



## Modeling the effect of surface energy on stressed grain growth in cubic polycrystalline bodies



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### ABSTRACT

A recently-developed constitutive theory of stressed grain growth is augmented to include the effect of excess surface energy via a surface effect state variable. The new constitutive theory is implemented into a coupled finite-element and phase-field computational framework. Through three-dimensional simulations, the new constitutive model is shown to be capable of predicting the experimental data of the annealing-induced texture transition in polycrystalline copper thin films of different thicknesses attached to a polyimide substrate. Our simulations show that the grain growth driving force arising from the through-film thickness grain boundary curvature plays a prominent role in such a transitional behavior.

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Grain-growth in polycrystalline bodies via grain boundary motion is one of the most extensively studied phenomena in engineering science. As the latest devices used in engineering practice are getting smaller, the role of excess energy at the external surfaces of the devices in controlling grain growth becomes more important [1,2]. Although grain growth is generally a three-dimensional (3D) phenomenon, Carel et al. [3] have performed two-dimensional simulations of stressed grain growth in a polycrystalline film by assuming that the grain-growth driving force due to release of excess surface energy at an external surface of the film is constant throughout the thickness of the film [3,4,5]. Recently, Lee et al. [6] have incorporated the effect of free surface in their 3D grain growth simulations but they ignored the effect of stress in their simulations. In our recent work [7], we have introduced a so-called surface effect variable which measures the degree of atomic rearrangement in a body due to the presence of external surfaces. Via using a surface effect variable, we are able to describe the variation of the excess surface energy in a 3D body [7].

Hence, the main objectives of this paper are to: (1) augment a previously-developed constitutive theory for elastic deformation

(stress)-driven grain growth [8] to include the effect of external surface energy through the use of surface effect variables [7]; and (2) quantitatively verify experimental trends of grain-growth in polycrystalline films of different thicknesses [4] through 3D numerical simulations.

Constitutive theory – we model a cubic polycrystalline body which has two unique single crystal orientations (or species), and two different types of external surfaces (free surface & film-substrate interface). The constitutive theory is formulated in the reference configuration cf. [8].

Let  $\nabla$ ,  $\text{Div}$  and  $\nabla^2$  denote the gradient, divergence and Laplacian operators in the reference configuration, respectively. The governing variables in the theory are: (a) the deformation gradient,  $\mathbf{F}$  with  $\mathbf{J} = \det \mathbf{F} > 0$ ; (b) the Helmholtz free energy per unit reference volume,  $\psi$ ; (c) the absolute temperature,  $\theta > 0$ ; (d) the Cauchy stress,  $\mathbf{T} = \mathbf{T}^T$ ; (e) the second Piola–Kirchoff stress,  $\mathbf{T}^* = \mathbf{J}\mathbf{F}^{-1}\mathbf{T}\mathbf{F}^{-T}$ ; (f) the Green strain,  $\mathbf{E} = (1/2)\{\mathbf{F}^T\mathbf{F} - \mathbf{I}\}$ ; (g) the volume fraction of species  $i$ ,  $\xi_i$  where  $0 \leq \xi_i \leq 1$  with  $i = 1, 2$ , and  $\sum_i \xi_i = 1$ . A value of  $\xi_i = 0$  means that species  $i$  is not present whereas a value of  $\xi_i = 1$  means that a particle is a single-crystal of species  $i$ . A particle which contains a mixture of two species represents a part of a grain-boundary region; (h) the surface effect variable associated with the external surface of the body,  $\lambda$ . The variable  $\lambda$  measures the magnitude of the atomic rearrangement in a body due to its external surface [7]. As a first-cut approach, we assume that the magnitude of the atomic rearrangement at the external surface is identical regardless of the type of external surface e.g. free surface, film-substrate interface etc., and crystal orientation. We take  $0 \leq \lambda \leq 1$  where  $\lambda = 1$  at the external surface, and  $\lambda$  vanishes at particles which are not affected by the presence of the external surface [7].

