An efficient method for computing microstructural evolution of elastically homogeneous media

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Received 3 August 2004; accepted 13 October 2004

Abstract

A boundary integral method is introduced to study the dynamics of the morphological evolution of a three-dimensional, coherent precipitate in an infinite, elastic matrix. The precipitate evolves diffusively in which the precipitate–matrix interface satisfies a generalized Gibbs–Thomson boundary condition, accounting for surface energy, elastic and interface kinetic energy. Elastically homogeneous systems, where the precipitate and matrix phases are taken to have the same elastic stiffness tensor of general anisotropy, are considered. A computationally efficient approach, which only involves surface integration, is developed to determine the elastic strain energy due to a misfit strain between the phases. The convergence rate of the numerical method is obtained, and the method is applied to simulate the evolution of a single precipitate in a cubic system. Results show that the number and the stability of equilibrium shapes of the precipitate change as the ratio between the elastic and surface energies is larger than a critical value. For ratios below the critical value, there is unique stable equilibrium shape of cubic symmetry; for a range of values beyond the critical value, at least two kinds of equilibrium shapes exist: one retains cubic symmetry and is metastable, and the other is tetragonal symmetric and more stable.

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PACS: 64.70Kb; 81.30Mh; 02.60L
Keywords: Microstructural evolution; Coherent precipitates; Phase transformations; Alloys; Equilibrium shapes; Boundary element method

1. Introduction

The boundary integral method has been an important tool in continuum mechanics. It is an effective numerical method for a problem that can be determined by the knowledge of boundary of the interested domain and the physical quantities.
on the boundary. In this case, boundary integral method reduces the dimensionality of the problem by one compared with other methods (such as finite element method or finite difference method). In solving the elasticity equation, the boundary integral formulation relating the boundary values of displacement and traction (referred to as the direct approach) was first developed by Rizzo [1] for two-dimensional isotropic elasticity. The direct boundary integral approach was extended to plane anisotropic (orthotropic) elasticity by Rizzo and Shippy [2] and to three-dimensional isotropic elasticity by Cruse [3–5].

Sharp interface modeling of microstructures consisting of matrix and particle phases usually employs boundary integral techniques. The elastic field arises due to the misfit, the difference in lattice parameters between the matrix and particle phases. For two-dimensional inhomogeneous (the elastic stiffness tensors for the two phases differ) systems, Rizzo and Shippy [6] and Jou et al. [7] derived coupled boundary integral equations for the displacement and traction on the interface between the two phases of isotropic elasticity; Schmidt and Gross [8] and Leo et al. [9] reformulated the integral equations for the case where the elastic constants of the matrix and particle phases are orthotropic based on the work in [2]. For three-dimensional inhomogeneous inclusion problems, Mueller and Gross [10] demonstrated that the same boundary integral equations derived in [3] for isotropic elasticity can be used for general anisotropic cases, while Li et al. [11] presented a different set of boundary integral equations for the same unknowns (the displacement and traction) that do not involve computation of singular integrals of Cauchy-type. Because the linear systems deduced from the discretized integral equations are dense and non-symmetric, the most computationally expensive part of the numerical simulation of the microstructural evolution is solving these coupled integral equations.

For homogeneous systems, where the elastic constants for the matrix and particles phases are identical, Voorhees et al. [12] obtained the expressions for the elastic field in terms of contour integrals for two-dimensional cubic elasticity. The formulation avoids solving the integral equations that is required in the inhomogeneous case. The derivation in [12] depends on the explicit expression of the Green’s function for plane cubic elasticity, which can not be extended to three dimensions due to lack of explicit formula of the Green’s function for general anisotropic elasticity (including cubic elasticity). In this work, we present a formulation for computing the elastic field of three-dimensional homogeneous systems with general anisotropic elasticity, which only involves evaluation of surface integrals, i.e., not requiring solution to integral equations.

The two-phase microstructure reaches an equilibrium when the sum of surface and elastic energies is at an extremum. We review the previous findings on equilibrium states for systems with cubic elasticity and in absence of external loading. For a single precipitate in infinite matrix, the number of equilibrium shapes and the stability change as the elastic effect increases through a bifurcation point. For two-dimensional homogeneous systems, the bifurcation is shown to be supercritical [13]: the equilibrium shape is fourfold symmetric (circular or squarish) for small ratios of elastic to surface energy; there are two kinds of equilibrium shapes beyond the bifurcation point, one retaining four-fold symmetry but unstable, and the other having twofold symmetry and globally stable. For two-dimensional inhomogeneous or three-dimensional (homogeneous or inhomogeneous) systems, the corresponding complete bifurcation diagram of equilibrium shapes has not been constructed using appropriate methods. However, numerous simulations (e.g., [14,9,11,15]) have shown that equilibrium shape bifurcates as the effect of elasticity increases. Before the bifurcation point, the equilibrium shape has a higher symmetry (fourfold in 2D and cubic in 3D) and is stable. After the bifurcation point, a stable equilibrium shape of a lower symmetry (twofold in 2D and tetragonal in 3D) emerges, and in 2D the fourfold symmetric equilibrium shape is stable with respect to fourfold symmetric perturbations but unstable to perturbations of lower symmetries. In this work, we will show, beyond the bifurcation point, there are two kinds of equilibrium shape for a three-dimensional homogeneous system, and discuss their stabilities through dynamic simulations.
In Section 2, we describe the mathematical model for the evolution of homogeneous inclusion in infinite matrix. In Section 3, we present the boundary integral formulation that is efficient for computing the elastic field. In Sections 4 and 5, we outline the numerical methods, demonstrate the convergence and investigate the dynamics of an isolated particle in infinite matrix.

