Inclusion problem in a two-dimensional nonlocal elastic solid

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We have examined the problem of incorporating an inclusion in a two-dimensional linear elastic solid that includes the nonlocal interactions via strain-gradient contributions, and determined an analytical solution for the strain field that minimizes the elastic energy. We have effected this analysis by representing the presence of the inclusion by an external stress field which the elastic solid relaxes around in order to accommodate the inclusion. This formulation of an old problem is extremely general, and is to be contrasted with the solution determined by Eshelby which requires the knowledge of the solid's elastic Green's function, an impractical requirement for either systems including nonlocal interactions, or anisotropic, or nonlinear elastic materials. One result that follows from our analytical solution is that we can say with certainty that the effect of the nonlocal interactions is restricted to at most a few angstroms near the parent-phase/inclusion interface in almost all materials. An analytic solution is presented for graphite, which is of special interest because it forms an exception to this rule.

The incorporation of any foreign object into a solid leads to a disturbance of the solid's structure. The displacement pattern representing this perturbation is well studied, and it is known[1] that the decay of the displacement pattern is algebraic, and that this leads to long-ranged interactions between the inclusion and other regions of the crystal. It is well understood that the long-ranged nature of this interaction is important in a variety of situations. For example, Kawasaki and Koga[2] have examined the dynamical evolution of a system towards equilibrium in the presence of such interactions. Ohta[3] has focused attention on the elastic misfit arising in order-disorder transitions, and shown how the long-ranged elastic interaction radically affects the product state.

The main focus of this paper is to reformulate the Eshelby inclusion problem in a manner that allows for more general energy functionals, for example, mean-field Ginzburg-Landau free-energy densities that include nonlocal interactions between different coarse-grained cells. We shall only consider the nonlocal elastic interactions that arise in the form of strain-gradient contributions to the elastic energy density.[4] Besides being a purely formal exercise, this formulation will eventually allow us to address the problem of defining the martensitic nucleus[5] via a nonlinear, nonlocal elastic energy density[6] which reflects the nonclassical character of this nucleation process. This is an important unsolved problem in the theory of solid-solid phase transitions. The considerations associated with the nucleus will appear as later papers in this series.

Let us begin by restating the solution to this problem that was completed several years ago by Eshelby.[1] In his formulation the inclusion is created by a series of hypothetical manipulations of an elastic solid. First, a portion of the solid (the future inclusion) is removed from the host lattice, and undergoes, a uniform, homogeneous strain. The inclusion at this point has zero total stress, and this deformation strain is called by Eshelby the "stress-free strain." This inclusion then has surface forces applied to it such that it returns to its original shape, acquiring an internal stress field in the process. It is reinserted into the host lattice, and "welded" across the interface so that sliding of the inclusion relative to the host lattice is not possible. The system then relaxes. In Eshelby's formulation, this relaxation is computed by solving the equations of elastic equilibrium in the presence of body forces exerted by the stressed inclusion on the host lattice. These forces are of course equal and opposite to the forces required to bring the inclusion back to its original shape, and are exerted on the system at the interface between the inclusion and the host lattice.

This paper demonstrates an equivalent formulation of the inclusion problem in terms of an externally applied, localized stress field. This stress field is applied to the region of the inclusion such that, in the absence of the restraining host lattice, the inclusion would acquire Eshelby's stress-free strain. The elastic energy is then variationally minimized in the presence of this stress field. This much more general formalism allows us to include different types of terms in the energy functional in a natural way. In this paper, we concentrate on the effect of the nonlocal, or strain gradient, terms. These terms are described at length in Ref. 7, and one instance in which they arise is in systems for which bond-bending forces are present. It is of importance in the nucleation problem to know, in the presence of the smearing-out effect of the gradient terms, whether the boundary between the inclusion and the host lattice is detectable. Specifically, we wish to know if the boundary is smeared out over length scales comparable to the size of the inclusion itself, which would be an important qualitative feature of such nuclei.