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Since  $\xi_2 = 1 - \xi_1$ , we therefore only need to track the volume fraction of one species i.e. either  $\xi_1$  or  $\xi_2$ . Therefore, we set  $\xi_1 \equiv \xi$ ,  $\xi_2 \equiv 1 - \xi$  and write the Helmholtz free energy density as

$$\psi = \psi^\xi + \psi^g + p(\xi)\psi_1 + [1 - p(\xi)]\psi_2 \quad (1)$$

where the exchange free energy between the species,  $\psi^\xi = \hat{\psi}^\xi(\xi) = \omega\xi(1-\xi)$  and the grain growth-related gradient free energy,  $\psi^g = (1/2)\kappa|\nabla\xi|^2$ . The material constant  $\omega > 0$  defines the potential energy barrier between the species in order to prevent spontaneous conversions between the species, and the material constant  $\kappa > 0$  introduces the characteristic length scale which controls the grain boundary thickness between the species. Hence, the gradient free energy penalizes the presence of grain boundaries. The smooth interpolation function  $p(\xi) = \xi^2(3 - 2\xi)$  ensures that spontaneous inter-species conversions do not occur within a single species [8].

With  $\theta_o$  representing the reference temperature, we take the free energy of species  $i$  as

$$\psi_i = \psi_i^e + \psi_i^\theta + \psi_i^x, \quad i = 1, 2 \quad (2)$$

where for species  $i$ , the thermo-elastic free energy,  $\psi_i^e = \hat{\psi}_i^e(\mathbf{E}, \theta) = (1/2)[\mathbf{E} - \alpha_i(\theta - \theta_o)] : C_i[\mathbf{E} - \alpha_i(\theta - \theta_o)]$  and the purely thermal free energy,  $\psi_i^\theta = \hat{\psi}_i^\theta(\theta) = c_i\{(\theta - \theta_o) - \theta \ln(\theta/\theta_o)\}$ . The material constants  $C_i$ ,  $\alpha_i$  and  $c_i$  respectively denote the fourth-order elastic moduli tensor, the coefficient of thermal expansion and the specific heat at constant volume, for species  $i$ . The excess surface free energy density of species  $i$  comprising the chemical energy caused by the presence of the external surface i.e.  $\psi_i^x$  is taken as [7]

$$\psi_i^x = \psi_i^{x,g} + \psi_i^{x,\lambda}, \quad i = 1, 2. \quad (3)$$

For a given species  $i$ ,  $\psi_i^{x,g} = \psi_i^{x,g}(\nabla\lambda) = (1/2)\varepsilon_i|\nabla\lambda|^2$  is the gradient energy portion of  $\psi_i^x$ , and  $\psi_i^{x,\lambda} = \hat{\psi}_i^{x,\lambda}(\lambda) = (1/2)\sigma_i\lambda^2$  is the potential (bulk) energy portion of  $\psi_i^x$ . The constant material coefficients  $\varepsilon_i > 0$  introduce characteristic length scales associated with the effect of the external surface on species  $i$ , and the constant-valued material coefficients  $\sigma_i > 0$  measure the height of the potential energy associated with the effect of the external surface on species  $i$  [7].

Guided by the theoretical framework developed by [8], we derive the key constitutive equations and kinetic relations for the elastic deformation (stress)-driven grain growth in polycrystalline bodies by accounting for the effect of external surface energy in the Supplementary Material [9]. The constitutive equation for stress is [9]:

$$\mathbf{T}^* = \mathcal{L}[\mathbf{E}] - (\theta - \theta_o)\mathbf{B} \quad (4)$$

where the composite elastic moduli  $\mathcal{L} \equiv p(\xi)C_1 + [1 - p(\xi)]C_2$ , and the composite stress-temperature moduli  $\mathbf{B} \equiv \{p(\xi)\alpha_1 C_1 + [1 - p(\xi)]\alpha_2 C_2\}[\mathbf{I}]$ . The kinetic relations for grain growth and the surface effect variable are respectively [9]:

$$\dot{\xi} = M^\xi^{-1} \left\{ \kappa \nabla^2 \xi - \omega(1 - 2\xi) - \frac{\partial p(\xi)}{\partial \xi} (\psi_1 - \psi_2) \right\} \quad (5)$$

and

$$\dot{\lambda} = M^\lambda^{-1} \left\{ \varepsilon \nabla^2 \lambda - \bar{\sigma} \lambda \right\}, \quad (6)$$