2. Governing equations

Consider the evolution of a homogeneous inclusion induced by a misfit strain between the matrix and the precipitate phases, \( \epsilon^T \). We assume that during the evolution, the dimensionless concentration \( c \) satisfies the quasi-static diffusion equation in both phases, denoted by \( \Omega^M \) and \( \Omega^P \) as sketched in Fig. 1,

\[
\nabla^2 c = 0 \quad \text{in} \quad \Omega^M, \Omega^P. \tag{1}
\]

The boundary condition is given by the generalized Gibbs–Thomson boundary condition [16]

\[
c = -\kappa - L g^{el} - \lambda v_n \quad \text{on} \quad \partial \Omega \tag{2}
\]

where \( \kappa \) is twice the mean curvature of the interface \( \partial \Omega \), \( g^{el} \) is the dimensionless elastic energy density defined later in Eq. (4), \( v_n \) is the magnitude of the normal velocity of the precipitate–matrix interface, and \( \lambda \) is the non-dimensional kinetic coefficient. The constant \( L \equiv \epsilon^2 C_{44} / \gamma^2 \), introduced in [12], characterizes the relative contribution of the elastic and surface energies, where \( \epsilon \) is the magnitude of the misfit strain, which is assumed to be independent of composition, \( C_{44} \) is an elastic constant for the solid (assumed equal in the matrix and the precipitate phases), and \( \gamma \) is the constant surface energy. The non-dimensionalization procedure for \( c \) can be found in [17], the characteristic length scale \( l \) is the equivalent radius of the precipitate \( (3V/4\pi)^{1/3} \) where \( V \) is the volume, and the strain and the stress are non-dimensionalized by \( \epsilon \) and \( C_{44} \) respectively. \( n \) is the unit normal of the surface pointing toward the matrix, and the normal velocity is given by \( v_n = k \left[ \frac{\sigma_n^{el}}{\kappa} \right]_{\Omega^P} - \frac{\sigma_n^{el}}{\kappa} \left[ \Omega^M \right] \) [18], where \( k \) is the diffusion coefficients in both phases and \( \frac{\sigma_n^{el}}{\kappa} \left[ \Omega^P \right] \) and \( \frac{\sigma_n^{el}}{\kappa} \left[ \Omega^M \right] \) denote the values of \( \frac{\sigma_n^{el}}{\kappa} \) evaluated from the precipitate side and the matrix side respectively.

The far-field condition for the diffusion problem is constant mass flux,

\[
J = \frac{1}{4\pi} \int_{\partial \Omega} v_n \, dA. \tag{3}
\]

To obtain the elastic energy density \( g^{el} \) in the boundary condition (2), we must calculate the related elastic quantities. The elastic fields arise because of the misfit strains, which is taken into account through the constitutive relation between the stress \( \sigma \) and strain \( \epsilon \), \( \sigma^P_{ij} = C_{ijkl}(\epsilon^P_{kl} - \epsilon^T_{kl}) \) and \( \sigma^M_{ij} = C_{ijkl}(\epsilon^M_{kl}) \), where \( C_{ijkl} \) denotes the stiffness tensor of the material and the superscripts \( P \) and \( M \) denote the precipitate and the matrix phases respectively.

