Eshelby instability pressure for nucleation of a phase change defect

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Abstract

The existence of a nucleation instability is demonstrated at the vanishing of the path-independent *M* integral in linear anisotropic elasticity so that a region that is arbitrarily small can grow at constant potential energy. It yields a quadratic equation for the critical pressure to balance the Eshelby dissipation and nucleate an inclusion undergoing both change in density and change in bulk modulus, and is independent of the radius of the defect. Regarding the shape of nucleation, the expression from Noether's theorem allows also a symmetry breaking mode as a penny-shape "pancake", and by comparison of the *M* integrals for the pancake and the sphere, it would require a greater loss of potential energy of the system to nucleate a pancake, but less to grow it larger.

I. Introduction

We are considering the problem of the nucleation of a phase change defect under pressure. It is shown that a "nucleation instability" exists, which allows a defect that is arbitrarily small to grow incrementally at constant potential energy when the pressure reaches a critical value depending on the phase change, but not on the radius. The nucleation instability occurs when the *M* integral, which is the energy-release rate under scaling of the defect (Budiansky and Rice, 1973) vanishes. The *M* integral was derived by Gunther (1962) based on Noether's (1918) theorem for invariance of the Lagrangean under scaling of the defect, and it is path-independent in anisotropic *linear* elasticity (Knowles and Sternberg, 1972). Lubarda and Markenscoff (2007) treated the dual integrals while Markenscoff and Singh (2015) analyzed the elastodynamic ones. The vanishing of the *M* integral determines a (quadratic) equation for the critical instability pressure in terms of the change in bulk modulus and concurrent change in density, and shows the Peach-Koehler type of terms that balance the Eshelby dissipation; the conditions for the existence of a positive root are investigated. The criterion of nucleation of defects proposed in the literature is that the interface becomes unstable point-wise when the "driving force" reaches a critical value [Stolz, 2018, and references within], while the *M* integral was proposed as a criterion for the growth of holes by Kienzler *et al* (2006) . Recently, Markenscoff (2019b) treated the problem of the dynamically expanding ellipsoidal region of phase change under pre-stress as an Eshelby (1957, 1961) inclusion, and showed, on the basis of Noether's (1918) theorem for invariance of the Hamiltonian under a group of infinitesimal translations, that the shape of a self-similarly expanding Eshelby ellipsoidal region may or may not preserve symmetry, in which case it can nucleate and expand as a flattened ellipsoid "pancake-like" inclusion with axisymmetric symmetry. Here, the comparison of the *M* integral for a sphere and a penny-shape "pancake" shows that it would require a bigger loss in potential energy to nucleate the "pancake" and but less to grow it. The phenomenon manifests itself in geophysics in deep focus earthquakes with phase transformation of volume collapse and change in moduli under high pressure .

II. The *M* integral and a "nucleation instability" for a phase change spherical defect under pressure.

The *M* integral is derived from Noether's theorem for invariance of the Lagrangean functional under scaling and is path-independent in anisotropic linear elasticity (Knowles and Sternberg, 1972). With l denoting the scaling parameter so that the rate of an increment in the radius *a* is $\delta\dot{a} = a\dot{l}$, the relation of the *M* integral to the rate of change of the potential energy Π of a purely mechanical system is (Budiansky and Rice, 1973)

$$d\Pi / dt = \dot{\Pi} = -\dot{l}M \qquad (1)$$

where the potential energy Π of the system is (e.g. Mura 1982, eqtn (25.19)).

$$\Pi = W^{elastic} - \int_S F_i(u_i + u_i^{(0)})dS\ , \qquad (2)$$

with F_i being the loading on the boundary surface S.

The expression for the *M* integral is (Budiansky and Rice, 1973)

$$M = \int_S (Wx_i n_i - T_j u_{j,i} x_i - (1/2)T_i u_i)dS \qquad (3)$$

with $\vec{T}$ denoting the traction vector, and for the spherical inclusion considered here, it takes the form (e.g. Kienzler and Herrmann, 2000),

$$M(r) = \int_0^{2\pi}\int_0^{\pi}(Wr - r\sigma_{rr}\,\partial u_r / \partial r - u_r\sigma_{rr} / 2)r^2 \sin\theta d\theta d\varphi \qquad (3a)$$

