MATERIAL FORCES IN MICROMORPHIC FRACTURE MECHANICS

James D. Lee*, Youping Chen, and Shiu-Wei Yin

ABSTRACT

The physical foundation, the balance laws and the constitutive relations of microcontinuum field theories are briefly reviewed. The concept of material forces, which may also be referred as Eshelbian mechanics, is extended to micromorphic theory. The balance law of pseudo-momentum is formulated. The detailed expressions of Eshelby stress tensor, pseudo-momentum, and material forces are derived. It is found that, for micromorphic thermoelastic solid, the material forces are due to (1) body force and body moment, (2) temperature gradient, and (3) the material inhomogeneities in density, microinertia, and elastic coefficients. It is shown that, at the crack front, material forces are reduced to generalized vectorial J-integral. The calculation of material forces, due to the presence of inhomogeneities or cracks, by finite element analysis and meshless analysis is discussed. Finite element analysis is performed for a multiphase material which is composed of randomly distributed and oriented grains and in between the grain boundaries in its amorphous phase. Each grain is modeled as a single crystal by specialized micromorphic theory. The grain boundaries are modeled with a thin and finite width by classical continuum mechanics. Numerical results, including Cauchy stresses, Eshelby stresses, and material forces, for a thin film of silicon subjected to thermal and/or mechanical loadings are obtained and discussed.

Key Words:

I. INTRODUCTION

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* (Maugin, 1995).

On the other hand, the concept of material forces was first introduced by Eshelby (1951), elaborated and further developed by Maugin (1993; 1995). Material forces are generated by displacement, not in physical space, but on material manifold. For example, they can be generated by (a) an infinitesimal rigid displacement of a finite region surrounding a point of singularity in an elastic body (Casal, 1978), (b) an infinitesimal displacement of a dislocation line (Peach and Koehler, 1950), (c) an infinitesimal increase in the length of a crack (Rice, 1968; Casal, 1978; Maugin 1992). Material forces drive the motion of defects of various dimensions in condensed matter physics, e.g. phase-transition fronts in elasticity, Bloch and Neel walls in ferromagnetism, and elastic solitons (Maugin, 1992; 1993). This 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

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scale, or it may change abruptly such as in laminated composite or in a body with foreign inclusions or cavities.

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. (Eringen and Suhubi, 1964; Eringen, 1964; 1999; 2001). A particle $P(\boldsymbol{X}, \Xi)$ in a microcontinuum is characterized by its centroid $\boldsymbol{C}$, located at the Lagrangian coordinate $\boldsymbol{X}$, and a generic vector Ξ attached to C. Deformation carries P to $p(\boldsymbol{x}, \xi)$ through the macromotion

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

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

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

which accounts for inner motions of the material within the particle. To secure the axiom of continuity, which requires that the matter is indestructible and impenetrable, the jacobians of the macromotion and micromotion must not vanish, i.e.,

$$J\equiv\det(x_{k,K})\neq 0,\ \ j\equiv\det(\chi_{kK})\neq 0 \quad (3)$$

Then the inverse motions can be expressed as

$$X_K=X_K(\boldsymbol{x}, t),\ \Xi_k=\overline{\chi}_{Kk}(\boldsymbol{x}, t)\xi_k \quad (4)$$

and three generalized Lagrangian strains are given as

$$E_{KL}\equiv x_{k,K}\overline{\chi}_{Lk}-\delta_{KL}$$

$$F_{KL}\equiv\chi_{kK}\chi_{kL}-\delta_{KL}$$

$$\Gamma_{KLM}\equiv\overline{\chi}_{Kk}-\chi_{kL,M} \quad (5)$$

Correspondingly, there are three stress measures: Cauchy stress $\boldsymbol{t}$, microstress average $\boldsymbol{s}$, and moment stress $\boldsymbol{m}$. Eringen and Suhubi (1964) derived the balance laws of micromorphic continuum through a “space averaging” process. Later, Eringen (1999) 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 (2003a; 2003b) and Chen *et al*. (2003) 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 and Lee (2003b) from an atomistic model agree perfectly with those by Eringen (1999).