In the absence of body forces, the field equations for elasticity are given by \( \sigma^\chi_{ij,\chi} = 0 \) in both phases, \( \Omega^\chi \) for \( \chi = M, P \). We assume the two-phase interface \( \partial \Omega \) is coherent, implying the displacement \( u \) and the traction \( t \) are continuous across the interfaces. \( g^{el} \) is computed as

\[
g^{el} = \frac{1}{2} \left( \sigma^P_{ij}(\epsilon^P_{ij} - \epsilon^T_{ij}) - \sigma^M_{ij}(\epsilon^M_{ij}) \right) + \sigma^M_{ij}(\epsilon^M_{ij} - \epsilon^P_{ij}) \quad \text{on} \quad \partial \Omega. \tag{4}
\]
The total energy of the system, $W_{tot}$, is the sum of the surface energy, $W_s$, and the elastic energy, $W_e$, where

$$W_s = \int \int_{\partial \Omega} dA,$$

$$W_e = \frac{L}{2} \left[ \int \int_{\Omega^M} \sigma^p \cdot (\epsilon^p - \epsilon^T) dV + \int \int_{\Omega^M'} \sigma^M \cdot \epsilon^M dV \right].$$

(5)

3. Boundary integral formulation

The diffusion equations (1) and (2) can be formulated as a boundary integral equation of second kind for the normal velocity $v_n$ [19]

$$\lambda v_n(x) + \frac{1}{4\pi} \int_{\partial \Omega} \frac{v_n(y)}{|x-y|} dA_y + c_{\infty} = -\kappa - L g^{el}.$$  

(6)

Together with the far-field condition (3), the boundary integral equation (6) determines the normal velocity $v_n(x)$ uniquely.

Next, we discuss the method for obtaining the displacement $u$ and the traction $t$ on the interface by solving the elastic field equations with a misfit inclusion $\Omega^P$. The computation of the elastic energy density $g^{el}$ defined by Eq. (4) in the right side of Eq. (6), based on the knowledge of $u$ and $t$ on $\partial \Omega$, is provided in Appendix A.

3.1. An effective formulation for the elasticity problem

For inhomogeneous systems, in which the elastic stiffness tensor $C$ for the precipitate phase is different than that for the matrix phase, the elastic energy density $g^{el}$ is obtained by solving two coupled boundary integral equations for the displacement vector $u$ and the traction vectors $t$ on the interface [11]. For every time-step of the evolution, if the total number of marker points on the surface is $M$, then a $6M \times 6M$ non-symmetric, dense matrix $A$ is built and a linear system with coefficient matrix $A$ is solved using an iterative method. The previous studies of inhomogeneous systems have shown that the computational cost of solving the elasticity equations is more than 98 percent of the overall expense, for sufficiently large $M(\geq 362)$ [11].

Here, we establish a formulation that finds the unknowns, the displacement $u$ and the traction $t$ on the interface, by evaluating surface integrals only, instead of solving integral equations.

Define the Green’s tensor $G$ as

$$C_{ijkl} G_{km,lj}(x) + \delta_{im} \delta(x) = 0,$$

(7)

where $\delta(x)$ is Dirac’s delta function and $G_{km,lj}(x)$ is the second-order derivative of $G_{km}(x)$ with respect to $x_i$ and $x_j$. $G_{km}(x)$ is the $m$th component of the displacement at point $x$ when a point body force in the axial direction $x_k$ is applied at the origin. In this paper, all the indices like $i,j,k$ run from 1 to 3, and the Einstein summation convention is used.

Integrating (7) over the closed region $\partial \Omega^P$ and using divergence theorem, we establish the identity

$$\int_{\partial \Omega} C_{ijkl} G_{km,lj}(y-x) n_j(y) dA_y + \delta_{im} k(x) = 0,$$

(8)

where $k(x) = 0$ or 1 depending on the point $x$ outside or inside $\Omega^P$.

It is well known, see for example Mura [20], that the displacement at point $x$ due to homogeneous inclusion is given by

$$u_j(x) = \int_{\partial \Omega} t^T_{j}(y) G_{ij}(y-x) dA_y,$$

(9)

where $t^T$ is the misfit traction, defined as $t^T_{ij} = C_{ijkl} e^T_{mp} n_l$. It should be emphasized that the displacement formula (9) is valid for any point $x$ in the space, i.e., it applies regardless whether $x$ is in the matrix phase $\Omega^M$ or in the particle $\Omega^P$, or on the interface $\partial \Omega$.

Difficulty lies in finding an effective method for computing the traction $t$ on the interface.

For a point $x$ not on the interface, taking partial derivatives of Eq. (9), we obtain the gradient of the displacement
\[ u_{j,k}(\mathbf{x}) = - \int_{\partial \Omega} t^T_i(y) G_{ij,k}(y - \mathbf{x}) \, dA_y. \]  

(10)

The displacement gradient \( u_{j,k} \) is continuous in \( \Omega^p \) and \( \Omega^M \) but discontinuous across the interface \( \partial \Omega \). From Eq. (10), we obtain the stress at a point \( \mathbf{x} \) in the matrix phase \( \Omega^M \)

\[ \sigma_{lm}(\mathbf{x}) = C_{lmjk} u_{j,k}(\mathbf{x}) \]

\[ = - \int_{\partial \Omega} t^T_i(y) C_{lmjk} G_{ij,k}(y - \mathbf{x}) \, dA_y. \]  

(11)