For a spherical inhomogeneity where the field quantities undergo jumps of the outside quantity minus the inside one (denoted by the double brackets) across the interface at $r = a$ (e.g., Markenscoff, 2015), we have from (1) and (3)

$$[[M]]\dot{l} = -\dot{\Pi} = -\{\partial\Pi / \partial a\}\partial a / \partial t = -\{\partial\Pi / \partial a\}\delta\dot{a} \qquad (4)$$

with $$[[M]]\dot{l} = \int_S \left(\left[\left[W\right]\right] - \vec{T}\cdot\left[\left[\frac{\partial\vec{u}}{\partial n}\right]\right] \right)\delta\dot{a}\, dS \qquad (4a)$$

where $\delta\dot{a} = a\dot{l}$. The third term in the 3-D expression for the *M* integral in (3) does not contribute a jump in (4a), which makes the connection to equation (20) below for invariance in translation.

An instability will occur when eqtn (4) vanishes for any incremental $\delta\dot{a}$, with the defect growing in scaling by $\delta\dot{a}$ without loss of potential energy, i.e., $\partial\Pi/\partial a = 0$, which provides the nucleation criterion as

$$[[M]]\dot{l} = \int_S \left(\left[\left[W\right]\right] - \vec{T}\cdot\left[\left[\frac{\partial\vec{u}}{\partial n}\right]\right] \right)\delta\dot{a}\,dS = -\{\partial\Pi/\partial a\}\delta\dot{a} = 0 \qquad (5)$$

The vanishing of the *M* integral marks the nucleation event, and it is independent of the radius for the sphere as shown below in eqtn (10).

We consider the nucleation of a region of phase change modeled as an Eshelby inclusion (Eshelby, 1957, 1961) and the matrix material will be assumed isotropic. The analysis is also valid in anisotropy with the Eshelby Tensor obtained by Willis (1971). The spherical inclusion undergoes change in density (superscript *"cd"*) with corresponding eigenstrain ε_{ij}^{*cd} (as the "plastic" eigenstrain in Mura's (1982) terminology) and a concurrent change in bulk modulus change ("inhomogeneous inclusion" according to Eshelby 1957, 1961) under remotely applied pressure $\varepsilon_{kk}^{(0)}$ producing an inhomogeneity with eigenstrain ε_{ij}^{*inh}.

The reason that two different types of eigenstrains are considered is because the transformation strain due to change in density occurs independently of the presence of an applied field at infinity, while the one due to the inhomogeneity is due to the presence of the applied field, and the interaction energies are different. The inhomogeneity (change in bulk modulus) under applied pressure has interaction energy depending only on the pressure acting on the eigenstrain, but *not* on the inclusion internal stresses acting on the eigenstrain (Eshelby 1957, eqtn (4.10)). By contrast, for an inclusion with the change in density ("inhomogeneous inclusion"), the interaction energy depends on the internal stresses acting on the eigenstrain (Eshelby, 1961, eqtn (3.21)) in addition to the applied stresses. This difference results in the corresponding terms affecting the *M* integral differently in eqtn (12) below.

We consider an infinite solid under pressure at infinity $p = -Ke_{kk}^{(0)}$, where *p* is a positive number related through the bulk modulus *K* to the dilatation $\varepsilon_{kk}^{(0)}$ (negative in this application) uniformly applied at infinity. We assume that the inclusion undergoes a change in bulk modulus from *K* to K^*, and simultaneously, at zero pressure $K\varepsilon_{kk}^{(0)}$, a change in density.

If the material of an inclusion with initial density ρ_0 as the matrix has a change in density to ρ^* given outside the matrix during the Eshelby (1957, 1975a) thought experiment, it can be considered as an eigenstrain $(\rho_0 - \rho^*)/\rho^* = dV^*/V = \varepsilon_{kk}^*$. When reinserted in the matrix (of the same material) it produces a change in volume in the constrained inclusion that corresponds to a density ρ' in the constrained inclusion

$$(\rho_0 - \rho')/\rho' = \varepsilon_{kk} = S_{kkij}\varepsilon_{ij}^* = (1+\nu)/3(1-\nu)\varepsilon_{kk}^{*cd} = (1+\nu)/(1-\nu)e^{*cd} \tag{6}$$

with $\varepsilon_{ij}^* = \delta_{ij}e^*$. For increase in density (volume collapse) the equivalent eigenstrain in (6) is negative $\varepsilon_{kk}^{*cd} < 0$.

