf{r})=\varepsilon_{ij}^e(\mathbf{r})+\varepsilon_{ij}^p(\mathbf{r})$. In other words, an additional phase field variable $\varepsilon_{ij}^p(\mathbf{r})$ is introduced, which requires an additional TDGL equation similar to Eq. (3). If the elastic-perfectly plastic constitutive relation is assumed, Eqs. (1)–(3) are still valid. One can see that the variational relaxing parameters $\varepsilon_{ij}^e(\mathbf{r})$ and $\varepsilon_{ij}^p(\mathbf{r})$ play the same role as the long-range order parameters in the phase field model during microstructure evolution. The plastic strain $\varepsilon_{ij}^p(\mathbf{r})$ describes the plastic deformation and the arbitrary plastic zone. An important property of $\varepsilon_{ij}^p(\mathbf{r})$ is that its magnitude depends only on the distortion strain energy at the location of concern. When the distortion strain energy equals or exceeds a value related to the yield stress of the materials, $\varepsilon_{ij}^p(\mathbf{r})$ starts to be nonzero. Following a similar procedure of Eq. (1), the distortion strain energy E^{dis} for the stress-controlled condition is given by

$$\begin{aligned} E^{\mathrm{dis}} &= \frac{1}{2}\int_V C_{ijkl}e_{ij}^0(\mathbf{r})e_{kl}^0(\mathbf{r})d^3r \\ &\quad - \frac{1}{2V}C_{ijkl}\int_V e_{kl}^0(\mathbf{r})d^3r\int_V e_{kl}^0(\mathbf{r}')d^3r' \\ &\quad - \frac{1}{2}\int_V \frac{d^3k}{(2\pi)^3}n_i\tilde{s}_{ij}^0(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{s}_{kl}^0(\mathbf{k})^* n_l \\ &\quad - s_{ij}^{\mathrm{appl}}\int_V e_{kl}^0(\mathbf{r})d^3r - S_{ijkl}s_{ij}^{\mathrm{appl}}s_{kl}^{\mathrm{appl}}V/2, \end{aligned} \qquad (4)$$

where $e_{ij}^0(\mathbf{r})=\varepsilon_{ij}^0(\mathbf{r})-1/3\varepsilon_{kk}^0(\mathbf{r})\delta_{ij}$ is the deviatoric strain, and the deviatoric stress in Fourier space is $\tilde{s}_{ij}^0(\mathbf{k})=\int_V C_{ijkl}e_{kl}^0(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})d^3r$. The evolution of the plastic zone can then be depicted by the solution of an additional TDGL equation

$$\frac{\partial \varepsilon_{ij}^p(\mathbf{r}_p,t)}{\partial t} = -K_{ijkl}\frac{\delta E^{\mathrm{dis}}}{\delta \varepsilon_{kl}^p(\mathbf{r}_p,t)}, \qquad (5)$$

where $\mathbf{r}_p$ denotes the domain of plastic deformation; in other words, Eq. (5) is valid only for the points inside plastic zones; K_{ijkl} is a kinetic coefficient characterizing the evolution rate of plastic deformation. Following Eq. (4), one can deduce the deviatoric stress field caused by the elastoplastic deformation, as follows:

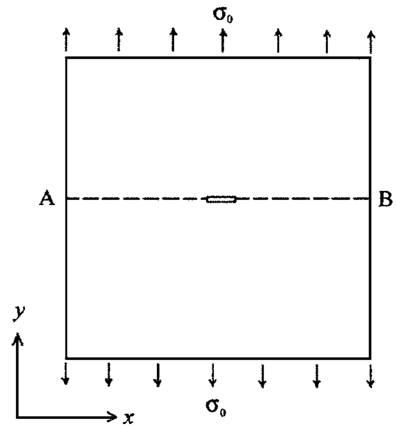

FIG. 1. Schematic illustration of a crack under uniaxial tension in the y direction.

$$\begin{aligned} s_{ij}(\mathbf{r}) = C_{ijkl}\Bigg\{ &\frac{1}{2}\int_V \frac{d^3k}{(2\pi)^3}[n_k\Omega_{lm}(\mathbf{n}) \\ &+ n_l\Omega_{km}(\mathbf{n})]\tilde{s}_{mn}^0(\mathbf{k})n_n\exp(i\mathbf{k}\cdot\mathbf{r}) - e_{kl}^0(\mathbf{r}) + \bar{e}_{kl}^0\Bigg\} \\ &+ s_{ij}^{\mathrm{appl}}. \end{aligned} \qquad (6)$$