The energy functional for the problem under study is bilinear in both the independent strain components and the strain gradients. It describes a linear, isotropic, two-dimensional solid. The elastic energy per unit area of this system is given by

$$\mathcal{F}=\tfrac{1}{2}\lambda(u_{ii})^2+\mu u_{ik}u_{ik}+d_1\zeta_{ijk}\zeta_{ijk}+d_2[(\zeta_{112}-\zeta_{211})^2+(\zeta_{212}-\zeta_{122})^2]-\sigma_{ik}u_{ik}\ . \quad (1)$$

With displacement field components u_i, the quantities $u_{ij}=\frac{1}{2}(u_{i,j}+u_{j,i})$ are the symmetric strain components, λ and μ are the Lamé coefficients,[8] σ_{ij} is an externally imposed stress field, and the ζ_{ijk} are the rotation-independent linear combinations of the gradients of the symmetric strain[9] given by

$$\zeta_{ijk}=u_{ij,k}+u_{ik,j}-u_{kj,i}\ . \quad (2)$$

Strain gradient terms of this type reflect the nonlocal character of the interactions included in the elastic energy functional, and are present to some degree in all solid systems. The particular terms included in Eq. (1), with coefficients d_1 and d_2, are the gradient terms allowed under the enforced isotropy of the system.

We undertake the examination of the response of the system to an inclusion by postulating an external stress field σ_{ij}, which is a uniform dilation within a circle of radius r_0 and zero outside. In the absence of a constraining matrix, the stressed region would respond to this field by uniformly expanding or contracting to a new radius r'. Such an object corresponds to the removed, deformed inclusion of the Eshelby formulation, and the acquired strain is the stress-free strain. That is, the inclusion would relax until the total stress is zero. In our case, the response of the system is obtained by variationally minimizing the total elastic energy of the full system in the presence of this externally applied stress field.

By symmetry, the displacement field of the solid will be everywhere radial. This reduces the problem to that of finding a single function, the radial displacement function $b(r)$. We shall express the quantities in Eq. (1) in terms of $b(r)$. The displacement field is given by

$$u_1=\frac{x}{r}b(r),\quad u_2=\frac{y}{r}b(r)\ . \quad (3)$$

In order to make the algebra in this paper accessible to the reader, we also include the strains and strain gradients in terms of $b(r)$:

$$u_{11}=\frac{y^2}{r^3}b(r)+\frac{x^2}{r^2}b'(r),\quad u_{22}=\frac{x^2}{r^3}b(r)+\frac{y^2}{r^2}b'(r),\quad u_{12}=u_{21}=-\frac{xy}{r^3}b(r)+\frac{xy}{r^2}b'(r)\ ; \quad (4)$$

$$\begin{aligned}
\zeta_{111}&=u_{11,1}=-\frac{3xy^2}{r^5}b(r)+\left[\frac{2x}{r^2}+\frac{xy^2-2x^3}{r^4}\right]b'(r)+\frac{x^3}{r^3}b''(r)\ ,\\
\zeta_{112}&=\zeta_{121}=u_{11,2}=\left[-\frac{3y^3}{r^5}+\frac{2y}{r^3}\right]b(r)+\frac{y^3-2x^2y}{r^4}b'(r)+\frac{x^2y}{r^3}b''(r)\ ,\\
\zeta_{122}&=2u_{12,2}-u_{22,1}=\left[-\frac{4x}{r^3}+\frac{3x^3+6xy^2}{r^5}\right]b(r)+\left[\frac{2x}{r^2}-\frac{x^3+4xy^2}{r^4}\right]b'(r)+\frac{xy^2}{r^3}b''(r)\ ,\\
\zeta_{211}&=2u_{21,1}-u_{11,2}=\left[-\frac{4y}{r^3}+\frac{3y^3+6yx^2}{r^5}\right]b(r)+\left[\frac{2y}{r^2}-\frac{y^3+4yx^2}{r^4}\right]b'(r)+\frac{yx^2}{r^3}b''(r)\ ,\\
\zeta_{221}&=\zeta_{212}=u_{22,1}=\left[-\frac{3x^3}{r^5}+\frac{2x}{r^3}\right]b(r)+\frac{x^3-2y^2x}{r^4}b'(r)+\frac{y^2x}{r^3}b''(r)\ ,\\
\zeta_{222}&=u_{22,2}=-\frac{3yx^2}{r^5}b(r)+\left[\frac{2y}{r^2}+\frac{yx^2-2y^3}{r^4}\right]b'(r)+\frac{y^3}{r^3}b''(r)\ .
\end{aligned} \quad (5)$$

