

Periodic Inclusion—Matrix Microstructures with Constant Field Inclusions

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We find a class of special microstructures consisting of a periodic array of inclusions, with the special property that constant magnetization (or eigenstrain) of the inclusion implies constant magnetic field (or strain) in the inclusion. The resulting inclusions, which we term E-inclusions, have the same property in a finite periodic domain as ellipsoids have in infinite space. The E-inclusions are found by mapping the magnetostatic or elasticity equations to a constrained minimization problem known as a free-boundary obstacle problem. By solving this minimization problem, we can construct families of E-inclusions with any prescribed volume fraction between zero and one. In two dimensions, our results coincide with the microstructures first introduced by Vigdergauz,^[1,2] while in three dimensions, we introduce a numerical method to calculate E-inclusions. E-inclusions extend the important role of ellipsoids in calculations concerning phase transformations and composite materials.

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I. INTRODUCTION

ELLIPSOIDS are widely used in micromagnetics and elasticity because they have the property that, given a uniformly magnetized/prestrained ellipsoid in three dimensions, the induced magnetic/strain field is uniform inside the ellipsoid. This property was identified by Poisson in 1826 in the context of partial differential equations,^[3] by Maxwell in 1873 for magnetics,^[4] and by Eshelby in 1957 for inclusions in linear elasticity.^[5,6] Because the induced field in ellipsoids is uniform, they play a central role in micromagnetics,^[7–10] the theory of composite materials,^[11,12] and micromechanics and phase transformation problems.^[6,13]

Motivated by the usefulness of ellipsoidal regions, we consider their periodic generalization, which we call E-inclusions. The terminology “E-inclusions” refers to three associations: (1) they can be parameterized by elliptic functions in two dimensions (Eq. [12]) and probably can also be parameterized by elliptic functions in three dimensions; (2) they are a generalization of ellipsoids, and, conversely, ellipsoids can be regarded as the limit of these special E-inclusions as the volume fraction goes to zero; and (3) this study was motivated by the Eshelby inclusion problem. The E-inclusions are characterized by a Bravais lattice, which determines their periodic arrangement in space, and by a semipositive definite matrix, which determines their shape.

We prove the existence of E-inclusions by mapping the micromagnetics/elasticity problem to a constrained

minimization problem known as a free-boundary obstacle problem. That is, we extremize a particular energy functional, where allowable functions are either above or touching a given function. This given function is subsequently referred to as the obstacle. With this formulation, we can show that for a piecewise quadratic obstacle, regions where the minimizer touches the obstacle define the E-inclusions. The existence of E-inclusions follows from the existence of minimizers for this variational inequality, which is proven by adapting existence theorems of Friedman^[14] and Caffarelli.^[15]

After we prove the existence of E-inclusions, we give examples in both two and three dimensions. In fact, the existence of E-inclusions has already been proven in the two-dimensional (2-D) case by Vigdergauz,^[1,2] this is now referred to as the Vigdergauz construction. Grabovsky and Kohn^[17] subsequently found an analytic solution of these inclusions and proved that they are in fact energy-minimizing structures for two-phase composites. In three dimensions, we have developed a numerical method to calculate E-inclusions by using generalized ellipsoids. We have as yet been unable to find an analytical solution for three-dimensional (3-D) E-inclusions, though we suspect that such a solution would involve elliptic functions.

The article is organized as follows. In Section II, we sketch the mathematical arguments leading to the existence of E-inclusions. We present the results in terms of the micromagnetics problem, which involves finding a scalar field (the magnetic potential). The corresponding elasticity problem involves a vector field (the displacement) and is more complicated. We can show that our results for the magnetics case apply to the isotropic elasticity case and we expect that they apply more generally. We give results without formal proofs (these can be found in Reference 16). In section III, we show examples of E-inclusions for different cases. Finally, in Section IV, we discuss our results and propose some applications.