Let \( \mathbf{z} \) denote the point on the surface such that the vector \( \mathbf{x} - \mathbf{z} \) is perpendicular to the surface. Extending the definition of the normal vector \( \mathbf{n} \) such that \( \mathbf{n}(x) = \mathbf{n}(z) \), multiplying Eq. (11) by \( \mathbf{n}(x) \) and adding the identity (8), we get

\[ \sigma_{lm}(\mathbf{x}) n_m(\mathbf{x}) = - \int_{\partial \Omega} t^T_i(y) C_{lmjk} G_{ij,k}(y - \mathbf{x}) n_m(\mathbf{x}) dA_y \]

\[ + \int_{\partial \Omega} t^T_i(\mathbf{x}) C_{lmjk} G_{ij,k}(\mathbf{y} - \mathbf{x}) n_m(\mathbf{y}) dA_y, \]

(12)

where the misfit traction \( t^T_i \) is extended into the matrix phase as \( t^T_i(x) = C_{ijkl} t^T_k n_j(x) \) and the following symmetry property is applied

\[ G_{ij}(\mathbf{y} - \mathbf{x}) = s_{ij}(\mathbf{y} - \mathbf{x}), \]

(13)

which is true for general free-space Green’s functions.

Taking the limit \( \mathbf{x} \to \mathbf{z} \), we have the expression of the traction along the interface

\[ t^T_i(\mathbf{x}) = \sigma_{lm}(\mathbf{x}) n_m(\mathbf{x}) \]

\[ = \int_{\partial \Omega} \left[ t^T_i(\mathbf{x}) n_m(\mathbf{y}) - t^T_i(\mathbf{y}) n_m(\mathbf{x}) \right] \]

\[ \times C_{lmjk} G_{ij,k}(\mathbf{y} - \mathbf{x}) dA_y \]

\[ = \int_{\partial \Omega} \left[ t^T_i(\mathbf{x}) n_m(\mathbf{y}) - t^T_i(\mathbf{y}) n_m(\mathbf{x}) \right] \]

\[ \times T_{lm}(\mathbf{y} - \mathbf{x}) dA_y, \]

(14)

for a point \( \mathbf{x} \) on \( \partial \Omega \). In the last expression, the corresponding Green’s functions associated with the stress \( T \) is defined as

\[ T_{ijk}(\mathbf{x}) = C_{ikmp} G_{jm,p}(\mathbf{x}). \]

(15)

If \( \partial \Omega \) is \( C^2 \)-smooth, i.e. the normal \( \mathbf{n} \) to the interface has continuous derivative, then \( [t^T_i(\mathbf{x}) n_m(\mathbf{y}) - t^T_i(\mathbf{y}) n_m(\mathbf{x})] \leq C_1 |x - y| \). Since the leading-order singularity in \( T_{ijk}(\mathbf{x}) \) is of \( O(|x|^{-2}) \), the integral in (14) is weakly singular for a smooth surface. It is interesting to note that, in the classic boundary integral formulation, it is necessary to find the explicit expression of the limit of \( \int_{\partial \Omega} t^T_i(\mathbf{y}) T_{lm}(\mathbf{y} - \mathbf{x}) dA_y \) as \( \mathbf{x} \) tends to \( \partial \Omega \). This approach has been successfully carried out for two-dimensional orthotropic elasticity and three-dimensional isotropic elasticity [2,3,21]. However, to author’s knowledge, the limit process is not available for general anisotropic elasticity in two or three dimensions.

The formulas (9) and (14) are used to compute the displacement and the traction on the interface respectively. Note that only evaluation of weakly singular surface integrals is involved in obtaining the unknowns \( \mathbf{u} \) and \( \mathbf{t} \). The components of the strain and stress tensors on both sides of the interface, \( \epsilon_{ij}^+ \) and \( \sigma_{ij}^+ \) for \( \chi = M, P, \) can be obtained from the knowledge of \( \mathbf{u} \) and \( \mathbf{t} \) by using the constitutive relations between the strain and the stress. The procedure is presented in Appendix A, which is an extension to that described in [7,14] for the two-dimensional case. Then, the elastic energy density \( g^\text{el} \) is computed by Eq. (4).

4. Numerical methods

In this section, we outline the main steps in simulating the evolution of the microstructure, and present the numerical algorithms for solving the elasticity problem in detail. For the rest of the details, we refer to the earlier work [11].

