Multiscale Modeling and Simulation of Crack Propagation in Polycrystalline Solids

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ABSTRACT

In this work, polycrystalline solid is considered as a multiphase material consisting of randomly distributed grains and grain boundaries. The randomly oriented and distributed grains in the shapes of polygons are created automatically with given statistical average of grain size by adopting the Wigner-Seitz approach, which is used in lattice dynamics to create unit cells. Each grain is modeled as crystallized solid by micromorphic theory, while the grain boundaries are modeled as in its amorphous phase by classical continuum theory. Meshless method is used as the numerical tool in this work. Due to the existence of material inhomogeneity, material forces and Eshelby stresses are obtained, that indicates the location of crack initiation. A fracture criterion, that determines the direction of crack propagation of mixed mode fracture problem in multiphase material, is proposed. Numerical results, showing the path of crack propagation and the ultimate strength of the materials, are presented and discussed.

1 MULTIPHASE MICROMORPHIC MATERIALS

In this work, polycrystalline solid is considered as a multiphase material consisting of randomly distributed grains and grain boundaries. The randomly oriented and distributed grains in the shapes of polygons are created automatically with a given statistical average of grain size by adopting the Wigner-Seitz approach, which is used in lattice dynamics to create unit cells. Each grain is modeled as crystallized solid by micromorphic theory, while the grain boundaries are modeled as in its amorphous phase by classical continuum theory.

In the general micromorphic theory, a material body is envisioned as a continuous collection of deformable particles of finite size and inner structure; each has 9 independent degrees of freedom describing the stretches and rotations of the particle, in addition to the 3 classical translational degrees of freedom of its center. The deformable particle may be considered as a polyatomic molecule, a primitive unit cell of a crystalline solid, or a chopped fiber in a composite, etc. [1-4]. A particle $P(\mathbf{X},\Xi)$ in a microcontinuum is characterized by its centroid **C**, located at the Lagrangian coordinate **X**, and a generic vector Ξ attached to C. Deformation carries P to $p(\mathbf{x},\boldsymbol{\xi})$ through the macromotion

$$x_k = x_k(\boldsymbol{X},t) \quad , \tag{1}$$

which defines the movement of the centroid of the particle and the micromotion

$$\xi_k = \chi_{kK}(\boldsymbol{X},t)\Xi_K \quad , \tag{2}$$

which accounts for inner motions of the material within the particle. Then the inverse motions can be expressed as

$$X_K = X_K(\mathbf{x}, t) \quad , \quad \Xi_K = \overline{\chi}_{Kk}(\mathbf{x}, t)\xi_k \quad . \tag{3}$$

In micromorphic theory, there are three generalized Lagrangian strains

$$E_{KL} \equiv x_{k,K}\overline{\chi}_{Lk} - \delta_{KL} \quad , \; F_{KL} \equiv \chi_{kK}\chi_{kL} - \delta_{KL} \quad , \; \Gamma_{KLM} \equiv \overline{\chi}_{Kk}\chi_{kL,M} \quad , \tag{4}$$

and, correspondingly, there are three stress measures: Cauchy stress $\mathbf{t}$, microstress average $\mathbf{s}$, and moment stress $\mathbf{m}$. The balance laws of micromorphic continuum were derived through a "space averaging" process by Eringen and Suhubi [1,2]. Later, Eringen [3] derived the balance laws of linear momentum and momentum moments by subjecting the energy balance law to the requirement of invariance under the Galilean group of transformation. Recently, Chen and Lee [5,6] and Chen et al. [7] identified all the instantaneous mechanical variables, corresponding to those in micromorphic theory, in phase space; derived the corresponding field quantities in physical space through the statistical ensemble averaging process; invoked the time evolution law and the generalized Boltzmann transport equation for conserved properties to obtain the local balance laws of mass, microinertia, linear momentum, momentum moments, and energy for microcontinuum field theory. In the case that the external field is the gravitational field, the balance laws obtained by Chen et al. [6,7] from an atomistic model agree perfectly with those by Eringen [3].