Then, Eq. (5) can be written as the form of $\partial\varepsilon_{ij}^p(\mathbf{r}_d,t)/\partial t = -K_{ijkl}s_{kl}$, which is similar to the classic Prandle-Reuss theory, $d\varepsilon_{ij}^p=\partial F/\partial\sigma_{ij}d\lambda = s_{ij}d\lambda$.[9]

In the first numerical example, a 1024×1024 pixel representative volume element (RVE) with a circular hole was subjected to normal stress of $\sigma_0=200$ MPa in the y direction. The radius of the hole is $R=25$. The Young's module of the RVE material is $E=100$ GPa, and the Poisson ratio is $\nu=0.3$. In our phase field computation, the elastic-perfectly plastic constitutive relation and the von Mises yield criteria are assumed. The yield stress is $\sigma_s=300$ MPa, and the deformation of the RVE is assumed to be plane strain. For simplicity, $L_{ijkl}=S_{ijkl}/\Delta t$ is chosen, where Δt is the unit time increment. In order to improve the speed of convergence of the TDGL kinetic equation, the fast Fourier transform technique is used to transform Eqs. (3) and (4) into reciprocal space. Also for simplicity, we set $K_{ijkl}=L_{ijkl}$ in our numerical simulations. For comparison, the same configuration was analyzed by the finite element method (FEM), (in ABAQUS). In the second example, as shown in Fig. 1, a central crack of 100 pixels length and five pixels width was analyzed by PFM and FEM, respectively. The material properties and loading condition are the same as those in the first example.

Our PFM simulations provide a dynamic evolution of stress, strain, and plastic deformation as a function of time under external loads. A stable distribution of stress, strain and plastic deformation will be reached at a sufficient time period. The plastic deformation zones around the hole and crack are illustrated in Fig. 2. Good agreement between PFM and FEM is achieved. Figure 3 illustrates the distribution of stress σ_{yy} obtained by these two methods. Both the distribution and the magnitude calculated by PFM are consistent with those calculated by FEM. The differences in maximum values predicted by PFM and FEM are about 1.6% and 3.7%, respectively. The variations in the normalized stress component σ_{yy} along horizontal line AB, which are shown in Fig. 4, also showed good agreement between the two methods. The difference was 1.6% for the hole and 2.0% for the crack,

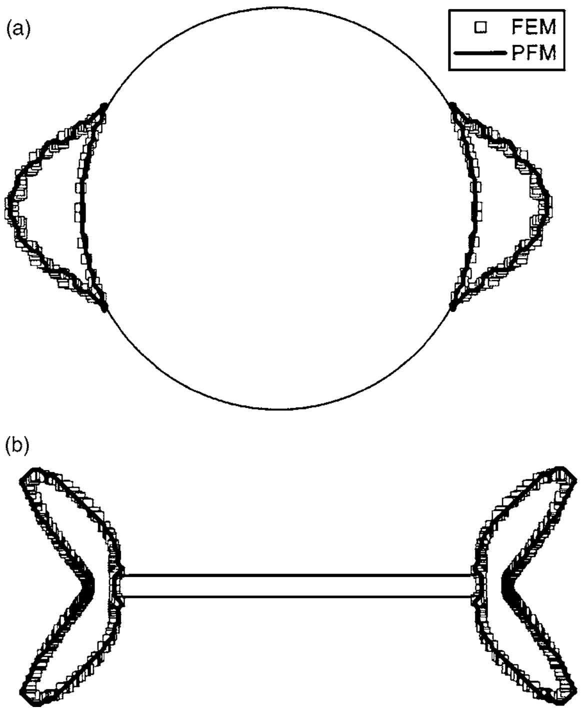

FIG. 2. Comparison of plastic zones calculated by PFM and FEM around (a) a circular hole and (b) a crack.

respectively. Other stress components also show a similar agreement.

In summary, both the elastic and plastic deformations of a system with a hole or a crack under applied loading were simulated by a proposed phase field approach. The evolution of field variables, stress-free elastic, and plastic strains, and the interaction among them are depicted by the solution of the time-dependent Ginzburg-Landau equations. Taking the yield and fracture criteria into account, the proposed PFM can be used to predict the crack propagation trajectory without priori assumed path. If the system also contains other defects, such as grain boundaries and precipitates, the dynamic evolution of the microstructure of the whole system can be described by the proposed PFM. One only has to add more free energy terms, such as the interface energy and stress-free strain of precipitates, into the TDGL equations (3).[10] Therefore, the proposed phase field model provides an opportunity to study the dynamic evolution of microstructures that involves plastic deformation.