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II. MATHEMATICAL ANALYSIS

Consider a Bravais lattice \mathcal{L} described by lattice vectors $\mathbf{e}_1, \dots, \mathbf{e}_2 \in \mathbb{R}^n$ ($n = 2, 3$). Given a particular unit cell Y for the lattice, we are interested in calculating the magnetic field induced by a region Ω contained in Y with prescribed magnetization $\mathbf{m} \in \mathbb{R}^n$. This field satisfies the Maxwell's equation:

$$\operatorname{div} [\nabla u_{\mathbf{m}}(\mathbf{y}) + \mathbf{m}\chi_{\Omega}(\mathbf{y})] = 0 \quad \text{in } Y \quad [1]$$

where $u_{\mathbf{m}}$ is the magnetic potential and χ_{Ω} is the characteristic function for Ω (so $\chi_{\Omega}(\mathbf{y}) = 1$ for $\mathbf{y} \in \Omega$ and zero otherwise). For completeness, we note that the corresponding equation for elasticity can be written as

$$\operatorname{div} [\mathbf{L}\nabla \mathbf{u} + \mathbf{P}\chi_{\Omega}] = 0 \quad \text{in } Y \quad [2]$$

where \mathbf{u} is the (vector) displacement field, \mathbf{L} is the elastic stiffness tensor, and \mathbf{P} is the eigenstress. Note that appropriate boundary conditions on the boundary of Y (e.g., periodic boundary conditions) are needed in order to solve Eqs. [1] and [2].

In terms of Eqs. [1] and [2], the special property of ellipsoids is that for $Y = \mathbb{R}^n$, uniform magnetization or eigenstress on ellipsoidal regions Ω induce uniform magnetic field or strain field in Ω . Roughly speaking, then, an E-inclusion is a region Ω in a unit cell Y with the same property. More formally, we state that the region Ω is a periodic E-inclusion associated with lattice \mathcal{L} if the overdetermined problem

$$\begin{cases} \operatorname{div}[\nabla u_{\mathbf{m}}(\mathbf{y}) + \mathbf{m}\chi_{\Omega}(\mathbf{y})] = 0 & \text{in } Y \\ \nabla u_{\mathbf{m}}(\mathbf{y}) = \text{const.} & \text{in } \Omega \\ \text{periodic boundary conditions on } \partial Y \end{cases} \quad [3]$$

has a solution for all $\mathbf{m} \in \mathbb{R}^n$

In order to make progress, it is convenient to pose the governing problem for E-inclusions in its simplest mathematical form:

$$\begin{cases} \Delta u = \theta - \chi_{\Omega} & \text{in } Y \\ \nabla \nabla u = -(1 - \theta)\mathbf{Q} & \text{in } \Omega \\ \text{periodic boundary conditions on } \partial Y \end{cases} \quad [4]$$

where \mathbf{Q} is a constant semipositive definite $n \times n$ matrix with trace $\operatorname{tr}(\mathbf{Q}) = 1$, and $\theta = |\Omega|/|Y|$ is the volume fraction of region Ω in unit cell Y . The matrix \mathbf{Q} sets the shape of the E-inclusion. The equivalence of Eqs. [3] and [4] can be seen by writing Eq. [4] in its weak or integral form:

$$\int_Y [\nabla u(\mathbf{y}) \cdot \nabla v(\mathbf{y}) + (\theta - \chi_{\Omega})v(\mathbf{y})] d\mathbf{y} = 0 \quad [5]$$

for all smooth functions v that are periodic in Y . Noting that for any $\mathbf{m} \in \mathbb{R}^n$, $\mathbf{m} \cdot \nabla v$ is a smooth periodic function in Y , we can replace v by $-\mathbf{m} \cdot \nabla v$ and integrate by parts to get

$$\begin{aligned} & \int_Y (\nabla u_{\mathbf{m}} + \chi_{\Omega}\mathbf{m} - \theta\mathbf{m}) \cdot \nabla v d\mathbf{y} \\ & = \int_Y (\nabla u_{\mathbf{m}} + \chi_{\Omega}\mathbf{m}) \cdot \nabla v d\mathbf{y} = 0 \end{aligned} \quad [6]$$