2 MATERIAL FORCES IN MICROMROPHIC MATERIALS

The gravitational forces, the Lorentz force on a charged particle, and a radiation force that causes damping are all physical forces in the usual Newtonian view of mechanics. They are the contributors to Newton's equation of motion (balance of linear momentum) or Euler-Cauchy equations of motion when we pass from discrete model to continuum field theory. Physical forces are generated by displacements in physical space. For a continuous body, this means a change in its actual position in its physical configuration at time t [8].

On the other hand, the concept of material forces was first introduced by Eshelby [9], elaborated and further developed by Maugin [8,10]. Material forces are generated by displacement, not in physical space, but on material manifold. The characteristic property of material forces also leads to their christening as inhomogeneity forces. Material inhomogeneity is defined as the dependence of properties (not the solution), such as density, elastic coefficients, viscosity, plasticity threshold, on the material point. These inhomogeneities may be more or less continuous such as in metallurgically superficially treated specimens or in a polycrystal observed at a mesoscopic scale, or it may change abruptly such as in laminated composite or in a body with foreign inclusions or cavities.

To derive the governing equations of material forces in micromorphic materials, we recall the balance laws of linear momentum and moment of momentum in terms of generalized Piola-Kirchhoff stresses as [11]:

$$(T_{KL}\bar{\chi}_{Ll})_{,K}+\rho^{o}(f_l-\dot{v}_l)=0 \qquad , \tag{5}$$

$$(M_{LMK}\bar{\chi}_{Ll}\chi_{mM})_{,K}+T_{ML}x_{m,M}\bar{\chi}_{Ll}-2S_{ML}\chi_{mM}\chi_{lL}+\rho^{o}(L_{lm}-\sigma_{lm})=0 \qquad . \tag{6}$$

Equation (5) multiplied by $x_{l,P}$ is added to eq. (6) multiplied by $\bar{\chi}_{Rm}\chi_{lR,P}$. After lengthy but straightforward derivation, it results

$$B_{KL,K}+F_L=\dot{P}_L \qquad , \tag{7}$$

where the pseudomomentum $\mathbf{P}$, Eshelby stress $\mathbf{B}$, and material force $\mathbf{F}$ for micromorphic thermoelastic solid are obtained to be

$$P_L\equiv-\rho^{o}(v_k x_{k,L}+i_{jm}\upsilon_{lj}\bar{\chi}_{Rm}\chi_{lR,L}), \tag{8}$$

$$B_{KL}=-(K-W)\delta_{KL}-T_{KM}E_{LM}-M_{NMK}\Gamma_{NML}, \tag{9}$$

$$\begin{aligned}
F_L=&-\rho^{o}f_l x_{l,L}-\rho^{o}L_{lm}\bar{\chi}_{Rm}\chi_{lR,L}\\
&+\tfrac{1}{2}v_k v_k(\rho^{o})_{,L}+\tfrac{1}{2}\upsilon_{mk}\upsilon_{ml}\chi_{kM}\chi_{lN}(\rho^{o}I_{MN})_{,L}\\
&+(\rho^{o}\gamma T/T^{o}+a_{KM}E_{KM}+b_{KM}F_{KM}+c_{KMN}\Gamma_{KMN})T_{,L}\\
&+(\rho^{o}\gamma)_{,L}\frac{T^2}{2T^{o}}+a_{KM,L}E_{KM}T+b_{KM,L}F_{KM}T+c_{KMN,L}\Gamma_{KMN}T\\
&-\tfrac{1}{2}A_{IJMN,L}E_{IJ}E_{MN}-\tfrac{1}{2}B_{IJMN,L}F_{IJ}F_{MN}-\tfrac{1}{2}C_{IJKMNP,L}\Gamma_{IJK}\Gamma_{MNP}\\
&-D_{IJMN,L}E_{IJ}F_{MN}-G_{IJKMN,L}E_{IJ}\Gamma_{KMN}-H_{IJKMN,L}F_{IJ}\Gamma_{KMN}
\end{aligned} \quad . \tag{10}$$

It is seen that the material force in micromorphic thermoelastic solid is due to (1) body force $\mathbf{F}$ and body moment $\mathbf{L}$, (2) temperature gradient ∇T, and (3) the material inhomogeneities in density, microinertia, and all the thermoelastic coefficients