II. FORMULATION

The balance laws of linear momentum and momentum moments can be written in terms of Cauchy stress $\boldsymbol{t}$, microstress average $\boldsymbol{s}$, and moment stress $\boldsymbol{m}$ as (Eringen, 1999; Chen and Lee, 2003b):

$$t_{kl,k}+\rho(f_l-\dot{v}_l)=0 \quad (6)$$

$$m_{klm,k}+t_{ml}-s_{lm}+\rho(L_{lm}-\sigma_{lm})=0 \quad (7$$

or in terms of the generalized Piola-Kirchhoff stresses as

$$(T_{KL}\overline{\chi}_{Ll})_{,K}+\rho^o(f_l-\dot{v}_l)=0 \quad (8)$$

$$(M_{LMK}\overline{\chi}_{Ll}\chi_{mM})_{,K}+T_{ML}x_{m,M}\overline{\chi}_{Ll}$$

$$-2S_{ML}\chi_{mM}\chi_{lL}+\rho^o(L_{lm}-\sigma_{lm})=0 \quad (9)$$

where $\boldsymbol{t}$, $\boldsymbol{s}$, $\boldsymbol{m}$ and the generalized Piola-Kirchhoff stress tensors are related as

$$T_{KL}=Jt_{kl}X_{K,k}\chi_{lL},\ t_{kl}=J^{-1}T_{KL}x_{k,K}\overline{\chi}_{Ll} \quad (10)$$

$$S_{KL}=\frac{1}{2}Js_{kl}\overline{\chi}_{Kk}\overline{\chi}_{Ll},\ s_{kl}=2J^{-1}S_{KL}\chi_{kK}\chi_{lL} \quad (11)$$

$$M_{KLM}=Jm_{mkl}X_{M,m}\chi_{kK}\overline{\chi}_{Ll},$$

$$m_{mkl}=J^{-1}M_{KLM}x_{m,M}\overline{\chi}_{Kk}\chi_{lL} \quad (12)$$

and the spin inertia is defined as

$$\sigma_{kl}\equiv i_{ml}(\dot{\upsilon}_{km}+\upsilon_{kn}\upsilon_{nm}) \quad (13)$$

Eq. (8) multiplied by $x_{l,P}$ is added to Eq. (9) multiplied by $\overline{\chi}_{Rm}\chi_{lR,P}$. After lengthy but straightforward mathematical manipulation, the governing equation of material force for micromorphic materials is obtained as

$$-(T_{KL}E_{PL}+M_{LMK}\Gamma_{LMP})_{,K}+T_{KL}E_{KL,P}+S_{KL}F_{KL,P}$$

$$+M_{LMK}\Gamma_{LMK,P}-K_{,P}+F_P^1+F_P^2=\dot{P}_P \quad (14)$$

where the kinetic energy density (per unit volume in Lagrangian coordinates) is defined as

$$K\equiv\frac{1}{2}\rho^o(v_k v_k+i_{kl}\upsilon_{mk}\upsilon_{ml}) \tag{15}$$

the pseudomomentum $\boldsymbol{P}$ is defined as

$$P_P\equiv-\rho^o(v_k x_{k,P}+i_{jm}\upsilon_{lj}\overline{\chi}_{Rm}\chi_{lR,P}) \tag{16}$$

the material force due to body force $\boldsymbol{f}$ and body moment $\boldsymbol{L}$ is equal to

$$F_P^1\equiv-\rho^o f_l x_{l,P}-\rho^o L_{lm}\overline{\chi}_{Rm}\chi_{lR,P} \tag{17}$$

and the material force due to the inhomogeneity of $\rho^o$and $\rho^o I_{KL}$ is equal to

$$F_P^2\equiv\frac{1}{2}v^2\{\frac{\partial\rho^o}{\partial X_P}\}+\frac{1}{2}\upsilon_{mk}\upsilon_{ml}\chi_{kK}\chi_{lL}\{\frac{\partial(\rho^o I_{KL})}{\partial X_P}\} \tag{18}$$