In the sharp interface model, depicted in Fig. 1, the entire microstructure is determined by the shape or location of the interface between the matrix and the precipitate phases. Since the interface is evolving in time, it’s impossible to have an analytical expression for the surface after the initial instant. At any time, we define a surface by the location of a set of the marker points, identified with the vertices \( \{ \forall, k = 1, 2, \ldots, N_\ell \} \) of its triangularization \( \mathcal{T} = \{ \hat{\Omega}_1, \ldots, \hat{\Omega}_N \} \). At a given time-
step, to evolve the surface, we first evaluate the surface integrals in the expressions for the displacement and the traction, Eqs. (9) and (14) at each marker point. Then, we calculate the elastic energy density $\tilde{g}^d$ in (4) and the right-hand-side of the integral equation (6) for normal velocity $n_m$. The dense linear system arising from the discretized integral equation (6) is solved by the iterative method GMRES. The solution, the normal velocity at each marker point, of the previous time-step provides the initial guess for the GMRES solver. Once the normal velocity at each marker point is available, the marker points are advanced according to the ordinary differential equation (5) using a second-order Runge–Kutta method. The process is repeated at the next time-step. Since the shape of precipitate can change substantially during its evolution, an adaptive mesh algorithm [22,23] is used for accurate and efficient simulations.

4.1. Approximation of the surface and quantities on the surface

At any instant, the interface $\partial \Omega$ between the phases is partitioned into a set of disjoint triangular elements $\{\Delta_k\}$, $\partial \Omega \approx \tilde{S} \equiv \bigcup_{k=1}^{N} \Delta_k$, and each triangular element $\Delta_k$ is traced by the six nodal points $\{x_{k,i}, i = 1, \ldots, 6\}$. As depicted in Fig. 2, the position of a point on the triangle $\Delta_k$ is obtained through quadratic polynomial interpolation $\tilde{m}_k$, a mapping from the unit simplex to a triangular patch on the interface, defined by

$$\tilde{m}_k : \{s, t\} \in \omega \rightarrow x_k(s, t) = \sum_{c=1}^6 x_{k,c} l_c(s, t) \in \tilde{\Delta}_k,$$

(16)

where $\{l_c(s, t)\}$ are the Lagrange basis functions with respect to the six nodes, $\omega$ is the unit simplex $\omega = \{(s, t)|s, t \geq 0, s + t \leq 1\}$, $\{q_c\}$ and $\{x_{k,c}\}, c = 1, \ldots, 6$, are respectively the six nodal points on the simplex $\omega$ and the triangle $\Delta_k$. Variables on the interface are approximated in a similar fashion. For example, a scalar surface quantity $g(y)$ is approximated by

$$g(y) \approx \sum_{c=1}^6 g(\tilde{m}_k(q_c)) l_c(s, t)$$

$$= \sum_{c=1}^6 g(x_{k,c}) l_c(s, t), \quad (s, t) \in \omega,$$

(17)

for a point $y$ on the triangle $\tilde{\Delta}_k$.

4.2. Evaluation of the traction $\mathbf{t}$

The evaluation techniques for the unknowns $\mathbf{u}$ and $\mathbf{t}$ are similar and we describe the methods for calculating $\mathbf{t}$, or equivalently the weakly singular surface integral in (14), as an example.

Since the kernel $T$ is singular when $x = y$, we divide the triangulation of the surface $\mathcal{F}$ into two sets: $\mathcal{F}(x)$, the set of triangles containing the point $x$, and $\mathcal{F}(x)$, the rest of the triangles. Then,

$$t_l(x) = \sum_{\tilde{\Delta}_k \in \mathcal{F}(x)} I_l^{(k)}(x) + \sum_{\tilde{\Delta}_k \in \mathcal{F}(x)} T_l^{(k)}(x),$$

(18)

where $I_l^{(k)}(x)$ and $T_l^{(k)}(x)$ are the surface integral over the $k$th triangle $\tilde{\Delta}_k$ depending on whether $\tilde{\Delta}_k \in \mathcal{F}(x)$ or $\bar{\mathcal{F}}(x)$, defined by

$$I_l^{(k)}(x) = \int_{\tilde{\Delta}_k} \left[ T_l^T(x)n_m(y) - T_l^T(y)n_m(x) \right]$$

$$\times T_{lim}(y - x) \, dA_s.$$

(19)

Recall that the variables on the surface are approximated as in Eq. (17). If the point $x$ is not on $\tilde{\Delta}_k$, transforming the integration on the element $\Delta_k$ onto the unit simplex $\omega$, the non-singular integrals are integrated as
\[ T_i^{(k)}(x) \approx \sum_{c=1}^{6} \left[ I_i^T(x)n_m(x_{k,c}) - I_i^T(x_{k,c})n_m(x) \right] \]
\[ \int \int_{\Omega} I_i(s,t)T_{im}(\tilde{m}_k(s,t) - x)|D_s\tilde{m}_k \]
\[ \times |D_s\tilde{m}_k|ds\,dt, \]  
(20)

where \(|D_s\tilde{m}_k \times D_s\tilde{m}_k|\) is the Jacobian of the mapping \(\tilde{m}_k\) defined in Eq. (16), and \(D_sx_k\) and \(D_sx_k\) are partial derivatives with respect to \(s\) and \(t\), respectively. The integral in Eq. (20) is numerically integrated using a 7-point quadrature over the unit simplic \(\omega\) from [24], which can be derived using orthogonal polynomials in two variables and has degree of precision equal to five.