with  $M^\xi$  and  $M^\lambda$  representing the damping coefficient for the grain growth process and the atomic rearrangement process caused by the presence of the external surface, respectively, and the external surface-related composite material coefficients  $\bar{\varepsilon} \equiv p(\xi)\varepsilon_1 + [1 - p(\xi)]\varepsilon_2$  and  $\bar{\sigma} \equiv p(\xi)\sigma_1 + [1 - p(\xi)]\sigma_2$ . For simplicity,

we take the external surface-related characteristic length scales  $l_i^\xi \equiv \sqrt{\varepsilon_i/\sigma_i}$  to be equal i.e.  $l_i^\xi \equiv l^s$  for  $i = 1, 2$ .

From molecular dynamics simulations [10,11], it is ascertained that the time required for the relaxation of atoms at the free surface of a body is in the order of femtoseconds to picoseconds. For simplicity, we assume that the time scale for the equilibration of the surface effect variable field do not depend on the type of external surface e.g. free surface, film-substrate interface, and it is also in the order of femtoseconds to picoseconds. Given that the time scale for grain growth i.e. inter-species conversions is in the order of milliseconds to seconds, we can conclude that the surface effect variable field relaxes very much faster than the species volume fraction field. To capture the kinetics of grain growth in a computationally-inexpensive manner, we choose a time increment in our numerical simulations for which the surface effect variable field has completely relaxed while inter-species conversions are still occurring. Hence, we set  $\dot{\lambda} = 0$ , and Eq. (6) reduces to

$$\varepsilon \nabla^2 \lambda - \bar{\sigma} \lambda = 0. \quad (7)$$

We model the grain-growth response in a polycrystalline film of initial thickness  $h_f$  which is perfectly bonded to a polymer substrate of initial thickness  $h_s$ . Hence, the polycrystalline film has an external surface which consists of two non-overlapping portions i.e. a free surface & a film-substrate interface. It is also assumed that for a given species  $i$ , the free surface of the film & the film-substrate interface have equal Gibbs surface free energies [4].

Let axis- $z$  describe the coordinates along the thickness direction of the polycrystalline film. The plane  $z = -h_f/2$  is taken to coincide with the free surface of the polycrystalline film, and the plane  $z = +h_f/2$  is taken to coincide with the polycrystalline film-polymer substrate interface. The in-plane dimensions of the polycrystalline film are assumed to be very much larger than the polycrystalline film thickness, and consequently Eq. (7) reduces to

$$l^{s2} \frac{\partial^2 \lambda}{\partial z^2} - \lambda = 0. \quad (8)$$

Since the highest degree of atomic rearrangement occurs at the external surface, we set  $\lambda = 1$  at  $z = \pm h_f/2$  and solve Eq. (8) to obtain:

$$\lambda = \cosh\left(\frac{z}{l^s}\right) / \left[ \cosh\left(\frac{h_f}{2l^s}\right) \right]. \quad (9)$$

By substituting Eq. (9) into Eq. (3), we can then obtain the variation of the external surface excess energies throughout the film. Since  $l^s \ll h_f$  for typical films used in engineering practice, we define

$$\gamma_i^x \equiv (1/2) \int_{-h_f/2}^{+h_f/2} \psi_i^x dz, \quad i = 1, 2 \quad (10)$$

where the material parameters  $\gamma_i^x > 0$  represent the Gibbs surface free energy (units of energy per unit area) associated with species  $i$ . Using Eqs. (3) and (9) in Eq. (10) yields  $\gamma_i^x = (1/2)\sqrt{\varepsilon_i}\sigma_i$  for  $i = 1, 2$  since  $l^s \ll h_f$ .

Numerical simulations — the coupled finite-element (FE) & phase-field (PF) multiscale numerical framework developed by [8] was employed to numerically implement the constitutive theory described above into the Abaqus [12] FE code through a user-material subroutine (UMAT) interface.

Fig. 1a shows the initially-undeformed FE mesh of a section of the perfectly-bonded polycrystalline film-polymer substrate ensemble modeled in this paper. Appropriate nodal displacement boundary conditions are imposed on the film-substrate ensemble shown in Fig. 1a to ensure that plane sections always remain plane.

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