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Displacement field inside a spherical dislocation cage and the Eshelby tensor

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The elasticity problem of a transformed inclusion constrained in an infinite matrix is solved by considering a dislocation cage made of uniformly stacked dislocation loops. The displacement, strain and stress are found using the Burgers' equation, directly yielding the Eshelby tensor. The model provides an alternative physical picture and solution of the transformed inclusion problem to Eshelby's method, and compares directly with transformations produced by a dislocation mechanism.

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INTRODUCTION

When a small volume of material, inside a large matrix, transforms, its displacements are constrained by the surrounding matrix. The elastic field in and around the transformed volume is important to the understanding of a range of solid-state phenomenon, such as solid-state phase transformations,[1–4] the onset of slip under high stresses,[5–8] composite materials,[9] and defects in crystals.[10] The elastic field inside a transformed inclusion is the key to the image stress in the cooperative nucleation of shear dislocation loops.[8]

Eshelby[11,12] calculated $\boldsymbol{\varepsilon}_{ij}^{C}$, the constrained strains inside a transformed inclusion, and related them to the stress-free transformation strains ε_{ij}^{T} by a tensor **S**, i.e., $\varepsilon_{ij}^{C} = \Sigma S_{ijkl}\varepsilon_{kl}^{T}$. He calculated **S** by imagining the small volume to be cut out of the matrix, transformed, returned to its original form elastically, welded back into the matrix, and then released. The Eshelby tensor has been calculated and tabulated for inclusions of various shapes.[13]

In this paper we give an alternative solution for the inclusion problem and for finding the Eshelby tensor. This approach, mentioned in passing but not used by Eshelby,[11] is to consider the transformation to occur *in situ* by the nucleation and growth of dislocation loops. The transformed inclusion constrained in the matrix is surrounded by a cage made of uniformly stacked dislocation loops (a spherical cage is shown in Fig. 1). The constrained displacement and strains are found directly using the Burgers' equation for dislocation loops. When the Burgers' vector and plane spacing are small, i.e., the transformation is homogeneous, the results agree exactly with Eshelby's calculations. This method gives identical results as Eshelby without invoking the cutting and welding procedure, and provides another physical picture for the problem. The picture is particularly valuable when the transformation is produced by a dislocation mechanism. For example, if a volume within a large solid were sheared (e.g., by glide or by twinning) then the dislocations in the cage are the actual dislocations which accomplished the shear. For a finite sample containing a large number of dislocation loops, the mean-field stress that drives the cooperative nucleation of these loops in the sample[8] includes the stress field inside the dislocation cage; the dislocations enveloping the sample are the unbalanced loops/dipoles on the surface.

RESULTS

We consider a large number of circular dislocation loops stacked uniformly along the z axis in the form of a spherical cage, as illustrated in Fig. 1. The dislocation loops have the same Burgers' vector **b** on which no restriction is placed. When **b** is in the loop plane, i.e., shear loops, the cage corresponds to a uniformly sheared inclusion. When **b** is perpendicular to the loop plane, i.e., prismatic loops, the inclusion's transformation is uniaxial dilation or compression. With three sets of loops, any general transformation strain can be represented. We will examine just one set of loops. The displacement field from more than one set can be found simply by symmetry and superposition.

To find the displacement, we start with the Burgers' equation[14] which gives the total displacement at **r** due to a complete dislocation loop

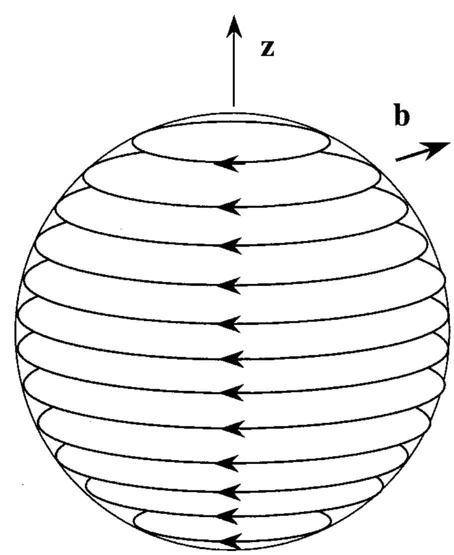

FIG. 1. A transformed inclusion is surrounded by a cage of dislocation loops stacked uniformly and having the same Burgers vector **b**.