If the point \(x\) is on \(\tilde{\Delta}_k\), we decompose the integrand
\[ I_i^T(x)n_m(y) - I_i^T(y)n_m(x) \]
\[ = I_i^T(x)[n_m(y) - n_m(x)] + [I_i^T(x) - I_i^T(y)]n_m(x) \]
\[ = I_i^T(x) \left[ \sum_{c=1}^{6} l_c(s,t)n_m(x_{k,c}) \right] - n_m(x) \left[ \sum_{c=1}^{6} l_c(s,t)I_i^T(x_{k,c}) \right] \]
\[ - n_m(x) \left[ \sum_{c=1}^{6} l_c(s,t)I_i^T(x_{k,c}) - \sum_{c=1}^{6} l_c(s,t)I_i^T(x_k) \right] \]
\[ = \sum_{c=1}^{6} \left[ I_i^T(x)n_m(x_{k,c}) - I_i^T(x_{k,c})n_m(x) \right] \]
\[ \times [l_c(s,t) - l_c(s_t,t)], \]  
(21)

where we have applied the identity \(g(x) = \sum_{c=1}^{6} l_c(s,t)g(x_{k,c})\) when \(x\) is one of the six nodal points \(x_{k,c}\) \(c = 1, \ldots, 6, k = 1, \ldots, N\) is a function of the number of triangular elements on the interface, \(N\), or the dimension of each triangular mesh, \(h\).

Consider a spherical precipitate of radius one in infinite matrix, purely dilatational misfit \(\epsilon = \text{diag}(1,1,1)\) and isotropic elasticity with the shear modulus \(\mu = 1\) and the Poisson’s ratio \(\nu = 1/4\). In Table 1, we compare our numerical values of \(g^{el}\) with the exact solution \(g^{el} = 10/3\) obtained from Mura [20]. The spherical surface is partitioned into \(N\) second-order triangular elements and the corresponding dimension of each equal-sized element is denoted by \(h\). As \(h\) decreases, the results in the table show that the order of convergence for \(g^{el}\) is between \(O(h^3)\) and \(O(h^4)\), closer to \(O(h^4)\).

5.2. Evolution of precipitate morphology

We consider an isolated precipitate with cubic elasticity in an infinite matrix with the same elastic stiffness tensor. The Voigt matrix for the elastic tensor has three independent non-zero elements: \(c_{11} = 1.98, c_{12} = 1.18\) and \(c_{44} = 1\), corresponding to pure nickel, the misfit between the two phases.
is dilatational, and the kinetic coefficient $\lambda$ is set to be 0.1.

When the net mass flux $J$ into the precipitate vanishes, the stable equilibrium shape of an isolated particle depends on the magnitude of elastic energy relative to the surface energy characterized by the “particle size” $L$. Similar to the corresponding two-dimensional system [13], for small values of $L$, the stable equilibrium shape has the higher symmetry (cubic); there exists a bifurcation point $L_c$ beyond which there exists stable equilibrium shape with the lower symmetry (tetragonal) [15]. For the three-dimensional homogeneous nickel-based system, denoted by [Ni–Ni], the estimated value of the bifurcation point $L_c$ fall in the range $3 < L_c < 4$ [15]. Here, we investigate the dynamics of the precipitates and the stability of the equilibrium shapes at different values of $L$.

Fig. 3 shows two time sequences of the precipitate shapes when the effect of elastic stress is relatively small, $L = 2.5$. The time sequence of the $y$–$z$ plane cross sections of the precipitate, as shown in Fig. 3(a), demonstrates that an initially spherical precipitate stretches along the elastically hard $\langle 111 \rangle$ directions and shrinks along the elastically soft $\langle 100 \rangle$ directions, where $\langle \rangle$ denotes all the symmetry-equivalent crystallographic directions. At dimensionless time $t = 0.036$, the precipitate reaches an equilibrium shape of cubic symmetry, shown in Fig. 3(b), where the regions that are perpendicular to the soft $\langle 100 \rangle$ directions are flatter and the curvature reaches the maximum along the hard $\langle 111 \rangle$ directions. During the evolution, the precipitate retains cubic symmetry and its cross sections in all coordinate planes are identical.