where we set $u_{\mathbf{m}} = \mathbf{m} \cdot \nabla u$. Equation [6] is exactly the weak or integral formulation of the first Eq. [3]; the second equation is clear from the definition of $u_{\mathbf{m}}$. Hence, from the uniqueness of the solution of Eq. [1], we conclude that $u_{\mathbf{m}} = \mathbf{m} \cdot \nabla u$. We also remark that if we take $v = u_{\mathbf{m}}$ in Eq. [5], we can conclude that \mathbf{Q} is semi-positive-definite, while the fact that \mathbf{Q} has a unit trace is easily seen by taking the trace of the second equation in problem [4].

A. Periodic Free-Boundary Obstacle Problem

To prove the existence of E-inclusions, we turn to a constrained minimization problem, also known as a *free-boundary obstacle problem* or *variational inequality problem* (References 14, 15, and 18):

$$G_f(u_f) \equiv \min_{v \in K_{\text{per}}} \left\{ G_f(v) \equiv \int_Y \left[\frac{1}{2} |\nabla v|^2 + f v \right] d\mathbf{y} \right\} \quad [7]$$

where the constant $f > 0$, and the admissible set K_{per} consists of periodic integrable functions (more precisely, periodic $W^{1,2}(Y)$ functions) v with $v \geq \phi_p$. The *obstacle* ϕ_p is a periodic continuous function; admissible functions v must be either on or above this obstacle.

The minimizer u_f is called the solution of the minimization problem [7]. The existence and uniqueness of the solution of problem [7] has been well established (Reference 14). Further, one can show that if the solution u_f is smooth enough, then it necessarily satisfies the Euler-Lagrange conditions:

$$\begin{aligned} & -\Delta u + f \geq 0, \quad u \geq \phi_p, \text{ and} \\ & (-\Delta u + f)(u - \phi_p) = 0 \quad \text{on } \mathbb{R}^n. \end{aligned} \quad [8]$$

Equation [8] can be used to show the equivalence between the minimization problem [7] and the E-inclusion problem [4]. Define a coincident or touching set Ω^f as the set in Y where the solution $u_f(\mathbf{y}) = \phi_p(\mathbf{y})$; similarly define the noncoincident set N^f as the set where $u_f(\mathbf{y}) > \phi_p(\mathbf{y})$. It is straightforward to extend these sets periodically. Then, the third Euler-Lagrange equation implies that $\Delta u_f = f$ in N^f and $u_f = \phi_p$ in Ω^f . Alternatively,

$$\begin{cases} \Delta u_f = f\chi_{\Omega^f} + \chi_{\Omega^f} \Delta \phi_p & \text{in } Y \\ \nabla \nabla u_f(\mathbf{x}) = \nabla \nabla \phi_p(\mathbf{x}) & \text{in } \Omega^f \\ \text{periodic boundary conditions on } \partial Y \end{cases} \quad [9]$$

where χ_{Ω^f} is the characteristic function of the noncoincident set. If the obstacle $\phi_p(\mathbf{x})$ is chosen to be a periodic continuous function that coincides with a quadratic polynomial on the unit cell Y , then the solution of problem [9] also solves the overdetermined problem [4] within a multiplicative constant. Therefore, finding a solution of the overdetermined problem [3] or [4] is equivalent to solving the minimization problem [7] for a piecewise quadratic obstacle.

We now give the main mathematical result of the paper; a full proof is given in Reference 16.

Theorem 1: Let u_f be the solution of problem [7] with respect to the obstacle:

$$\phi_p(\mathbf{x}) = \max \left\{ -\frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}(\mathbf{x} + \mathbf{r}) : \mathbf{r} \in \mathcal{L} \right\}$$

where \mathbf{Q} is a semi-positive-definite matrix and trace $\text{tr}(\mathbf{Q}) = 1$, and let Ω^f be the coincident set of all \mathbf{x} in Y such that $u_f(\mathbf{x}) = \phi_p(\mathbf{x})$. For any $f \in (0, \infty)$, then

- (1) Ω^f is an E-inclusion,
- (2) $\Omega^f \subset \mathbb{R}^n$ is a convex region and its boundary is an analytic surface, and
- (3) the volume fraction $\theta = |\Omega^f|/|Y|$ of the E-inclusion is given by $\theta = f/(1 + f)$.