If there is a change in density simultaneously with change in bulk modulus under remote pressure (pre-stress) $\varepsilon_{kk}^{(0)}$, then the total eigenstrain, due to the inhomogeneity and the change in density under pressure is $\varepsilon_{ij}^{**} = \varepsilon_{ij}^{*inh} + \varepsilon_{ij}^{*cd}$, where (e.g. Mura, 1982, eqtn (22.25))

$$\varepsilon_{kk}^{**} = \{3[(K-K^*)\varepsilon_{kk}^{(0)} + K^*\varepsilon_{kk}^{*cd}](1-\nu)\}/\{2(1-2\nu)K + (1+\nu)K^*\} \tag{7}$$

Equation (7) indicates that without applied pressure, but only change in bulk modulus, the eigenstrain due to change in density with concurrent change in bulk modulus produces an "inhomogeneous inclusion" with equivalent eigenstrain given from the second term in (7), as

$$\begin{aligned} &3K^*\varepsilon_{kk}^{*cd}(1-\nu)/\{2(1-2\nu)K + K^*(1+\nu)\} = \\ &9(1-\nu)/(1+\nu)\varepsilon_{kk}^{*cd}/[3+4\mu/K^*] \end{aligned} \tag{8}$$

which depends on the ratio of the shear modulus of the matrix over the bulk modulus of the inclusion, and with the expression in (8) being in agreement with Eshelby (1975c).

The eigenstrain due to the inhomogeneity of different bulk modulus does not only include the effect of pressure on the change of bulk modulus, but also the effect of the change in density as "loading" on a material with a different bulk modulus, and is

$$\begin{aligned} &3e^{*inh} = \varepsilon_{kk}^{*inh} = \varepsilon_{kk}^{**} - \varepsilon_{kk}^{*cd} = \{3[(K-K^*)\varepsilon_{kk}^{(0)} + K^*\varepsilon_{kk}^{*cd}](1-\nu)\}/\{2(1-2\nu)K + (1+\nu)K^*\} - \varepsilon_{kk}^{*cd} = \\ &3(1-\nu)/(1+\nu)(1-K^*/K)(-p/K)/\{2(1-2\nu)/(1+\nu) + K^*/K\} \\ &+9(1-\nu)/(1+\nu)\varepsilon_{kk}^{*cd}/[3+4\mu/K^*] - \varepsilon_{kk}^{*cd} \end{aligned} \tag{9}$$

The total change in volume is

$$\Delta V/V = \varepsilon_{kk} = S_{llmm}\varepsilon_{kk}^{**}/3 = (1+\nu)/3(1-\nu)\varepsilon_{kk}^{**}. \tag{10}$$

and, with (7) and (9), it is

$$\Delta V/V = \varepsilon_{kk} = (1+\nu)/3(1-\nu)\varepsilon^{**}_{kk} = (1-K^*/K)(-p/K)/\{2(1-2\nu)/(1+\nu)+K^*/K\}$$
$$+3\varepsilon^{*cd}_{kk}/[3+4\mu/K^*] \tag{11}$$

For the calculation of the *M* integral according to (4), the change of the potential energy of the system in (2) for an inclusion with eigenstrains $\varepsilon^{*cd}_{ij}, \varepsilon^{*inh}_{ij}$ under an applied stress field $\sigma^{(0)}_{ij}$ is evaluated as equal to the "interaction energy" , which according to Mura (1982, eqtn (25.24)) is

$$\Delta W = -1/2\int_{\Omega}\sigma^{(0)}_{ij}\varepsilon^{*inh}_{ij}dV - \int_{\Omega}\sigma^{(0)}_{ij}\varepsilon^{*cd}_{ij}\,dV - 1/2\int_{\Omega}\sigma_{ij}\varepsilon^{*cd}_{ij}dV \tag{12}$$