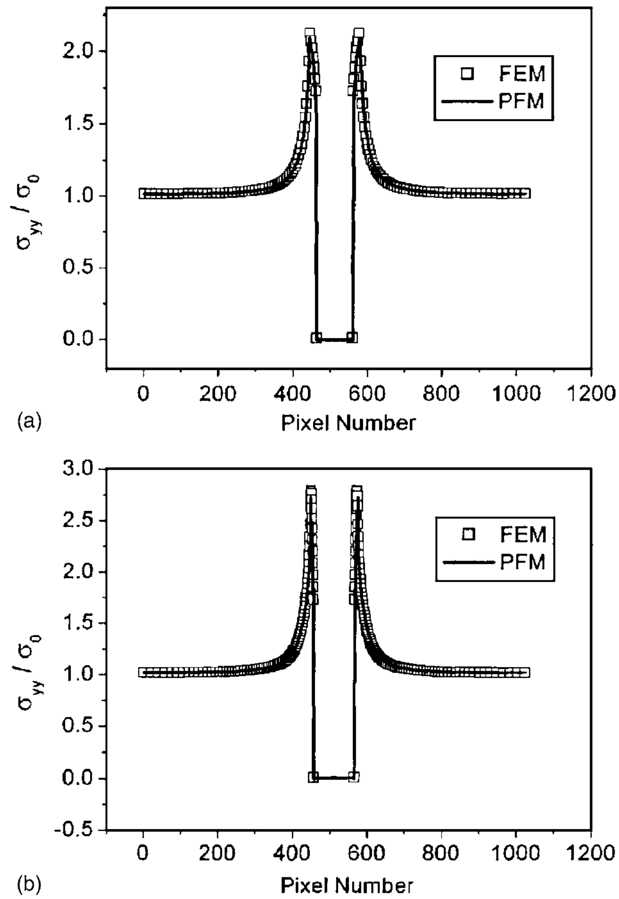

FIG. 4. The variations of σ_{yy} along a horizontal line *AB* (see Fig. 1) that crosses (a) the centre of a circular hole and (b) the crack line.

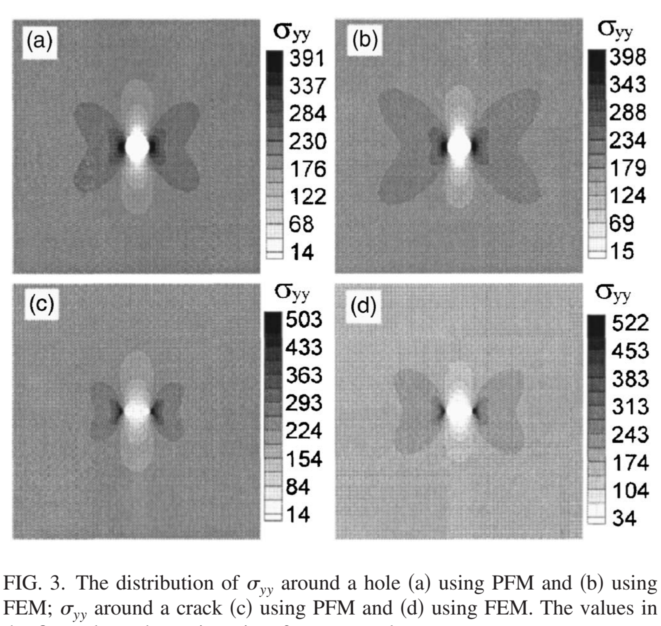

FIG. 3. The distribution of σ_{yy} around a hole (a) using PFM and (b) using FEM; σ_{yy} around a crack (c) using PFM and (d) using FEM. The values in the figure legends are in units of megapascal.

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[1] L. Q. Chen, Annu. Rev. Mater. Res. **32**, 113 (2002).
[2] Y. L. Li, S. Choudhury, Z. K. Liu, and L. Q. Chen, Appl. Phys. Lett. **83**, 1608 (2003).
[3] X. Q. Ma, S. Q. Shi, C. H. Woo, and L. Q. Chen, Mater. Sci. Eng., A **334**, 6 (2002).
[4] W. Dreyer and W. H. Muller, Int. J. Solids Struct. **37**, 3841 (2000).
[5] A. Onuki, *Phase Transition Dynamics* (Cambridge University Press, Cambridge, 2002).
[6] A. G. Khachaturyan and G. A. Shatalov, Sov. Phys. JETP **29**, 557 (1969).
[7] A. G. Khachaturyan, *Theory of Structural Transformations in Solids* (Wiley, New York, 1983).
[8] Y. M. Jin, Y. U. Wang, and A. G. Khachaturyan, Philos. Mag. **83**, 1587 (2003).
[9] J. Chakrabarty, *Theory of Plasticity* (McGraw-Hill, New York, 1998).
[10] S. Q. Shi and X. N. Jing, *Proceedings of International Conference on Computational & Experimental Engineering and Sciences*, 26–29 July 2004, Funchal, Portugal.