To find the stability of the equilibrium shape with cubic symmetry, Fig. 3(d) shows another time sequence of the $y$–$z$ plane cross sections starting from a perturbed shape with lower symmetry (tetragonal) displayed in Fig. 3(c). Initially, the dimension along the shorter side of the plate-like shape expands as well as the dimensions along the other two axes as demonstrated by the cross section (the dashed line) at $t = 0.035$. Then, the dimensions perpendicular to the shorter side slowly decreases while the length of the shorter side increases, and finally at $t = 2.494$ it reaches the same cubically symmetric equilibrium shape evolved from a unit sphere (Fig. 3(b)). The result illustrates that the equilibrium shape with cubic symmetry is stable for $L < L_c$. The time it takes for the precipitate to reach the equilibrium from the perturbed tetragonal shape is more than 60 times longer than it does from the highly symmetric spherical shape. Experimentally, it implies that, if the initial shape of the precipitate has a lower symmetry than cubic and the effect of elasticity is sufficiently small, obtaining the equilibrium shape might take a long time [12].

We turn to investigate the evolution of a precipitate when elastic effect is stronger at $L = 5$ which is larger than $L_c$. Starting from the spherical shape, the precipitate reaches an equilibrium shape of cubic symmetry as shown in Fig. 4(a) at $t = 0.110$. A time sequence of the cross sections in the $y$–$z$ plane is shown in Fig. 4(b). Comparing with the corresponding equilibrium shape at $L = 2.5$, flatter facets form perpendicular to the elastically soft directions $\langle 100 \rangle$, and the edges and the corners of the cubic symmetric precipitate are sharper. As an indication of the shape geometry, we measure the particle diameters along the three coordinate axes, denoted by $d_x$, $d_y$, and $d_z$. When the coordinate planes are aligned with the symmetry planes, the values of $d_x$, $d_y$, and $d_z$ are equal to 1.720 and 1.812 for cubic symmetry equilibrium shapes at $L = 5$ and 2.5 respectively. Here we note that, in our numerical simulations, we have not taken advantage of the symmetries of the physical shape of the precipitate, and the adaptive surface mesh [22] on the precipitate is not symmetric with respect to

<table>
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<th>$N$</th>
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<th>500</th>
<th>720</th>
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<tr>
<td>Error $E_g$</td>
<td>$2.6 \times 10^{-2}$</td>
<td>$5.7 \times 10^{-3}$</td>
<td>$2.0 \times 10^{-3}$</td>
<td>$9.1 \times 10^{-4}$</td>
<td>$5.0 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Table 1
The rate of convergence for evaluating the elastic energy density $g^e$, shown by the maximum error $E_g$ as functions of the number of triangles $N$ and the size of the triangles $h$.
any planes. Consequently, small-amplitude asymmetric perturbations are always present during the evolution, due to the existence of numerical errors and the non-symmetric surface meshes. This implies that, at $L = 5 > L_c$, the cubic symmetric equilibrium shape in Fig. 4(a) is stable with respect to small perturbations.

The equilibrium shape in Fig. 4(a) is unstable to larger disturbances with a lower symmetry. Starting with the perturbed shape of a rectangular parallelepiped ($d_x:d_y:d_z = 1.720:1.746:1.672$), we obtain an equilibrium shape with tetragonal symmetry as shown in Fig. 4(c). A time sequence of the precipitate sliced through the $y-z$ plane is shown in Fig. 4(d). It takes dimensionless time $t = 0.917$ to reach the steady state, an order of magnitude longer than the previous evolution from the unit sphere to cubic symmetric equilibrium shape. The dimensions of the equilibrium shape are given by $d_x:d_y:d_z = 2.402:2.402:0.884$. Thus, we have shown through dynamic simulations, between the two equilibrium shapes, the
one with the lower symmetry (Fig. 4(c)) is more stable than that with the higher symmetry (Fig. 4(a)). Furthermore, the non-dimensional total energy $W_{\text{tot}}$ defined in (5) for the configuration with the tetragonal symmetry is 63.633, which is smaller than 64.010 for the cubic symmetric configuration. Though the difference in total energy appears to be small, it is significant because $W_{\text{tot}}$ is a weak function of the geometry for a fixed-size particle. For example, $W_{\text{tot}} = 65.124$ for the configuration of the unit sphere at $L = 5$, which is comparable to the previous two values.

Finally, further numerical simulations (not shown here) demonstrate that, for $4 \leq L \leq 6$, the equilibrium shapes keep the same properties: there are two kinds of stable equilibrium shapes; the first kind has the cubic symmetry and is metastable, and the other has the tetragonal symmetry and is more stable than the first. The result suggests that the behavior of equilibrium shapes hold for a range of values $L$ beyond the bifurcation point. Whether it remains true for much larger values of $L$ is beyond the scope of this work and will be investigated in future.
6. Conclusions

We have shown that the elasticity problem for homogeneous inclusion can be solved by surface integration only, instead of solving integral equations required for inhomogeneous systems. The integrals in the expressions for the displacement and traction are weakly singular and can be integrated accurately with a coordinate transformation. We have presented numerical methods for approximating an evolving surface of arbitrary shape using second-order triangular elements and for numerically integrating singular integrals on such surfaces.