III. EXAMPLES OF E-INCLUSIONS

We now consider some examples of E-inclusions in both two and three dimensions. From the discussion in Section II, the choice of parameters we have to change the shape of the E-inclusions includes the lattice \mathcal{L} or the unit cell Y , the matrix \mathbf{Q} specifying the quadratic obstacle, and the volume fraction θ of the inclusion phase.

A. Two-Dimensions: Vigdergauz Microstructure

The existence of E-inclusions for rectangular cells in two dimensions was first proved by Vigdergauz.^[1,2] Grabovsky and Kohn^[17] found a corresponding analytic solution for these ‘‘Vigdergauz microstructures.’’ Here, we present a formula to calculate E-inclusions for rectangular lattices (References 17 and 16 provide details).

Consider a rectangular lattice \mathcal{L} with unit cell $[-c_x, c_x] \times [-c_y, c_y]$, and choose the half lengths a_x and a_y of the E-inclusion projected on the x -axis and y -axis, respectively. We explicitly parameterize an E-inclusion by using the incomplete elliptic integral of the first kind:

$$F[x, m] = \int_0^x \frac{1}{(1-t^2)(1-m^2t^2)} dt$$

and the complete elliptic integral of the first kind, $K[m] = F[1, m]$ (Reference 20). We first solve the equations

$$\begin{cases} c_x = a_x + a_y K[1 - m_y]/K[m_y] \\ c_y = a_x K[1 - m_x]/K[m_x] + a_y \end{cases} \quad [10]$$

to find values m_x and m_y between zero and one. Using these values, we compute a curve of dummy variables x' and y' satisfying

$$(1 - (x')^2)(1 - (y')^2) = M \quad [11]$$

where $M = (1 - m_x)(1 - m_y)/(m_x m_y)$ is between zero and one, and we choose the branch of the curve with $x', y' \in [-\sqrt{1-M}, \sqrt{1-M}]$. The curve (x, y) describing the boundary of an E-inclusion is then computed from the curve (x', y') through the mapping

$$\begin{cases} x = \frac{a_x}{K[m_x]} F[x', m_x] \\ y = \frac{a_y}{K[m_y]} F[y', m_y] \end{cases} \quad [12]$$

With this representation, the matrix \mathbf{Q} is

$$\mathbf{Q} = \frac{1}{1 - \theta} \begin{pmatrix} 1 - a_x/c_x & 0 \\ 0 & 1 - a_y/c_y \end{pmatrix} \quad [13]$$

where the volume fraction

$$\theta = a_x/c_x + a_y/c_y - 1 \quad [14]$$

We obtain different E-inclusions by adjusting parameters a_x , a_y , c_x , and c_y . In the following, we define a relative aspect ratio,

$$r = \frac{1 - a_y/c_y}{1 - a_x/c_x} \quad [15]$$

and we take $c_y = 1$ and use c_x , r , and θ as the control variables. Figure 1 shows E-inclusions, plotted for different values of c_x with $r = 1$ and $\theta = 0.5$. Because of symmetry, we show a quarter of the E-inclusion. From left to right, the regions bounded by the curves correspond to $c_x = 0.5, 0.8, 1, 1.25,$ and 2 . Figure 2 shows E-inclusions plotted for different values of r with $\theta = 0.5$ and $c_x = 1$, *i.e.*, a square unit cell. Going from the top of the figure to the bottom, the shapes have values $r = 1/5, 1/4, 1/3, 1/2, 1, 2, 3, 4,$ and 5 . Note that