Then, substituting Eqs. (4) and (5) into $\mathcal{F}$, the various components of the energy density expressed in terms of $b(r)$ become

$$\mathcal{F}=\tfrac{1}{2}\lambda\left[\frac{1}{r}b+b'\right]^2+\mu\left[\frac{1}{r^2}b^2+b'^2\right]+d_1\left[b''^2+\frac{3}{r^2}\left[\frac{b}{r}-b'\right]^2\right]-\sigma(r)\left[\frac{1}{r}b+b'\right], \quad (6)$$

where $\sigma(r)$ is the radial profile of the purely dilational or compressional external stress. Due to the radial nature of the deformation, the d_2 gradient term of the general elastic energy density, Eq. (1), does not contribute.

The total elastic energy of the system is then given by the integral of the circularly symmetric energy density $\mathcal{F}$ over the whole system, which we take to be an infinite plane. The energy is a functional of the function $b(r)$,

$$\begin{aligned}
E&=2\pi\int r\,dr\,\mathcal{F}\\
&=2\pi\int_0^\infty dr\left\{\frac{1}{2}\lambda r\left[\frac{1}{r}b+b'\right]^2+\mu r\left[\frac{1}{r^2}b^2+b'^2\right]\right.\\
&\qquad+d_1 r\left[b''^2+\frac{3}{r^2}\left[\frac{b}{r}-b'\right]^2\right]\\
&\qquad\left.-\sigma(r)r\left[\frac{1}{r}b+b'\right]\right\}\ .
\end{aligned} \quad (7)$$

The problem of finding the two-dimensional configuration of the system has therefore been reduced to a well-posed, one-dimensional variational problem. It is necessary to variationally solve[10] for the function $b(r)$ on the interval $[0,\infty)$ with cost function $F=r\mathcal{F}$, the integrand in Eq. (7).

The circular inclusion is modeled by choosing the appropriate stress term in the cost function. We take the external stress to be a radial step function, with values

$$\sigma(r)=\begin{cases}\sigma_0 & \text{for } r<r_0\\ 0 & \text{for } r>r_0 .\end{cases} \tag{8}$$

The differential equation for the displacement profile $b(r)$ is obtained from the Euler-Lagrange equation using the cost function F,

$$F_b-\frac{d}{dr}F_{b'}+\frac{d^2}{dr^2}F_{b''}=0 , \tag{9}$$

giving rise to the differential equation

$$b^{(4)}+\frac{2}{r}b'''-\left[q^2+\frac{3}{r^2}\right]b''-\left[\frac{q^2}{r}-\frac{3}{r^3}\right]b' +\left[\frac{q^2}{r^2}-\frac{3}{r^4}\right]b=\frac{\sigma_0}{2d_1}\delta(r-r_0) , \tag{10}$$

with

$$q^2=\left[\frac{\lambda+2\mu}{2d_1}\right] . \tag{11}$$

The quantity q has dimensions of inverse length, showing how the gradient term coefficient d_1 controls the length scale in this problem.

This high-symmetry special case represented by Eq. (11) can be solved analytically. The homogeneous ($\sigma_0=0$) case has four linearly independent solutions

$$qr,\quad \frac{1}{qr},\quad I_1(qr),\quad K_1(qr) , \tag{12}$$

where I_1 and K_1 are modified Bessel functions of order 1. Within the regions $[0,r_0]$ and $[r_0,\infty)$, the function $b(r)$ will be some linear combination of these four functions, the precise combination being determined by the boundary conditions. There are therefore eight parameters required to specify the solution, which will be labeled according to the following convention:

$$b(r)=\begin{cases} b_-(r)=c_1^-qr+c_2^-\dfrac{1}{qr}+c_3^-I_1(qr)\\ \qquad +c_4^-K_1(qr),\quad r<r_0\\ b_+(r)=c_1^+qr+c_2^+\dfrac{1}{qr}+c_3^+I_1(qr)\\ \qquad +c_4^+K_1(qr),\quad r>r_0 . \end{cases} \tag{13}$$