$$\mathbf{u}^C(\mathbf{r})=\frac{\mathbf{b}}{4\pi}\int\frac{(\mathbf{r}'-\mathbf{r})\cdot d\mathbf{A}'}{|\mathbf{r}'-\mathbf{r}|^3}-\frac{1}{4\pi}\oint\frac{\mathbf{b}\times d\mathbf{l}'}{|\mathbf{r}'-\mathbf{r}|}+\frac{1}{8\pi(1-\nu)}\nabla\oint\frac{\mathbf{b}\times(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|}\cdot d\mathbf{l}' \tag{1}$$

where $d\mathbf{A}'$ is an area element in the surface enclosed by the dislocation loop, $d\mathbf{l}'$ is a segment along the dislocation line, $\mathbf{r}'$ gives the position of these elements, ν is the Poisson ratio, and C stands for "constrained." The line integrals can be converted into area integrals using the Stokes' theorem (Appendix A), after which the Burgers' equation consists entirely of area integrals

$$\mathbf{u}^C(\mathbf{r})=\frac{\mathbf{b}}{4\pi}\int\frac{(\mathbf{r}'-\mathbf{r})\cdot d\mathbf{A}'}{|\mathbf{r}'-\mathbf{r}|^3}-\frac{1}{4\pi}\int\frac{\mathbf{b}\times[(\mathbf{r}'-\mathbf{r})\times d\mathbf{A}']}{|\mathbf{r}'-\mathbf{r}|^3}+\frac{1}{8\pi(1-\nu)}\nabla\left[\int\frac{\mathbf{b}\cdot d\mathbf{A}'}{|\mathbf{r}'-\mathbf{r}|}+\mathbf{b}\cdot\int\frac{(\mathbf{r}'-\mathbf{r})(\mathbf{r}'-\mathbf{r})\cdot d\mathbf{A}'}{|\mathbf{r}'-\mathbf{r}|^3}\right]. \tag{2}$$

The area integral form of the Burgers' equation is used next to find the total displacement due to a large number of dislocation loops.

Now consider a large number of dislocation loops stacked with uniform density n along the z axis. $d\mathbf{A}'=dA_z'\hat{\mathbf{z}}$, where $\hat{\mathbf{z}}$ is the unit vector in the z direction. For a cage of radius R, the total displacement at any point $\mathbf{r}$ is the sum of the displacements from the loops,

$$\mathbf{U}^C(\mathbf{r})=n\int_{-R}^{R}\mathbf{u}^C(\mathbf{r})dz'=\frac{n}{4\pi}\left[\mathbf{b}I_1-\mathbf{b}\times(\mathbf{I}_2\times\hat{\mathbf{z}})+\frac{1}{2(1-\nu)}\nabla(b_zI_3+\mathbf{b}\cdot\mathbf{I}_4)\right], \tag{3}$$

where

$$I_1=\int_{\text{sphere}}\frac{(z'-z)dV'}{|\mathbf{r}'-\mathbf{r}|^3},\quad \mathbf{I}_2=\int_{\text{sphere}}\frac{(\mathbf{r}'-\mathbf{r})dV'}{|\mathbf{r}'-\mathbf{r}|^3},\quad I_3=\int_{\text{sphere}}\frac{dV'}{|\mathbf{r}'-\mathbf{r}|},\quad \mathbf{I}_4=\int_{\text{sphere}}\frac{(\mathbf{r}'-\mathbf{r})(z'-z)dV'}{|\mathbf{r}'-\mathbf{r}|^3}, \tag{4}$$

and $dV'=dA_z'dz'$.

For any point inside the sphere $|\mathbf{r}|\leqslant R$, the integrals are $I_1=-(4\pi/3)z$, $\mathbf{I}_2=-(4\pi/3)\mathbf{r}$, $I_3=(2\pi/3)(3R^2-r^2)$, and $\mathbf{I}_4=(2\pi/15)[4z\mathbf{r}+(5R^2-3r^2)\hat{\mathbf{z}}]$ (See Appendix B for details for finding these integrals.) The total displacement at any point $\mathbf{r}$ inside the sphere is therefore

$$\mathbf{U}^C(\mathbf{r})=-\frac{n\mathbf{b}}{3}z+\frac{n}{3}\mathbf{b}\times(\mathbf{r}\times\hat{\mathbf{z}})+\frac{n}{15(1-\nu)}[z\mathbf{b}-4b_z\mathbf{r}+(\mathbf{b}\cdot\mathbf{r})\hat{\mathbf{z}}]. \tag{5}$$