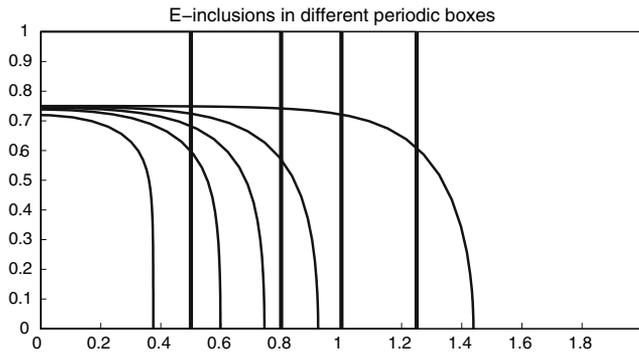


Fig. 1—E-inclusions are shown for five different unit cells. The relative aspect ratio $r = 1$ and volume fraction $\theta = 0.5$. The height of these five quarter-unit cells is fixed at 1 and their widths are 0.5, 0.8, 1, 1.25, and 2. The regions bounded by the curves are the quarter-E-inclusions.

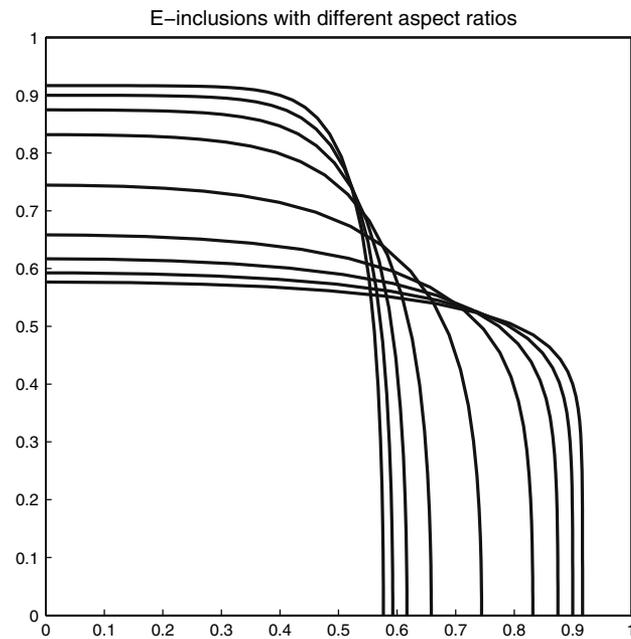


Fig. 2—E-inclusions are shown for five different relative aspect ratios r . The volume fraction $\theta = 0.5$ and the quarter-unit cell is a unit square. From top to bottom, the regions bounded by the curves are quarter-E-inclusions with $r = 1/5, 1/4, 1/3, 1/2, 1, 2, 3, 4,$ and 5 .

the shapes are all convex with smooth boundaries, consistent with Theorem 1.

Figure 3 shows E-inclusions for different volume fractions, with $c_x = 1$ and $r = 1$. The volume fractions increase from inward to outward and are $\theta = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7,$ and 0.8 . The “+” denotes numerical solutions that will be presented in Section B. As volume fraction increases, the E-inclusion moves from a circular shape to a squarish shape, consistent with a square unit cell and $r = 1$. Conversely, one can show that as the volume fraction θ tends to zero, the parameterization [12] of the E-inclusion is precisely that of an ellipse.