The cost function F must be integrable, and since it contains the second derivative of b, both $b(r)$ and $b'(r)$ must be continuous at r_0. Furthermore, from the variational analysis,[10] there are two corner conditions which apply—the quantities $F_{b''}$ and $F_{b'}-(d/dr)F_{b''}$ must be continuous at r_0. The effect of the inclusion must be relaxed to zero at infinite distances, so that $b(\infty)=0$. Further, for a purely dilational or compressional distortion, obviously the displacement of the center of the distortion is zero, and thus $b(0)=0$. This variational analysis also provides us with the so-called "free-boundary conditions," which allow the slope of b at zero and infinity to take the value which minimizes the total energy. This condition imposes the constraint that the quantity $rb''(r)$ be zero at the boundaries.

In summary, the eight conditions which fix the constants in Eq. (13) are

$$\begin{aligned} &b(r),\ \ b'(r),\ \ F_{b''},\ \ F_{b'}-\frac{d}{dr}F_{b''} ,\ \ \text{continuous at } r=r_0 ,\\ &b=0,\ \ \lim_{r\to x} rb''(r)=0,\ \ \text{for } x=0,\ \ x=\infty . \end{aligned} \tag{14}$$

With the given cost function, Eq. (7), the first corner condition gives

$$F_{b''}=2d_1rb'' \tag{15a}$$

so that continuity of $F_{b''}$ clearly implies continuity of b''. The second corner condition gives

$$F_{b'}-\frac{d}{dr}F_{b''}=(\tfrac{1}{2}\lambda+\mu)(2rb')+\left[\lambda-\frac{6d_1}{r^2}\right]b +\frac{6d_1}{r}b'-\sigma_0r-\frac{d}{dx}(2d_1rb'') . \tag{15b}$$

Since all but the last two terms are continuous, this condition reduces to

$$(-\sigma_0r-2d_1b''-2d_1rb''')|_{r_0-}^{r_0+}=0 . \tag{16}$$

However, since b'' is also known to be continuous, and the stress field has a discontinuous jump of magnitude σ_0 at r_0, we thus have

$$b_+'''-b_1'''=\frac{\sigma_0}{2d_1} \tag{17}$$

for the discontinuity in the third derivative of b at r_0. Physically, these corner conditions correspond to integrating the differential equation, Eq. (10), through the δ-function source term at r_0.

From the above relation it is possible to solve for the constants in Eq. (13). We have examined the implications of these relations for the constants $c_1^-\cdots c_4^-$ and $c_1^+\cdots c_4^+$ and determined that the boundary conditions give

$$c_1^+=c_3^+=c_2^-=c_4^-=0 \tag{18}$$

and that the continuity equations at r_0 give

$$
\begin{aligned}
&c_1^- q r_0 - c_2^+ \frac{1}{q r_0} + c_3^- I_1 - c_4^+ K_1 = 0 , \\
&c_1^- q + c_2^+ \frac{1}{q r_0^2} + c_3^- \left[q I_0 - \frac{I_1}{r_0} \right] + c_4^+ \left[q K_0 + \frac{K_1}{r_0} \right] = 0 , \\
&-c_2^+ \frac{2}{q r_0^3} + c_3^- \left[-\frac{q I_0}{r_0} + \left[q^2 + \frac{2}{r_0^2} \right] I_1 \right] \\
&\qquad\qquad - c_4^+ \left[\frac{q K_0}{r_0} + \left[q^2 + \frac{2}{r_0^2} \right] K_1 \right] = 0 , \\
&-c_2^+ \left[\frac{6}{q r_0^4} \right] - c_3^- \left[\frac{3+q^2 r_0^2}{r_0^3} \right] (q r_0 I_0 - 2 I_1) \\
&\qquad\qquad - c_4^+ \left[\frac{3+q^2 r_0^2}{r_0^3} \right] (q r_0 K_0 + 2 K_1) = \frac{\sigma_0}{2 d_1} ,
\end{aligned}
\tag{19}
$$