The displacement varies linearly with the coordinates, and hence the strains are constant. The constrained strains inside the dislocation cage, defined by $\varepsilon_{ij}^C=(\partial U_i^C/\partial x_j+\partial U_j^C/\partial x_i)/2$, are

$$\begin{aligned}\varepsilon_{xx}^C&=\varepsilon_{yy}^C=\frac{5\nu-1}{15(1-\nu)}\varepsilon_{zz}^T,\\ \varepsilon_{zz}^C&=\frac{7-5\nu}{15(1-\nu)}\varepsilon_{zz}^T,\\ \varepsilon_{xz}^C&=\frac{4-5\nu}{15(1-\nu)}\varepsilon_{xz}^T,\\ \varepsilon_{yz}^C&=\frac{4-5\nu}{15(1-\nu)}\varepsilon_{yz}^T,\\ \varepsilon_{xy}^C&=0,\end{aligned} \tag{6}$$

where $\varepsilon_{zz}^T=-nb_z$, $\varepsilon_{xz}^T=-nb_x$, and $\varepsilon_{yz}^T=-nb_y$ are the transformation strains. Note that, for the Burgers' equation, the Burgers vector is defined by displacing the material above the loop plane by -**b** relative to the material below it.[14] This accounts for the negative sign in the transformation strains. Equation (6) leads to the following terms of the Eshelby tensor:

$$\begin{aligned}S_{1133}&=S_{2233}=\frac{5\nu-1}{15(1-\nu)},\\ S_{3333}&=\frac{7-5\nu}{15(1-\nu)},\\ S_{1313}&=S_{2323}=\frac{4-5\nu}{15(1-\nu)}.\end{aligned} \tag{7}$$

Other non-zero terms in the Eshelby tensor can be obtained similarly using symmetry, giving $S_{iiii}=(7-5\nu)/15(1-\nu)$, $S_{iijj}=(5\nu-1)/15(1-\nu)$, $S_{ijij}=(4-5\nu)/15(1-\nu)$. All other terms (e.g., S_{iiij}) are zero. These results are the same as given by Eshelby's method.[12,13]

The relation $2S_{ijij}=S_{iiii}-S_{iijj}$ in Eq. (7) can be understood by considering two sets of prismatic dislocation loops with opposite signs stacked perpendicularly, one along the i axis with b and the other along the j axis with b. The two sets of prismatic loops produce opposite normal strains (of nb and $-nb$) which are equivalent to two shear strains of the same sign, resulting in $2S_{ijij}=S_{iiii}-S_{iijj}$. Two sets of prismatic dislocation loops of opposite signs stacked perpendicularly produce the same constrained strains as two sets of shear loops bisecting the prismatic loops.

The elastic field in the dislocation cage can now be described using Eshelby's language. The dislocation cage is the transformed inclusion. If completely unconstrained by the matrix, the displacement inside the dislocation cage would be entirely plastic, i.e., $\mathbf{U}^P(\mathbf{r})=-nz\mathbf{b}$ from which the stress-free transformation strain can be found. With the matrix constraint, the displacement is $\mathbf{U}^C(\mathbf{r})$ [Eq. (5)], from which the constrained strain is derived [Eq. (6)].

The elastic displacement in the dislocation cage—the displacement that would be gained if the matrix were dissolved away-is the difference between the transformation and constrained displacements, i.e., $\mathbf{U}^e=-(\mathbf{U}^P-\mathbf{U}^C)$, from which the elastic strains and stresses in the cage can be found. Take a shear dislocation cage, with $\mathbf{b}=b\hat{\mathbf{x}}$, as an example. $U_x^P=-nbz$, $U_x^C=-nb\beta z$, and $U_z^C=-nb\beta x$ [Eq. (5)], where $\beta=(4-5\nu)/15(1-\nu)$. The elastic displacements are $U_x^e=(1-\beta)nbz$ and $U_z^e=-\beta nbx$. The x component of the displacement varies linearly with z, and the z component with x. The only stress in the dislocation cage is hence a shear stress $\sigma_{xz}^C=G(\partial U_x^e/\partial z+\partial U_z^e/\partial x)=(1-2\beta)Gnb=Gnb(7-5\nu)/15(1-\nu)$, the same as given by Eshelby.[12,13] The field inside ellipsoidal dislocation cages and cages of complex shapes can be treated similarly; we will report these in the future.

A hydrostatically dilated or compressed inclusion can be modeled by three sets of prismatic dislocation loops, along three orthogonal directions, each producing a strain given by $\varepsilon_{ii}^T=\Delta^T/3$, where Δ^T is the amount of dilatation in the unconstrained state. The constrained strains are $\varepsilon_{ii}^C=(S_{iiii}+2S_{iijj})\varepsilon_{ii}^T=\varepsilon_{ii}^T(1+\nu)/3(1-\nu)$. Hence the constrained dilation is $\Delta^C=\Delta^T(1+\nu)/3(1-\nu)$, another result given by Eshelby.[10] Since both dilation and shear may be modeled by prismatic loops, the constrained strains and stresses resulting from a general transformation may always be obtained from cages containing three sets of prismatic dislocations with appropriate densities n.