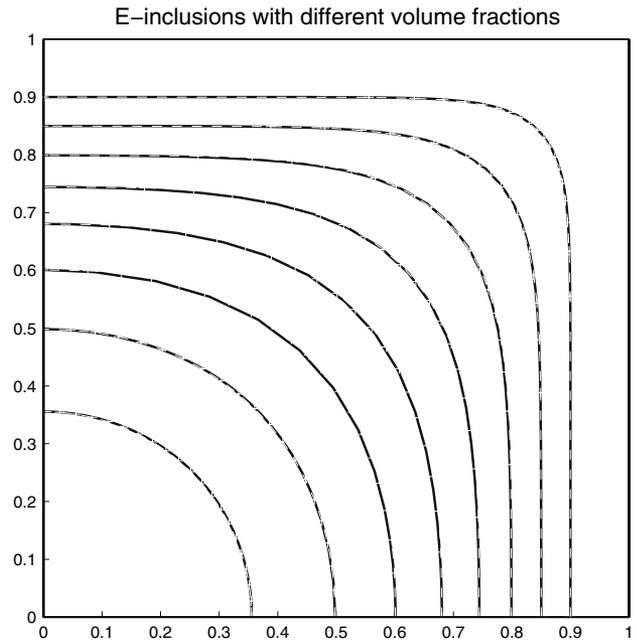


Fig. 3—E-inclusions are shown for increasing volume fractions. The relative aspect ratio $r = 1$ and the quarter-unit cell is a unit square. From inward to outward, the regions bounded by the curves are quarter E-inclusions with $\theta = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7,$ and 0.8 . The “+” symbols are numerical solutions based on generalized ellipses.

B. Three Dimensions: a Numerical Solution

In three dimensions, an analytic solution for E-inclusions is not yet available. Therefore, we have developed numerical methods to compute E-inclusions. Motivated by the 2-D results, we restrict our attention to E-inclusions with the shape of a generalized ellipsoid:

$$\Omega(l) \equiv \left\{ \mathbf{x} : \frac{x^l}{a_x^l} + \frac{y^l}{a_y^l} + \frac{z^l}{a_z^l} \leq 1 \right\} \quad [16]$$

where $l \geq 2$ because the shape must be convex. Suppose that the unit cell Y , values $a_x, a_y,$ and $a_z,$ and the volume fraction θ are given. (Note that setting the a_i values is equivalent to choosing \mathbf{Q} , e.g., Eq. [13].) Because $\nabla \nabla u$ is uniform inside an E-inclusion (Eq. [4]), we seek the optimal $l = l^*$ to minimize the standard deviation of the second derivatives of the periodic solution of $\Delta u_1(\mathbf{y}) = \theta - \chi_{\Omega(l)}$. That is, we minimize the error $s(l)$ associated with deviation from uniformity:

$$s(l^*) = \min_{l \geq 2} \left\{ s(l) \equiv \int_{\Omega(l)} \left| \nabla \nabla u_l(\mathbf{x}) - \int_{\Omega(l)} \nabla \nabla u_l(\mathbf{y}) d\mathbf{y} \right|^2 d\mathbf{x} \right\} \quad [17]$$

Note that when $l = 2$, $\Omega(l)$ is an ellipsoid. In contrast, when l becomes large, $\Omega(l)$ approaches a rectangle. Practically speaking, increasing l beyond about 15 has little effect on either $\Omega(l)$ or $s(l)$, and so, for the actual computation if $l^* > 15$, we stop the computation and take optimal l^* as $+\infty$.

We have carried out numerical computations in both two and three dimensions. We consider square or cubic unit cells and vary volume fraction of the inclusion. Numerical results show that the optimal shapes $\Omega(l^*)$ are very close to E-inclusions in the sense that $s(l^*)$ is very close to 0 (order 10^{-3}). Table I shows values for

the optimal l^* as a function of volume fraction θ in both two and three dimensions. Note that as $\theta \rightarrow 0$, $l^* \rightarrow 2$, as expected. Also note that the “+” marks in Figure 3 are calculated according to the optimal l^* listed in the second row of the table. There is excellent agreement between the exact shapes and our calculated shapes.

Calculated E-inclusions in three dimensions are shown in Figure 4. In all cases, we consider a cubic unit cell and we set $a_x = a_y = a_z$, so \mathbf{Q} is proportional to the identity matrix. The volume fraction ranges from $\theta = 0.1$ in Figure 4(a) to $\theta = 0.7$ in Figure 4(d). As in

Table I. Optimal Value of l to Minimize Deviation from Uniformity is Shown as a Function of θ in Both Two and Three Dimensions

θ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$n = 2$	2.00	2.14	2.46	2.83	3.48	4.59	6.50	10.56	$l^* \rightarrow \infty$
$N = 3$	2.14	2.64	3.03	3.73	4.92	6.75	9.50	$l^* \rightarrow \infty$	$l^* \rightarrow \infty$