III. MICROMORPHIC THERMOELASTIC SOLID

For micromorphic thermoelastic solid, the Helmholtz free energy density function ψ and the heat flux $\boldsymbol{Q}$ may be obtained as

$$\rho^o\psi=W(\boldsymbol{E},\boldsymbol{F},\boldsymbol{\Gamma},\theta,\boldsymbol{X}) \tag{19}$$

$$Q_K=Q_K(\boldsymbol{E},\boldsymbol{F},\boldsymbol{\Gamma},\theta,\nabla\theta,\boldsymbol{X}) \tag{20}$$

subjected to (due to Clausius-Duhem inequality)

$$Q_K\theta_{,K}\le 0 \tag{21}$$

where θ is the absolute temperature; and the dependence of W explicitly on the Lagrangian coordinate $\boldsymbol{X}$ indicates the inhomogeneity of material properties. Then the entropy and the generalized Piola-Kirchhoff stresses can be derived as

$$\eta=-\frac{\partial\psi}{\partial\theta}=-\frac{1}{\rho^o}\frac{\partial W}{\partial\theta} \tag{22}$$

$$T_{KL}=\frac{\partial W}{\partial E_{KL}} \tag{23}$$

$$S_{KL}=\frac{\partial W}{\partial F_{KL}} \tag{24}$$

$$M_{KLM}=\frac{\partial W}{\partial\Gamma_{KLM}} \tag{25}$$

Notice that the gradient of the potential function can be written as

$$\begin{aligned}W_{,K}&=\frac{\partial W}{\partial E_{MN}}E_{MN,K}+\frac{\partial W}{\partial F_{MN}}F_{MN,K}+\frac{\partial W}{\partial\Gamma_{MNL}}\Gamma_{MNL}\\&\quad+\frac{\partial W}{\partial\theta}\theta_{,K}+\{\frac{\partial W}{\partial X_K}\}\\&=T_{MN}E_{MN,K}+S_{MN}F_{MN,K}+M_{MNL}\Gamma_{MNL,K}-\rho^o\eta\theta_{,K}\\&\quad+\{\frac{\partial W}{\partial X_K}\}\end{aligned} \tag{26}$$

Define the Lagrangian L as the difference between the kinetic energy and the potential energy W, i.e.,

$$L\equiv K-W=\rho^o(\frac{1}{2}v_k v_k+\frac{1}{2}i_{kl}\upsilon_{mk}\upsilon_{ml}-\psi) \tag{27}$$

then the governing equation for material force in micromorphic thermoelastic solid can be expressed as

$$B_{KL,K}+F_L=\dot{P}_L \tag{28}$$

where the generalized Eshelby stress tensor obtained as

$$B_{KL}=-L\delta_{KL}-T_{KM}E_{LM}-M_{NMK}\Gamma_{NML} \tag{29}$$

and the material force becomes

$$F_L=F_L^1+\rho^o\eta\theta_{,L}+\{\frac{\partial L}{\partial X_L}\} \tag{30}$$

where $\{\frac{\partial L}{\partial X_L}\}$ can be rewritten as

$$\begin{aligned}\{\frac{\partial L}{\partial X_K}\}&=\frac{1}{2}v_k v_k\{\frac{\partial\rho^o}{\partial X_K}\}+\frac{1}{2}\upsilon_{mk}\upsilon_{ml}\chi_{kM}\chi_{lN}\{\frac{\partial(\rho^o I_{MN})}{\partial X_K}\}\\&\quad-\{\frac{\partial W}{\partial X_K}\}\end{aligned} \tag{31}$$

Now, let the strain energy density function W, Eq. (19), be written as a polynomial up to second order terms as

$$\begin{aligned}W=&W^o-\rho^o\eta^o T+T_{KL}^o E_{KL}+S_{KL}^o F_{KL}+M_{KLM}^o\Gamma_{KLM}\\&-\frac{\rho^o r}{2T^o}T^2-a_{KL}E_{KL}T-b_{KL}F_{KL}T-c_{KLM}\Gamma_{KLM}T\\&+\frac{1}{2}A_{KLMN}E_{KL}E_{MN}+\frac{1}{2}B_{KLMN}F_{KL}F_{MN}\\&+\frac{1}{2}C_{IJKLMN}\Gamma_{IJK}\Gamma_{LMN}+D_{KLMN}E_{KL}F_{MN}\\&+G_{IJKLM}E_{IJ}\Gamma_{KLM}+H_{IJKLM}F_{IJ}\Gamma_{KLM}\end{aligned} \tag{32}$$

where T^o is the constant reference temperature, T the temperature variation, and