CONCLUSIONS

The elasticity problem of a transformed inclusion constrained in an infinite matrix can be solved by considering a dislocation cage made of uniformly stacked dislocation loops. The displacement, strain and stress are found using the Burgers' equation, yielding directly the Eshelby tensor. The model provides an alternative physical picture and solution of the inclusion problem to Eshelby's cutting and welding procedure. The model compares directly with transformations produced by a dislocation mechanism.

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APPENDIX A

Here are the details used in converting the line integrals in the Burgers' equation [Eq. (1)] into area integrals [Eq. (2)]. Starting with Stokes' theorem, we have

$$\begin{aligned}\oint \frac{\mathbf{b}\times(\mathbf{r}'-\mathbf{r})\cdot d\mathbf{l}'}{|\mathbf{r}'-\mathbf{r}|} &= \int \nabla'\times\frac{\mathbf{b}\times(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|}\cdot d\mathbf{A}' \\ &= \int \left[\mathbf{b}\nabla'\cdot\frac{(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|}-(\mathbf{b}\cdot\nabla')\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|}\right]\cdot d\mathbf{A}' \\ &= \int \frac{\mathbf{b}\cdot d\mathbf{A}'}{|\mathbf{r}'-\mathbf{r}|}+\mathbf{b}\cdot\int\frac{(\mathbf{r}'-\mathbf{r})(\mathbf{r}'-\mathbf{r})\cdot d\mathbf{A}'}{|\mathbf{r}'-\mathbf{r}|^3}\end{aligned} \tag{A1}$$

where, in the second step, use is made of $\mathbf{A}\times(\mathbf{B}\times\mathbf{C})=(\mathbf{A}\cdot\mathbf{C})\mathbf{B}-(\mathbf{A}\cdot\mathbf{B})\mathbf{C}$. The above takes care of the third term in the Burgers' equation.

For the second integral in the Burgers' equation, we look at its projection along an arbitrary unit direction $\hat{\mathbf{e}}$, i.e.,

$$\begin{aligned}\oint \frac{\mathbf{b}\times d\mathbf{l}'}{|\mathbf{r}'-\mathbf{r}|}\cdot\hat{\mathbf{e}} &= \oint\frac{(\hat{\mathbf{e}}\times\mathbf{b})\cdot d\mathbf{l}'}{|\mathbf{r}'-\mathbf{r}|}=\int\nabla'\times\frac{(\hat{\mathbf{e}}\times\mathbf{b})}{|\mathbf{r}'-\mathbf{r}|}\cdot d\mathbf{A}' \\ &= \left[\int\frac{(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}\mathbf{b}\cdot d\mathbf{A}'-\int\frac{(\mathbf{r}'-\mathbf{r})\cdot\mathbf{b}}{|\mathbf{r}'-\mathbf{r}|^3}d\mathbf{A}'\right]\cdot\hat{\mathbf{e}},\end{aligned} \tag{A2}$$

where the third step is handled similarly as the second step in Eq. (A1). Since $\hat{\mathbf{e}}$ is arbitrary,

$$\begin{aligned}\oint\frac{\mathbf{b}\times d\mathbf{l}'}{|\mathbf{r}'-\mathbf{r}|} &= \int\frac{(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}\mathbf{b}\cdot d\mathbf{A}'-\int\frac{(\mathbf{r}'-\mathbf{r})\cdot\mathbf{b}}{|\mathbf{r}'-\mathbf{r}|^3}d\mathbf{A}' \\ &= \int\frac{\mathbf{b}\times[(\mathbf{r}'-\mathbf{r})\times d\mathbf{A}']}{|\mathbf{r}'-\mathbf{r}|^3}.\end{aligned}$$

APPENDIX B

The displacement in Eq. (5) is obtained from Eq. (3) by making use of the following integrals over a sphere for any point $\mathbf{r}$ inside the sphere:

$$\begin{aligned}&\int_{\text{sphere}}\frac{x'-x}{|\mathbf{r}'-\mathbf{r}|^3}dV'=-\frac{4\pi}{3}x \\ &\int_{\text{sphere}}\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^3}dV'=-\frac{4\pi}{3}\mathbf{r} \\ &\int_{\text{sphere}}\frac{1}{|\mathbf{r}'-\mathbf{r}|}dV'=\frac{2\pi}{3}(3R^2-r^2) \\ &\int_{\text{sphere}}\frac{(\mathbf{r}'-\mathbf{r})(z'-z)}{|\mathbf{r}-\mathbf{r}'|^3}dV'=\frac{2\pi}{15}[4z\mathbf{r}+\hat{\mathbf{z}}(5R^2-3r^2)].\end{aligned} \tag{B1}$$