We have remarked earlier why there is a difference on how ε^{*inh}_{ij} and ε^{*cd}_{ij} affect differently the interaction energy in (12). We need to evaluate the stress σ_{ij} in the last term in (12) for the spherical inhomogeneity with transformation strain $\varepsilon^{**}_{ij} = \varepsilon^{*inh}_{ij} + \varepsilon^{*cd}_{ij}$ with a superposed field of radial stress $\sigma^{(0)}_{rr} = -p$ at infinity. The displacement field external and internal to the spherical inclusion is given by Mura (1982,eqtns (11.44)/(11.45)), and the stress field is calculated accordingly. The internal stresses in the inhomogeneous inclusion are

$$\sigma_{11} = \sigma_{22} = \sigma_{33} = -(4/3)(1+\nu)/(1-\nu)\mu e^{**} \tag{13}$$

Thus, (12) yields

$$\Delta W = 2\pi p e^{*inh}a^3 + 4\pi p e^{*cd}a^3 + 8\pi\mu\{(1+\nu)/3(1-\nu)\}(e^{*inh}+e^{*cd})e^{*cd}a^3 \tag{14}$$

III. Instability pressure for nucleation of a phase change defect

The instability criterion of the vanishing of the *M* integral in eqtn (5), for a defect of phase change under pressure to grow in scaling incrementally under no loss in potential energy, in view of eqtn (14), takes the form

$$[[M]]\dot{l} = -\partial\Pi/\partial a\delta\dot{a} = -\partial(\Delta W)/\partial a\delta\dot{a} = -$$
$$\{-6\pi p e^{**} - 6\pi p e^{*cd} - 8\pi\mu\{(1+\nu)/(1-\nu)\}e^{**}e^{*cd}\}a^2\delta\dot{a} = 0 \tag{15}$$

with $\delta\dot{a} = a\dot{l}$. We may note that ΔW in (15) is related to $[[W]]$ since the LHS of (15) is given by (4a). The expression (15) is in agreement with the calculation of the change in potential energy in eqtn (2) using the above fields for a spherical inhomogeneity under a radial applied stress performed by S. P.V. Singh. (To be noted here that the domain has always to be considered finite when the derivative with respect to the radius is taken, and then take the limit for the outside boundary to go to infinity).

For any infinitesimally small nonzero radius a, the vanishing of the term in curls in eqtn (15) with eqtns (6), (7), (8) and (9) gives an equation for the critical pressure for nucleation of a defect with change in density and bulk modulus; it is independent of the radius. Equation (15) yields a quadratic equation for the instability pressure

$$A(p/K)^2 + B(p/K) + C = 0 \tag{16}$$

with

$$A = -\frac{(1-K^*/K)}{[2(1-2\nu)/(1+\nu)+K^*/K]} \tag{17}$$

$$\begin{aligned} B = [&\{9\{(1-\nu)/(1+\nu)\}/[3+4\mu/K^*]+1\} \\ &-2\{(1-2\nu)/(1+\nu)\}\frac{(1-K^*/K)}{[2(1-2\nu)/(1+\nu)+K^*/K]}](1+\nu)/3(1-\nu)\varepsilon_{kk}^{*cd} \end{aligned} \tag{18}$$

$$C = 2\{(1-2\nu)/(1-\nu)\}(\varepsilon_{kk}^{*cd})^2/[3+4\mu/K^*]] \tag{19}$$

The investigation of the signs of the roots in terms of their product and sum gives the conditions for the existence of a positive root p/K so that nucleation will occur. For drop in bulk modulus ($K^* < K$) a positive root always exists since the product of the roots C/A is negative, so a positive nucleation pressure exists. For $K^* > K$ the sum of the roots depends the sign of the change in density: for increase in density $\varepsilon_{kk}^* < 0$ there will be two positive roots. For decrease in density and $K^* > K$ no positive root exists. The root (smaller) is plotted in Figure 1.