$$\theta = T^o + T,\ T^o > 0,\ |T| \ll T^o \tag{33}$$

W^o, η^o, $\boldsymbol{T}^o$, $\boldsymbol{S}^o$, $\boldsymbol{M}^o$, γ, $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$, $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$, $\boldsymbol{D}$, $\boldsymbol{G}$ and $\boldsymbol{H}$ are material constants, and because of inhomogeneities, they are functions of the Lagrangian coordinate $\boldsymbol{X}$. From Eqs. (22-25) one obtains

$$\rho^o\eta = \rho^o\eta^o + \rho^o\gamma T/T^o + a_{KL}E_{KL} + b_{KL}F_{KL} + c_{KLM}\Gamma_{KLM} \tag{34}$$

$$T_{KL} = T^o_{KL} - a_{KL}T + A_{KLMN}E_{MN} + D_{KLMN}F_{MN} + G_{KLMNP}\Gamma_{MNP} \tag{35}$$

$$S_{KL} = S^o_{KL} - b_{KL}T + B_{KLMN}F_{MN} + D_{MNKL}E_{MN} + H_{KLMNP}\Gamma_{MNP} \tag{36}$$

$$M_{KLM} = M^o_{KLM} - c_{KLM}T + C_{KLMNPQ}\Gamma_{NPQ} + G_{PQKLM}E_{PQ} + H_{PQKLM}F_{PQ} \tag{37}$$

In this work, it is assumed that the strain energy W, the entropy η and the stresses $\boldsymbol{T}$, $\boldsymbol{S}$, $\boldsymbol{M}$ vanish when the temperature variation T and the strains $\boldsymbol{E}$, $\boldsymbol{F}$, $\boldsymbol{\Gamma}$ are zero. This assumption leads to

$$W^o = \eta^o = \boldsymbol{T}^o = \boldsymbol{S}^o = \boldsymbol{M}^o = 0 \tag{38}$$

Now the material force can be rewritten as

$$\begin{aligned} F_P = & -\rho^o f_l x_{l,P} - \rho^o L_{lm}\overline{\chi}_{Rm}\chi_{lR,P} \\ & + \frac{1}{2}v_k v_k(\rho^o)_{,P} + \frac{1}{2}\upsilon_{mk}\upsilon_{ml}\chi_{kM}\chi_{lN}(\rho^o I_{MN})_{,P} \\ & + (\rho^o\gamma T/T^o + a_{KL}E_{KL} + b_{KL}F_{KL} + c_{KLM}\Gamma_{KLM})T_{,P} \\ & + (\rho^o\gamma)_{,P}\frac{T^2}{2T^o} + a_{KL,P}E_{KL}T + b_{KL,P}F_{KL}T \\ & + c_{KLM,P}\Gamma_{KLM}T - \frac{1}{2}A_{KLMN,P}E_{KL}E_{MN} \\ & - \frac{1}{2}B_{KLMN,P}F_{KL}F_{MN} - \frac{1}{2}C_{IJKLMN,P}\Gamma_{IJK}\Gamma_{LMN} \\ & - D_{KLMN,P}E_{KL}F_{MN} - G_{IJKLM,P}E_{IJ}\Gamma_{KLM} \\ & - H_{IJKLM,P}F_{IJ}\Gamma_{KLM} \end{aligned} \tag{39}$$

It is seen that the material force in micromorphic thermoelastic solid is due to (1) body force and body moment, (2) temperature gradient, and (3) the material inhomogeneities in ρ^o, I_{KL}, and all the thermoelastic coefficients.

The balance law of energy can now be expressed as (Lee and Chen, 2003):

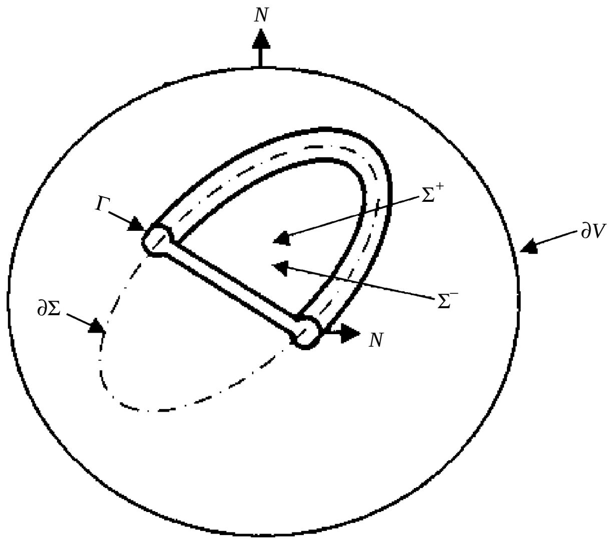

Fig. 1 Finite disk-shaped crack

$$\rho^o\theta\dot{\eta} = -Q_{K,K} + \rho^o h \tag{40}$$

and the heat flux is related to temperature gradient as

$$Q_K = -h_{KL}\theta_{,L} \tag{41}$$

where h_{KL} is the heat conductivity tensor, symmetric and positive definite.