where $I_0 = I_0(q r_0)$, $K_0 = K_0(q r_0)$, $I_1 = I_1(q r_0)$, and $K_1 = K_1(q r_0)$. These equations can be solved numerically for given combinations of σ_0 and d_1, and the results substituted into the appropriate part of Eq. (13), thus giving the displacement field due to the inclusion.

In order to examine the implications of the nonlocality, we have substituted the elastic constants and gradient constants of example systems into the above equations. We have applied our two-dimensional formalism to these three-dimensional crystals since we simply wish to obtain the characteristic length scale of the interfacial region for such inclusions. To be specific, the two-dimensional inclusion problem is the first nontrivial problem involving the effects of accommodation (one-dimensional domain walls do not involve this restriction), and so we content ourselves with a formal solution to this problem. This thus gives a qualitative description of the inclusion profile.

For the case of bcc La, the relevant elastic constants and gradient constants can be deduced from the phonon dispersion relation[11] of the T_1 branch in the [110] direction. This branch was chosen because the gradient coefficient is positive, and because this is the shear involved in the martensitic bcc to hcp transformation which we ultimately wish to describe. The phonon dispersion relations for both longitudinal and transverse phonons, in the presence of gradient couplings, are of the form $\omega^2 = a_1 k^2 + a_2 k^4$, where a_1 depends only on the elastic constants of the system, and a_2 depends only on the gradient coefficients. The La system has a characteristic length scale $\sqrt{a_2/a_1} = 1/q$ of ≈ 1 Å, compared to a lattice constant of ≈ 4 Å. This result suggests that gradient effects in cubic systems are very small, and that the interface between the transformed region of a product-phase nucleus and the host lattice should have a characteristic length scale smaller than the unit-cell length. In the exterior region, the Bessel function $K_1(qr)$ decays rapidly to zero with the same characteristic length scale $1/q$, so that at distances large compared to this length scale, the displacement field is dominated by the algebraic $1/r$ term.

We have also examined this solution for a system in which the length scale is large compared to the unit-cell size. This effect may be expected in weakly first-order structural transitions where the elastic constant of a soft mode, corresponding to a_1, is small, but the gradient coefficients, corresponding to a_2, are not. A long length scale is also realized in graphite, due to the relative strength of the bond-bending forces in the hexagonal planes in comparison to the c_{44} elastic constant corresponding to a shearing of the planes. This unusual characteristic of the lattice gives rise to anomalies in the specific heat of graphite.[12] The length scale can be estimated from the thermodynamic data. The authors in Ref. 12 have found that a crossover in the behavior of the specific heat occurs at 10 K. Assuming that at the energy corresponding to this temperature, the elastic term $a_1 k^2$ and the gradient term $a_2 k^4$ contribute equally to the phonon energy, and given the value of the a_1 elastic constant, one can compute the ratio a_2/a_1 and thus the length scale. For representative data for graphite, the resulting length is 33 ± 9 Å. corresponding to several lattice constants. Figure 1 shows the radial displacement function for a homogeneous circular system with a length scale $1/q$ of 33 Å, an inclusion diameter of 100 Å, and a stress field strength of 9.2×10^{10} dyn cm^{-2}. This stress corresponds to a nongradient radial strain of 0.02, using the value of 2.3×10^{10} dyn cm^{-2} for a_1 from Ref. 12.

These two analyses indicate that the length scale is a good indicator of the extent to which the inclusion/host interface is modified by gradient effects. Gradient forces may be expected to be important in layered systems which resist bending, as demonstrated by graphite, but will be of considerably lesser importance in cubic systems unless the elastic constants are anomalously small.