Also, for 2-D problems in the presence of propagating crack, the material force associated with the crack tip is obtained as

$$\mathbf{F}=\lim_{\Gamma\to 0}\int_{\Gamma}\mathbf{N}\cdot(\mathbf{V}\otimes\mathbf{P}-\mathbf{B})d\Gamma \qquad , \tag{11}$$

where Γ denotes the cross-sectional circuit around the crack tip; $\mathbf{N}$ is the unit vector normal to Γ pointing away from the crack tip; $\mathbf{V}$ is the velocity of crack propagation. Notice that crack propagation is a movement on material manifold, not in physical space, therefore, $\mathbf{V}$ is not equal to the material time rate of change of the position vector (velocity) of any particle. It can be shown that, in a very special case, the projection of $\mathbf{F}$ in the direction tangent to the crack path behind the crack tip is reduced to the J-integral, which is path-independent if the material within Γ is homogeneous.

3 MESHLESS METHODS

Meshless methods can be constructed solely in terms of nodes without the need of a highly structured mesh as required in finite element (FE) method. For a variety of problems with large deformation, moving boundary discontinuities, or in optimization problems where re-meshing may be required, meshless methods are very attractive [12-14]. The meshless methods are based on the moving least squares technique in which the approximation of any scalar-valued function, $\tilde{U}(\mathbf{x})$, can be expressed as an inner product between a vector of shape functions, $\mathbf{\Phi}(\mathbf{x})$, and a vector of nodal values, $\mathbf{U}$, as

$$\tilde{U}(\mathbf{x}) = \mathbf{\Phi}(\mathbf{x}) \cdot \mathbf{U} \quad , \tag{12}$$

which has the same form as in the FE method. However, there is a characteristic difference between FE method and meshless method: eq. (12) is an approximation rather than an interpolation, i.e., in meshless method, $\tilde{U}(\mathbf{x}_i) \neq U_i$. This character requires special and careful treatments of essential boundary conditions, mirror symmetries, and moving discontinuities, such as crack propagation [14-15]. It should also be emphasized that it is almost impossible and even erroneous to calculate the derivatives of the material properties in eq. (10) through FE method, and, on the other hand, it is natural and easy to do so through meshless method.

4 CRACK PROPAGATION

In two dimensional fracture problems, Mode I fracture may lead to self-similar crack extension due to symmetry. In general case, especially in case of multiphase material, we encounter mixed mode fracture problems. Therefore, to determine the direction of crack extension is an unavoidable task. Usually, we use the maximum opening stress criterion or the maximum energy release rate criterion to determine the direction of crack propagation. For example, using maximum opening stress criterion, the current crack tip will extends to $\{r_c,\ \theta\}$ if the Cauchy stress $t_{\theta\theta}$ is maximum at $\{\theta\ ;\ r_c\}$, where $r_c > 0$ is small and finite constant. One may consider that $t_{\theta\theta}(r_c\ ,\ \theta)$ is the driving force distributed along an arc with a radius r_c with respect to the current crack tip. If the material is homogeneous, the maximum opening stress criterion is reasonable, i.e., the information of driving force is enough to determine the direction of crack extension. However, if the material is inhomogeneous, one has to consider the resistance, i.e., the toughness, distributed in front of crack tip. In this work, we propose that the current crack tip will extend to $\{r_c, \ \theta\}$ if the ratio

$$R(r_c,\theta) \equiv \frac{t_{\theta\theta}(r_c,\theta)}{t_c(r_c,\theta)} \quad , \tag{7}$$

reaches a maximum at $\{r_c, \ \theta\}$, where t_c is the toughness associated with the opening stress. Crack propagation process can be viewed as a changing of crack tip with a moving barrier following the advancing of the crack tip. It is noticed that meshless analysis of crack propagation does not involve the formidable task of constantly remeshing the cracking specimen. It only needs the updating of the barrier and the sprinkle of additional nodes in front of the current crack tip to enhance the solution accuracy.

5 NUMERICAL RESULTS

In this work material forces and Eshelby stresses, due to the existence of material inhomogeneity, are calculated and can be employed as the indicator for the location of crack initiation. The fracture criterion, based on the ratio of the opening stress over the material toughness distributed in front of the crack tip, is proposed to determine the direction of crack propagation of mixed mode fracture problem in multiphase micromorphic material. Numerical results, including deformation, stresses, path of crack propagation, failure process and the ultimate strength of the multiphase material, are presented and discussed.

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