IV. MATERIAL FORCES AT THE CRACK FRONT

In this section we focus our attention to the case that (1) it is static, (2) it has no body force and body moment, (3) the material is elastic and homogeneous, and (4) the material body has a finite disk-shaped crack. The disk-shaped crack Σ, as shown in Fig. 1, has an upper surface Σ^+, a lower surface Σ^-, and a crack front $\partial\Sigma$, i.e., $\Sigma = \Sigma^+ \oplus \Sigma^- \oplus \partial\Sigma$. Based on the first three conditions mentioned above, one has

$$P_L = F_L = 0 \tag{42}$$

$$B_{KL,K} = 0 \tag{43}$$

and the Eshelby stress tensor is reduced to

$$B_{KL} = W\delta_{KL} - T_{KM}E_{LM} - M_{NMK}\Gamma_{NML} \tag{44}$$

One may verify Eq. (43) by using Eqs. (44, 23-25) and

$$W = W(\boldsymbol{E}, \boldsymbol{F}, \boldsymbol{\Gamma}) \tag{45}$$

Provided that V contains no singularity, i.e., the crack front $\partial\Sigma$ is not in V, the integration of Eq. (43) over a material volume V implies the following

$$\int_V B_{KL,K} dV = \oint_S B_{KL} N_K dS = 0 \tag{46}$$

where S is the enclosing surface of V and $\boldsymbol{N}$ is the unit outward normal of S. We rewrite Eq. (46) as

$$\oint_S \boldsymbol{B}\cdot\boldsymbol{N} dS = \int_{\partial\Sigma} dL\{\int_{\Gamma} \boldsymbol{B}\cdot\boldsymbol{N} d\Gamma\} = 0 \tag{47}$$

where dL is the differential length along the crack front $\partial\Sigma$; Γ denotes the closed cross-sectional circuit on the plane perpendicular to tangent of $\partial\Sigma$; Γ can be decomposed into four parts $\Gamma=\Gamma_1\oplus\Gamma_2^*\oplus\Gamma^+\oplus\Gamma^-$, as shown in Fig. 2. Notice that Γ_1 traces clock-wise around the crack front with its outward unit normal $\boldsymbol{N}(\Gamma_1)$ pointing away from the crack friont; Γ_2^* traces counter-clock-wise around the crack front with its outward unit normal $\boldsymbol{N}(\Gamma_2^*)$ pointing toward the crack front. A vector $\boldsymbol{I}_L$ is defined along the crack front as

$$\boldsymbol{I}_L \equiv J_L(\Gamma_1)+J_L(\Gamma_2^*)+J_L(\Gamma^+)+J_L(\Gamma^-) \tag{48}$$

where

$$J_L(\Gamma_1) \equiv \int_{\Gamma_1} B_{KL} N_K d\Gamma \tag{49}$$

and, similarly, for $J_L(\Gamma_2^*)$, $J_L(\Gamma^+)$, and $J_L(\Gamma^-)$. Actually, J_L defined in Eq. (49) is the generalized vectorial J-integral. It can be readily shown that

$$\int B_{KL} N_K d\Gamma = \int \{WJ^{-1} x_{k,L} - t_{km}(x_{m,L} - \chi_{mL}) - m_{knm} \overline{\chi}_{Mm} \chi_{nM,L}\} n_k d\Gamma \tag{50}$$

and it is noticed that

$$t_m^* = t_{km} n_k,\ m_{nm}^* = m_{knm} n_k \tag{51}$$

are the surface traction and surface moment, which are vanishing at Γ^+ and Γ^-. Now Eq. (48) can be rewritten as

$$\boldsymbol{I}_L = J_L(\Gamma_1) - J_L(\Gamma_2) + \int_{\Gamma^+} W N_L d\Gamma + \int_{\Gamma^-} W N_L d\Gamma \tag{52}$$

where $\Gamma_2 \equiv -\Gamma_2^*$, i.e., $\boldsymbol{N}(\Gamma_2) = -\boldsymbol{N}(\Gamma_2^*)$ and Γ_2 traces clock-wise around the crack front just like Γ_1. This leads to $J_L(\Gamma_2) = -J_L(\Gamma_2^*)$. Since Eq. (47) means