Here we give details leading to the first integral in Eq. (B1); the others in Eq. (B1) can be worked out similarly. Let $x'=x+\rho\sin\theta\cos\phi$, $y'=y+\rho\sin\theta\sin\phi$, and $z'=z+\rho\cos\theta$, where $\theta=0\sim\pi$ and $\phi=0\sim2\pi$ are the latitude and azimuth angles. We have $dV'=\rho^2\sin\theta d\theta d\phi d\rho$ and hence

$$\int_{\text{sphere}} \frac{x'-x}{|\mathbf{r}-\mathbf{r}'|^3} dV' = \int_0^{\pi}\int_0^{2\pi}\int_0^{\rho_M} \sin^2\theta\cos\phi d\rho d\theta d\phi$$

$$= \int_0^{\pi}\int_0^{2\pi} \rho_M(\theta,\phi)\sin^2\theta\cos\phi d\theta d\phi. \tag{B2}$$

$\rho_M(\theta,\phi)$ is the integration limit of ρ on the surface of the sphere, satisfying

$$(x+\rho_M\sin\theta\cos\phi)^2+(y+\rho_M\sin\theta\sin\phi)^2 + (z+\rho_M\cos\theta)^2 = R^2, \tag{B3}$$

where R is the radius of the sphere. The solution for $\rho_M(\theta,\phi)$ from Eq. (B3) gives

$$\rho_M(\theta,\phi) = \sqrt{B^2+C} - B,$$

where $B = x\sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta$ and $C = R^2 - (x^2+y^2+z^2)$. Note that $C \geqslant 0$, since the point $\mathbf{r}$ is inside the sphere and hence $\rho_M(\theta,\phi) \geqslant 0$. The integral in Eq. (B2) can be further simplified since

$$\int_0^{\pi}\int_0^{2\pi} \sqrt{B^2+C}\sin^2\theta\cos\phi d\theta d\phi = 0$$

because the integrand $\sqrt{B^2+C}\sin^2\theta\cos\phi$ is antisymmetrical with respect to inversion $(\theta\rightarrow\pi-\theta, \phi\rightarrow\pi+\phi)$. Hence

$$\int_{\text{sphere}} \frac{x'-x}{|\mathbf{r}-\mathbf{r}'|^3} dV' = -\int_0^{\pi}\int_0^{2\pi} B\sin^2\theta\cos\phi d\theta d\phi$$

$$= -\int_0^{\pi}\int_0^{2\pi}(x\sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta)\sin^2\theta\cos\phi d\theta d\phi$$

$$= -\frac{4\pi}{3}x. \tag{B4}$$

[1] J. W. Christian, *The Theory of Transformations in Metals and Alloys* (Pergamon, Oxford, 1975).
[2] P. C. Clapp, Phys. Status Solidi A **57**, 561 (1973).
[3] W. Klein *et al.*, Phys. Rev. Lett. **88**, 085701 (2002).
[4] Z. Nishiyama, *The Martensite Transformation* (Academic, New York, 1979).
[5] M. Khantha, D. P. Pope, and V. Vitek, Phys. Rev. Lett. **73**, 684 (1994).
[6] M. Khantha, D. P. Pope, and V. Vitek, Mater. Sci. Eng., A **234–236**, 629 (1997).
[7] A. Loveridge-Smith *et al.*, Phys. Rev. Lett. **86**, 2349 (2001).
[8] Y. Q. Sun, P. M. Hazzledine, and P. B. Hirsch, Phys. Rev. Lett. **88**, 065503 (2002).
[9] T. W. Clyne and P. J. Withers, *An Introduction to Metal Matrix Composites* (Cambridge University Press, Cambridge, 1993).
[10] J. D. Eshelby, in *The Physics of Metals: Defects*, edited by P. B. Hirsch (Cambridge University Press, Cambridge, 1975), p. 2.
[11] J. D. Eshelby, Proc. R. Soc. London, Ser. A **241**, 376 (1957).
[12] J. D. Eshelby, Prog. Solid Mech. **11**, 89 (1961).
[13] L. M. Brown and D. R. Clarke, Acta Mater. **23**, 821 (1975).
[14] J. P. Hirth and J. Lothe, *Theory of Dislocations* (Krieger, Malabar, FL, 1982).