As an application, we have investigated the dynamics of a precipitate in an infinite matrix using the efficient scheme described in this work. When the precipitate volume is conserved, the equilibrium configuration depends on the “particle size” $L$. Assuming the elasticity is cubic, we find that there is a unique equilibrium shape of cubic symmetry for small values of $L$; there are at least two kinds of equilibrium shapes for a range of values of $L$ larger than a critical value $L_c$, one with cubic symmetry and one with tetragonal symmetry (plate-like). More importantly, using dynamical simulations, we find that, for these values of $L$ greater than $L_c$, the equilibrium state with the higher symmetry (cubic) is metastable, but the one with the lower symmetry (tetragonal) is more stable and has smaller total energy. Further, for $L > L_c$, the times required to evolve to the two equilibrium shapes are different: it takes much longer time to evolve to the tetragonal symmetric equilibrium shape than it does from a spherical particle to the cubic symmetric equilibrium shape. It indicates that cubic symmetric shapes might be easier to be observed than those of lower symmetry in physical experiments.

Acknowledgements

The author would like thank Vittorio Cristini for providing the adaptive surface mesh package for this research, and Peter Voorhees and John Lowengrub for valuable discussions. The numerical simulations were done on a Beowulf clusters acquired with the help of NSF-SCREMS funding at the Illinois Institute of Technology.

Appendix A. Computation of the elastic energy density

The boundary condition (2) for the diffusion equations requires the knowledge of the elastic energy density $\varepsilon^{el}$. To compute the elastic energy density $\varepsilon^{el}$ defined in (4), we need all components of the stress and strain tensors, $\sigma$ and $\varepsilon$, on both sides of the interface.

At a point $x$ on the interface $\partial \Omega$, we introduce a new Cartesian coordinate, denoted by $(x_1', x_2', x_3')$, which consists of two mutually perpendicular tangent vectors $e_1', e_2'$ and the normal vector $e_3'$ to the interface at the point $x$. The original coordinate system is denoted by $(x_1, x_2, x_3)$. The stress and strain tensors can be obtained from the displacement $u$ and the traction $t$, given by surface integrals (9) and (14). To illustrate, we consider the tensors on the matrix side and omit the superscript $M$.

First, three components of the stress tensor $\sigma_{i3}, \sigma_{23}, \sigma_{33}$ and three components of strain tensor $\varepsilon_{11}, \varepsilon_{12}, \varepsilon_{22}$ can be written explicitly in terms of $u$ and $t$ in the original coordinates as

$$\sigma'_{i3} = t_i, \quad i = 1, 2, 3, \quad (A.1)$$

and

$$\varepsilon'_{ij} = u'_{ij} = \frac{\partial (u \cdot e_j)}{\partial x_i} = \frac{\partial u}{\partial x_i} e_j', \quad i = 1, 2, \quad (A.2)$$

$$\varepsilon'_{12} = \frac{1}{2} \left( u'_{12} + u'_{21} \right) = \frac{1}{2} \left( \frac{\partial u}{\partial x_1} e_2' + \frac{\partial u}{\partial x_2} e_1' \right), \quad (A.3)$$

where

$$u'_i = u \cdot e_i', \quad t'_i = t \cdot e_i', \quad i = 1, 2, 3. \quad (A.4)$$

Second, because the stress and strain tensors are symmetric, the remaining 6 components of the stress and strain can be solved from the following linear system,

$$\sigma'_{ij} = C'_{ijkl} \varepsilon'_{kl}, \quad i, j = 1, 2, 3, \quad (A.5)$$
where \( C'_{ijkl} \) are the elastic constants in \((x'_1, x'_2, x'_3)\)-coordinate. The relation between the constants \( C'_{ijkl} \) and \( C_{ijkl} \) is given by
\[
C'_{mnrs} = a_{im}a_{jm}a_{kr}a_{ls}C_{ijkl},
\]
where \( 3 \times 3 \) matrix \((a_{ij})\) are the directional cosines of the new axes with respect of the original axes [25]
\[
A = (a_{ij}) = \begin{bmatrix}
\cos \theta_{11} & \cos \theta_{12} & \cos \theta_{13} \\
\cos \theta_{21} & \cos \theta_{22} & \cos \theta_{23} \\
\cos \theta_{31} & \cos \theta_{32} & \cos \theta_{33}
\end{bmatrix}.
\]
The columns of the transformation matrix are the direction cosines of the new axes
\[
\cos \theta_{ij} = e_i \cdot e'_j,
\]
where \( \{e_i\} \) are unit vectors of the original axes and \( e'_j \) is the unit vector in the direction of new axis \( x'_j \).
Finally, the value of \( g^{el} \) is independent of coordinate system and is calculated according to the formula (4) in the new coordinates.

References