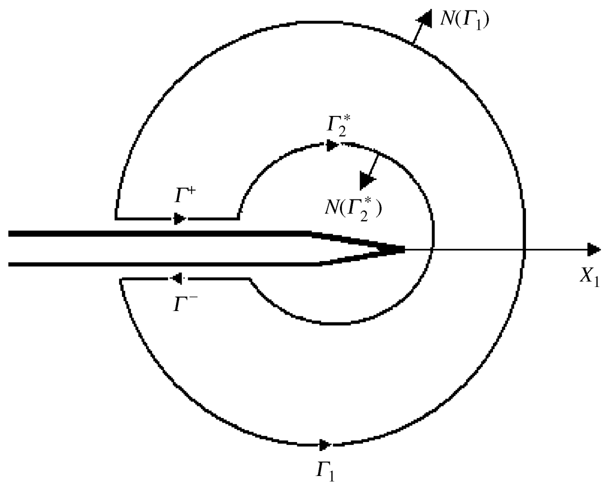

Fig. 2 J-integral contour around crack tip

$$\int_{\partial\Sigma} \boldsymbol{I}_L dL = 0 \tag{53}$$

For any case that $\boldsymbol{I}_L$ is constant along the crack front such as (1) a straight-through crack in a plane problem ($\partial\Sigma$ becomes a straight line perpendicular to the X-Y plane as shown in Fig. 2 and (2) a circular crack front in an axis symmetric problem, it results

$$\boldsymbol{I}_L = 0 \tag{54}$$

Since $N_1=0$ on Γ^+ and Γ^-, Eq. (52) leads to

$$J_1(\Gamma_1) = J_1(\Gamma_2) \tag{55}$$

which means the X-component of the vectorial J-integral is path independent while X-direction is the tangent to $\Sigma^+(\Sigma^-)$ in the wake of the crack front. It is further noticed that the vectorial J-integral is path independent, i.e.,

$$J_L(\Gamma_1) = J_L(\Gamma_2) = \cdots = J_L(\Gamma_i) = \cdots \tag{56}$$

provided that both starting and ending points of Γ_i (i=1, 2, ⋯) are approaching the crack front from its wake in the limit. Also, it is worthwhile to note that when the micro- and macro-deformations are small, i.e.,

$$x_{k,K} \approx (\delta_{kl} + u_{k,l})\delta_{lK}, \quad \chi_{kK} \approx (\delta_{kl} + \phi_{kl})\delta_{lK}, \quad \overline{\chi}_{Kk} \approx (\delta_{lk} - \phi_{lk})\delta_{Kl} \tag{57}$$

the expression of J-integral becomes

$$J_l = \int_{\Gamma} \{W\delta_{kl} - t_{km}(u_{m,l} - \phi_{ml}) - m_{knm}\phi_{nm,l}\} n_k ds \tag{58}$$

where u_k is the displacement vector; ϕ_{kl} is the micro-deformation tensor; δ_{kK} is the shifter between the Lagrangian and Eulerian coordinate systems. Thus, the concept of material force (Eshelby mechanics) is used to derive the driving force of crack propagation, the J-integral, which is generalized to a vector for large-strain micromorphic elastic materials. The vectorial feature of $\boldsymbol{J}$ may be used as an indicator to predict the direction of crack propagation in future studies.

V. FINITE ELEMENT ANALYSIS

In this work, attention is focused on small-strain theory; Eq. (57) leads to

$$E_{KL}\approx(u_{l,\,k}-\phi_{lk})\delta_{kK}\delta_{lL},\ \dot{E}_{KL}\approx(v_{l,\,k}-\upsilon_{lk})\delta_{kK}\delta_{lL}$$

$$F_{KL}\approx(\phi_{kl}+\phi_{lk})\delta_{kK}\delta_{lL},\ \dot{F}_{KL}\approx(\upsilon_{kl}+\upsilon_{lk})\delta_{kK}\delta_{lL}$$

$$\Gamma_{KLM}\approx\phi_{kl,\,m}\delta_{kK}\delta_{lL}\delta_{mM},\ \dot{\Gamma}_{KLM}\approx\upsilon_{kl,\,m}\delta_{kK}\delta_{lL}\delta_{mM} \tag{59}$$

where v_k is the velocity; υ_{kl} the micro-gyration tensor.