In light of the length-scale results for cubic systems, it is instructive to examine the short-length-scale limit of Eq. (10), which is obtained by multiplying by d_1 and then taking the limit $d_1 \to 0$. The resulting equation is

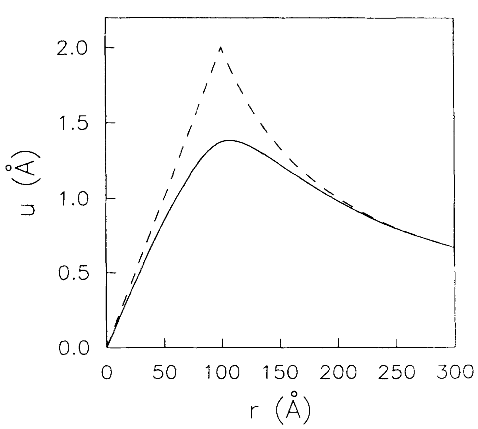

FIG. 1. Radial displacement function $u(r)$ for a two-dimensional, isotropic solid with elastic parameters consistent with those of graphite, subject to a circular dilational stress field. The magnitude of the stress is chosen to yield a 2% expansion of the inclusion in the host lattice in the absence of gradient forces. The dashed curve is this nongradient elastic response, and the solid curve is the response of the system with an additional gradient effect giving rise to a characteristic interfacial length scale of 33 Å.

$$(\lambda+2\mu)\left[-b''-\frac{b'}{r}+\frac{b}{r^2}\right]=\sigma_0\delta(r-r_0) \tag{20}$$

with two linearly independent solutions for the homogeneous case,

$$r,\ \frac{1}{r}\ . \tag{21}$$

The solution to the inclusion problem is therefore given, including the continuity constraint on b and the discontinuity in b' at r_0, by

$$b(r)=\begin{cases}\dfrac{\sigma_0}{2(\lambda+2\mu)}r & \text{for } r<r_0\\[2ex] \dfrac{\sigma_0 r_0^2}{2(\lambda+2\mu)}\dfrac{1}{r} & \text{for } r>r_0\ .\end{cases} \tag{22}$$

We can now show that this particular version of the problem corresponds exactly to a special case of the problem studied by Eshelby. His formulation starts from the equation for elastic equilibrium, given here in terms of the Lamé constants,[8]

$$\mu\nabla^2\mathbf{u}+(\lambda+\mu)\vec{\nabla}(\vec{\nabla}\cdot\mathbf{u})=-\mathbf{f}\ , \tag{23}$$

where $\mathbf{u}$ is the displacement field and $\mathbf{f}$ is the body force field generated by inserting the inclusion into the solid. This force field will, for this problem, be radially directed, and confined to the boundary of the inclusion. Thus the body force may be written

$$\mathbf{f}=\sigma_0\delta(r-r_0)\hat{\mathbf{r}}\ , \tag{24}$$

where we have written the amplitude as σ_0 to correspond with the notation of the preceding text. Physically, the force exerted by the inclusion on the matrix is the change in the stress field at the boundary of the inclusion prior to insertion, so that the amount of compression in fact determines the stress. This underscores the equivalence of these two approaches to the same problem. Writing the displacement field $\mathbf{u}$ in terms of the radial displacement function $b(r)$ and substituting it and Eq. (24) into Eq. (23), the resulting differential equation is

$$(\lambda+2\mu)\left[-b''-\frac{b'}{r}+\frac{b}{r^2}\right]=\sigma_0\delta(r-r_0)\ , \tag{25}$$

which is identical to Eq. (20).

The external stress field formulation of the inclusion problem is formally identical to the Eshelby method of solution of the equations of equilibrium. While the Eshelby model is well adapted for differing inclusion geometries, the stress field model is better adapted for exploring the implications of different types of terms in the elastic energy functional. In particular, we have shown here that the effect of adding gradient terms to the energy is to smear out the inclusion/host interface over a characteristic length scale obtained from the ratio of the gradient coefficient to the elastic constant. We have also shown that the gradient effect is generally small for real cubic systems, but that it can be quite large for systems with unusual elastic properties. In a later publication, we shall be examining a further generalization of this problem which includes nonlinear terms in the energy functional in order to represent actual martensitic nuclei.

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