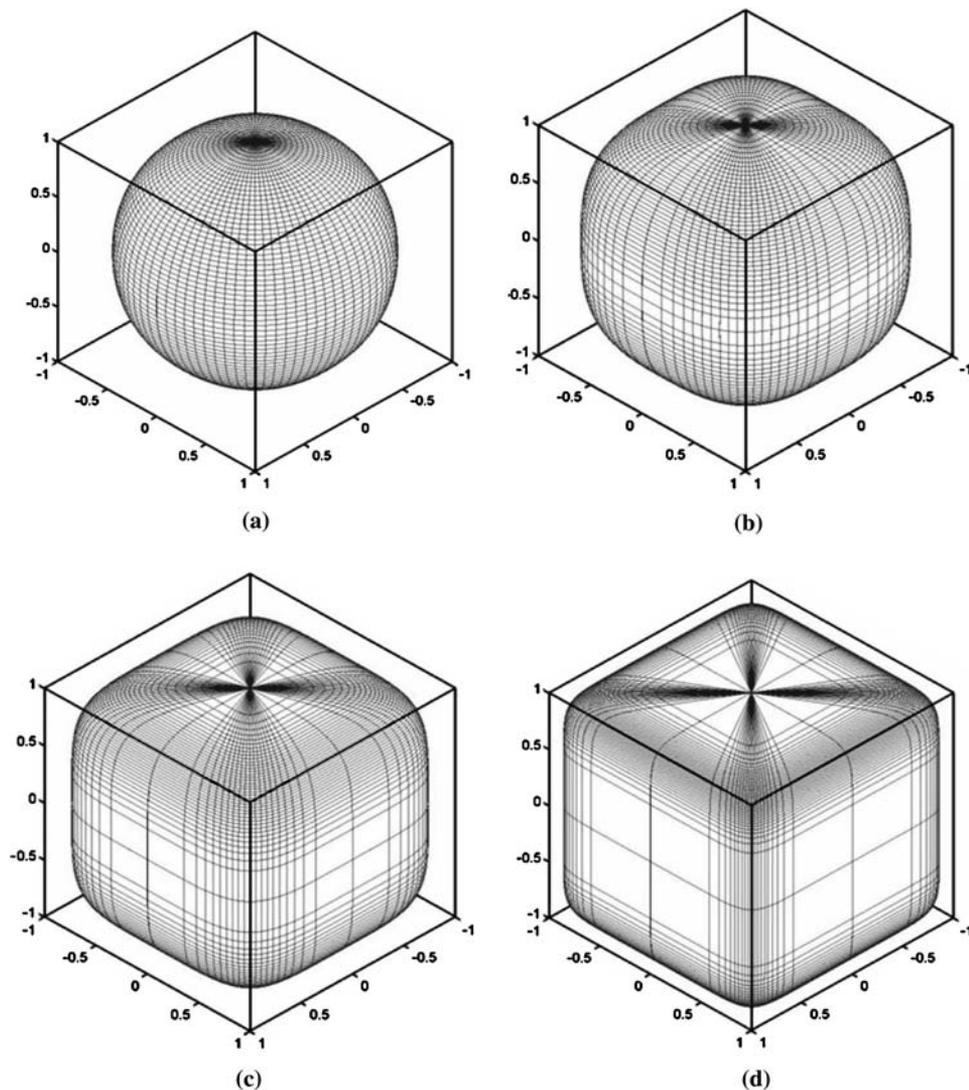


Fig. 4—A series of 3-D E-inclusions are shown for cubic symmetry and volume fractions: (a) 0.1, (b) 0.3, (c) 0.5, and (d) 0.7.

the 2-D case, the E-inclusion goes from being roughly spherical at low volume fractions to cuboidal at high volume fractions. Changing either the lattice or the ratio of the a_i will lead to roughly ellipsoidal shapes at low volume fractions and rectangular parallelepiped-like shapes at higher volume fractions.