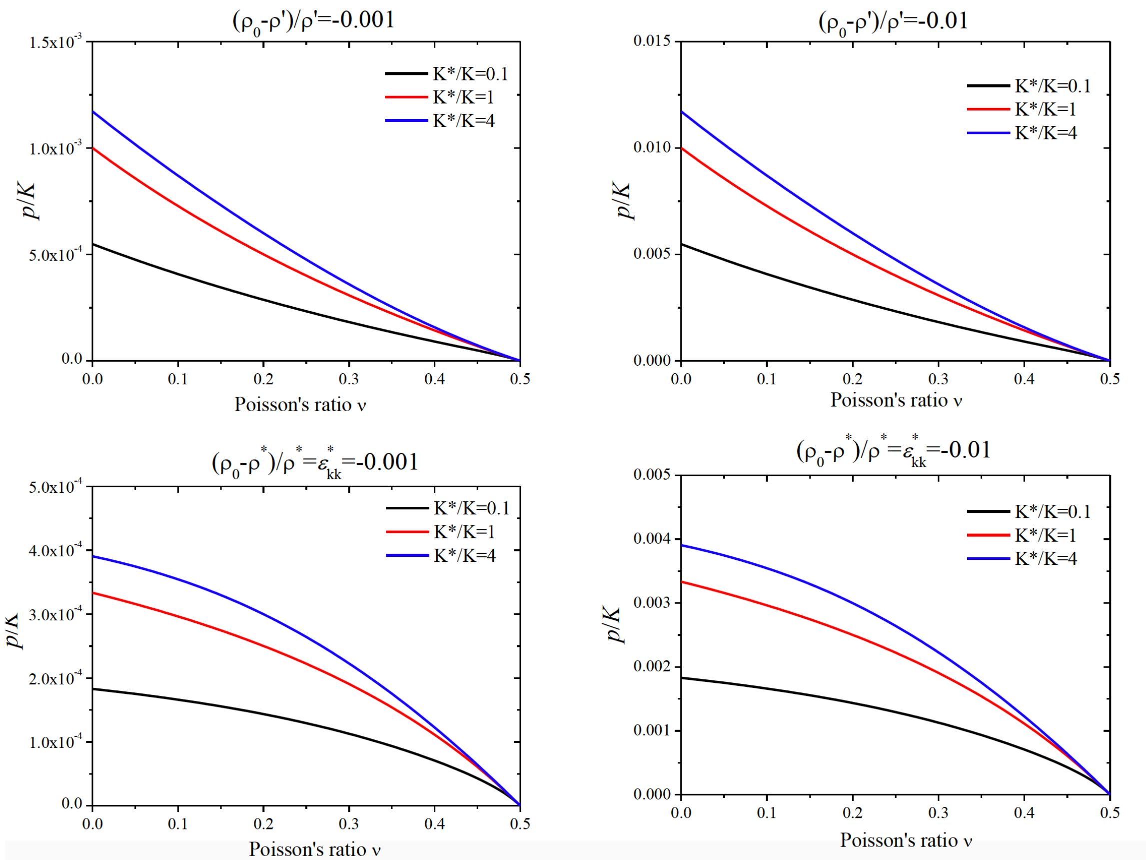

Figure 1: Critical pressure for nucleation of a spherical defect of change in density and bulk modulus

The first two terms in the curly brackets in (15) represent a Peach-Koehler type of force to balance the third term, which is the self-force (Eshelby dissipation). We note that for pressures lower than the critical pressure the M integral is negative. For one material with change in density only, with bulk modulus $K = K^*$, the coefficient A in eqtn (16) vanishes, and we observe that equations (15)/ (16) equate the Peach-Koehler force $-p\varepsilon_{kk}^*$ to the third term $-2\mu(1+\nu)/(1-\nu)(e^{*cd})^2 = -2\mu(3\lambda+2\mu)/(\lambda+2\mu)(e^{*cd})^2$ which is the Eshelby dissipation (Eshelby, 1951, 1956, 1970, 1975a) for a spherical inclusion with eigenstrain as given by Eshelby (1978). The self-force in the equation of motion *with inertia* (Markenscoff, 2010, 2019b)) includes the above term, which shows that the solution of the dynamically self-similarly expanding spherical inclusion automatically expends the energy needed to nucleate a static inclusion from non-existence before growing it (which is the nonzero term at expansion speed V=0). This is to be expected, since the governing system of equations for the self-similarly expanding inclusion is starting from zero initial conditions.