The balance laws of linear momentum, momentum moments, and energy, Eqs. (6, 7, 40), together with the constitutive equations, Eqs. (34-37, 41), lead to the following dynamic finite element equations:

$$M_{\alpha\beta}\ddot{u}_\beta+K^1_{\alpha\beta}u_\beta+K^2_{\alpha\beta}\phi_\beta+K^3_{\alpha\beta}T_\beta=F_\alpha \tag{60}$$

$$J_{\alpha\beta}\ddot{\phi}_\beta+K^4_{\alpha\beta}u_\beta+K^5_{\alpha\beta}\phi_\beta+K^6_{\alpha\beta}T_\beta=L_\alpha \tag{61}$$

$$\gamma_{\alpha\beta}\dot{T}_\beta+G^1_{\alpha\beta}\dot{u}_\beta+G^2_{\alpha\beta}\dot{\phi}_\beta+H_{\alpha\beta}T_\beta=Q_\alpha \tag{62}$$

where the detailed expressions of $\boldsymbol{M}$, $\boldsymbol{J}$, γ, $\boldsymbol{K}^i$ (i=1, 2, ⋯, 6), $\boldsymbol{G}^1$, $\boldsymbol{G}^2$, $\boldsymbol{H}$, $\boldsymbol{F}$, $\boldsymbol{L}$, and $\boldsymbol{Q}$ can be found in (Lee and Chen, 2003).

It is noticed that, from Eqs. (60-62), the temperature, displacement and micro-motion fields are coupled in the dynamic case, while in static case Eqs. (60-62) are reduced to

$$H_{\alpha\beta}T_\beta=Q_\alpha \tag{63}$$

$$K^1_{\alpha\beta}U_\beta+K^2_{\alpha\beta}\phi_\beta=F_\alpha-K^3_{\alpha\beta}T_\beta \tag{64}$$

$$K^4_{\alpha\beta}U_\beta+K^5_{\alpha\beta}\phi_\beta=L_\alpha-K^6_{\alpha\beta}T_\beta \tag{65}$$

which means the temperature field can be obtained by solving the heat equation, Eq. (63), and then it serves as the forcing terms in Eqs. (64, 65) which are the governing equations for the coupled displacement and micro-motion fields.

In molecular crystal or crystal containing complex ions, both internal modes (the stretching and distortion of the molecules) and external modes (molecules move as rigid units) may exist. While for a lot of solid crystallines, the atomic motion involves no external modes. Examples include metallic, covalent and ionic crystals, i.e., materials like silicon, diamond, germanium, ZnO, NaCl, *et al*. For those solid crystallines, phonon dispersion relations only present the internal modes. With the absence of external rotational modes, the deformable particle thus only has 6 independent degrees of freedom describing the stretches within the microstructure in addition to the 3 translational degrees of freedom of its center. The micro-deformation tensor and the gyration tensor are then symmetric, i.e.,

$$\phi_{[kl]}=\upsilon_{[kl]}=0 \tag{66}$$

and then it is shown that the number of elastic moduli for general cubic crystal and diamond structure crystal is reduced to 10 and 7, respectively. Through phonon dispersion relations from shell model (Cochran, 1993), *ab initio* calculation (Van Camp *et al*., 1983), valence force model (Bruessh, 1982), and experimental data (Cochran, 1993, Warren *et al*., 1965), all the elastic moduli in special micromorphic theory for diamond and silicon are obtained (Chen and Lee, 2003c).