IV. DISCUSSION

We have presented a calculation that generalizes to a periodic setting the special properties that ellipsoids possess in three dimensions. In magnetics, ellipsoids have the property that a uniformly magnetized ellipsoid induces a uniform magnetic field inside the ellipsoid. In elasticity, ellipsoids have the property that a uniform eigenstrain induces a uniform strain inside the ellipsoid. We have shown that shapes—E-inclusions—with these properties exist in a periodic setting and we have presented calculations of such shapes. Because ellipsoidal shapes are commonly used to solve micromagnetics and elasticity problems involving composite properties in the low volume fraction limit, we expect that E-inclusions may play a similar role at higher volume fractions.

Our analysis is based on the micromagnetics problem [3] or the equivalent elliptic problem [4]. It is straightforward to generalize the analysis to the elliptic equation

$$\operatorname{div}[\mathbf{A}\nabla u(\mathbf{x})] = \theta - \chi_\Omega \quad \text{in } Y$$

by a linear transformation, where \mathbf{A} is a positive definite $n \times n$ matrix. We can also extend the analysis to the elasticity case by considering the problem

$$\begin{cases} \operatorname{div}[\mathbf{L}\nabla \mathbf{u}(\mathbf{x}) + \mathbf{P}\chi_\Omega(\mathbf{x})] = 0 & \text{in } Y \\ \nabla \mathbf{u}(\mathbf{x}) = - (1 - \theta)\mathbf{R}\mathbf{P} & \text{in } \Omega \end{cases} \quad [18]$$

where \mathbf{u} is the unknown vector displacement, \mathbf{L} is the elastic stiffness tensor, \mathbf{P} is the eigenstress, and \mathbf{R} is a constant tensor analogous to the Eshelby tensor.[6] We can prove that E-inclusions exist if \mathbf{L} is the fourth-rank identity tensor, $L_{ijkl} = \delta_{ij}\delta_{kl}$. We can also show that E-inclusions exist in the important case where \mathbf{P} is proportional to the identity (a dilatational eigenstress) and \mathbf{L} is the isotropic linear elastic tensor, $L_{ijkl} = \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ij}\delta_{kl}$, with Lamé moduli μ , λ . We believe, based on both our analysis and numerical results, that E-inclusions also exist in more general cases, and we are working on a formal proof of this conjecture.

As mentioned previously, E-inclusions may play an important role in computing properties of multiphase magnetic and elastic materials. For example, one can adapt Eshelby's equivalent inclusion argument^[5,6,19] to the elasticity problem^[18] to construct solutions for inhomogeneous inclusion problems;^[10,16] this solution can be used to compute bounds on effective elastic constants for composite materials.^[11,12] In fact, we can show that E-inclusions can be used to characterize the set of *all* possible conductivity tensors of a composite, called the G_θ closure of two-phase composite

systems.^[21,16] Finally, E-inclusions can be shown to be the energy minimizing microstructure of two-phase composites.^[16] This property could have applications in magnetics, *e.g.*, to minimize loss in magnetic storage media. E-inclusions would also form a natural class of shapes to categorize equilibrium microstructures that arise in diffusional phase transformations, such as those that arise in coherent $\gamma - \gamma'$ nickel-based superalloys.^[22,23,24] In this case, one must consider the surface energy of the inclusion-matrix interfaces as well as the elastic energy of the microstructure.

We have explored E-inclusions by direct analysis of the underlying partial differential equations. We are also working on using Fourier methods to study E-inclusions. Fourier methods are widely used in micromechanics, and they work especially well in the dilute case where E-inclusions are ellipsoids.^[6,25] In particular, we hope that Fourier methods give some insight into constructing an analytical solution for the shapes of 3-D E-inclusions. On the other hand, we note that our method has the advantages that one can consider multiple inclusions in the unit cell Y by introducing multiple obstacles in Y . We can also extend our method to find special shapes that give *any* induced field in the shape, simply by changing the second condition of the overdetermined problem [4]. This flexibility may lead to many new and exciting applications beyond those discussed previously.

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