IV. Symmetry breaking instability as a penny-shape (*"pancake"*) growing inclusion

It was shown in Markenscoff, 2019b, that the shape which a self-similarly expanding ellipsoidal inclusion will assume is the one for which the Hamiltonian remains invariant under a group of infinitesimal translations of the inhomogeneity position. From Noether's theorem (dynamic *J* integral), under total loading, the energy -release rate through a contour surrounding the surface of discontinuity and shrinking onto it was obtained as

$$\delta \dot{E}^{tot} = -\lim_{S^d \to 0} \int_{S^d} \dot{l}([[W]] - <\sigma_{ij}>[[u_{i,j}]])dS = 0 \quad (20)$$

so that the moving phase boundary does not become a source or sink of energy. The quantity in parenthesis in (20) is the energy-momentum tensor, Eshelby, 1970, 1975a, 1978), where the square brackets [[.]] denote jumps across the interface, <.> the average , $\dot{l}$ the normal boundary velocity (not the scaling parameter as in the previous sections, in order to maintain consistency with notations in the pertinent literature), and $W = 1/2\sigma_{ij}(\varepsilon_{ij} - \varepsilon^*_{ij}) = 1/2C_{ijkl}(\varepsilon_{kl} - \varepsilon^*_{kl})(\varepsilon_{ij} - \varepsilon^*_{ij})$ is the strain energy density; the expression in parenthesis in (20) coincides with the expression in parenthesis in eqtns (4) and (5). The field quantities include both the applied pre-stress loading and the self-stresses due to the motion of the self-similarly expanding inclusion. It should be noted that before the inclusion starts to nucleate/expand the integral in (20) is a negative quantity under total loading.

In eqtn (20) two possibilities exist: either the quantity in parenthesis is zero (symmetry preserving) or to have the normal boundary velocity $\dot{l} = 0$ on the upper and lower surfaces, in the limit of a flattened ellipsoid ("pancake"), which has only axisymmetric symmetry (symmetry-breaking). The two modes are in competition for nucleation and growth, as will be shown below. In self-similar expansion the nucleated shape does not change, it only scales.

The evaluation of the *M* integral (eqtns (4) with (14)) shows that the *M* integral for the sphere depends on the radius as a^3 .The *M* integral for the circular pancake of phase change is not calculated at this point, but we can make the following remarks: As shown in Eshelby, 1975b, Freund, 1978, Rice (1985), the M integral M_O about the origin will be shifted with regard to the crack tip by $x_i^0 J_i$. For a circular penny-shape crack in tension the stress intensity factor is $K_I = (2/\pi)\sigma\sqrt{a\pi}$, so that $J \sim K_I^2 \sim a$. Thus, for the circular penny-shape, M_O would vary as $aJ \sim a^2$. While this holds for cracks (which are a special limit of inclusions, e.g., Mura (1982), Markenscoff (2019b), the singularity at the tip of the flattened ellipsoidal inclusion with eigenstrain will also be square-root singular. The square root singularity at the tip of the inclusion was obtained by the integration of distributed centers of eigenstrain inside the flattened elliptical cylinder in Markenscoff (2019a), where the principal value of the resulting integral gives a square-root singularity according to Kaya and Erdogan, 1987.

The fact that the M_O integral for the sphere varies as a^3, while for the pancake it varies as a^2 , implies that, for small a (as $a \to 0$), initial growth at nucleation requires a smaller loss of the potential energy of the system, while for growth into a larger shape, as $a \to \infty$ the pancake mode is energetically favored , as the M_O integral tends to infinity at a slower rate. From the above, we may infer that, if there is enough energy to nucleate an inclusion as a "pancake", it will then grow planarly with less energy expenditure, while a spherically nucleated one may not have the energy to grow large.

V. Conclusions

The path-independent *M* integral in linear anisotropic elasticity, as the energy-release rate under scaling of the defect, provides an instability criterion for nucleation of a defect, for incremental growth of an arbitrarily small defect to grow without loss of potential energy under scaling. The instability pressure for nucleation of an inclusion of phase change in density and concurrent change in bulk modulus was obtained as a quadratic equation (independent of the radius), in which the Peach-Koehler forces balance the self-force of Eshelby dissipation, with the conditions for the existence of a positive root investigated. As shown in Markenscoff, 2019b, Noether's theorem allows both for a symmetry preserving nucleation shape and also for a symmetry breaking axisymmetric one, as a "pancake"-like ellipsoidal limit, under conditions of total symmetry in the loading and material properties. The comparison of the *M* integrals shows that the two geometries are in competition for nucleation and growth, and the results are also valid for self-similarly expanding inclusions of phase change with inertia, which in self-similarity start with zero initial conditions and include the nucleation energy. Indeed, as shown in Markenscoff and Ni (2016) the dynamic solution includes the static Eshelby energy to nucleate them, so that the above comparisons also hold in dynamic expansion of regions of phase change.

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