A polycrystalline material is composed of randomly distributed and oriented grains, and the grain boundaries are usually in the amorphous phase (Stemmer *et al*., 2000). In this work, a statistical model of polycrystalline solid is adopted. The randomly oriented and distributed grains in the shape of polygons can be created and meshed automatically with given statistical average of grain size by adopting the Wigner-Seitz approach (Kittel, 1967), an approach that has been used in lattice dynamics to create unit cells. Each grain is modeled as a single crystal by specialized micromorphic theory. Between the grains, the grain boundaries are modeled as in its amorphous phase with a thin and finite width by classical continuum mechanics. Material constants for amorphous silicon are estimated to be λ=0.278E-7 N/nm^2, μ= 0.417E-7 N/nm^2 (Chiou; 2003, Peterson, 1972; Muller and Kamins, 1986, Stannowski *et al*., 2002).

A thin film of silicon subjected to simple tension/compression along X-direction is modeled and simulated. Cauchy stresses, Eshelby stresses, and material forces are obtained. The von Mises stresses calculated from the Cauchy stress tensor, Eshelby stress tensor and the material force (in the X-direction) F_x are shown in Fig. 3, Fig. 4 and Fig. 5, respectively.

VI. DISCUSSIONS

(1) If the material under the loading of simple tension/compression as in this case had been

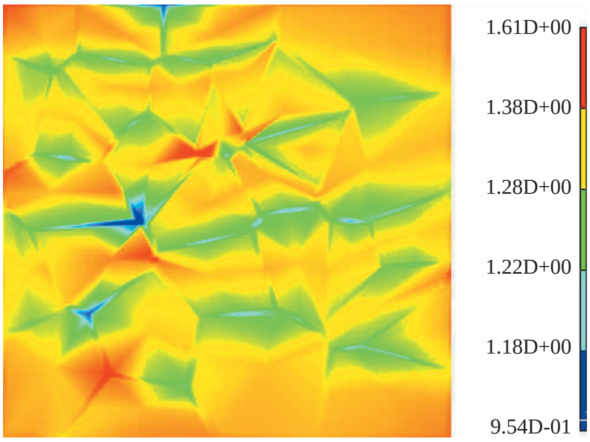

Fig. 3 Cauchy stress (von Mises)

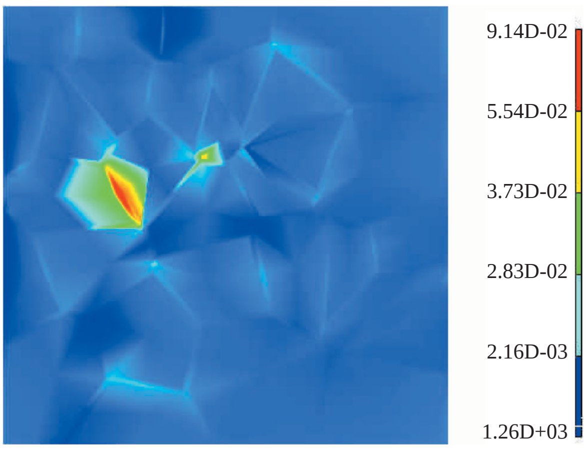

Fig. 4 Eshelby stress (von Mises)

homogeneous, there would have been no Eshelby stresses, no material forces and no shear stresses either. However, the simulation does show that there are Eshelby stresses, material forces and considerable shear stresses as well. This is due to the existence of material inhomogeneities - the difference of material behavior between crystallized grains and amorphous grain boundaries.

(2) The maximum Cauchy stresses and Eshelby stresses exist in the grain boundaries. Also, it is seen that the material forces, one side positive and the other negative, are acting at the two sides of grain boundaries indicating a tendency to pull the grains apart. As a consequence, cracks would initiate and propagate at grain boundaries. This explains why cracks observed in polycrystalline materials seldom appear as straight lines; they are curved instead.

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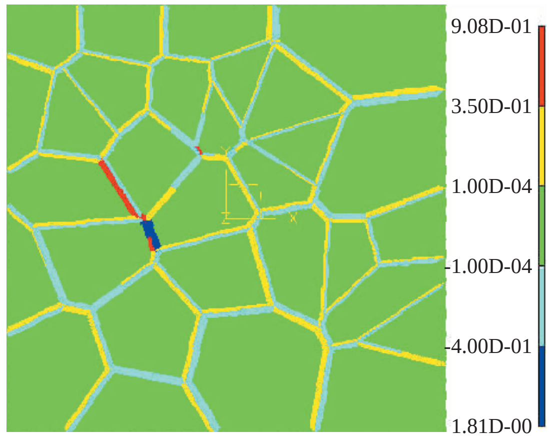

Fig. 5 Material force (F_x)

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