Elastic Image Corrections for Double-force Displacement Fields[†]

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ABSTRACT

The elastic effects of a free surface are found for double-force defects distributed throughout elastically isotropic spheres and cylinders. This permits separation of the rapidly fluctuating displacement fields found near the defects from the slowly varying image displacements. The spherically asymmetric displacement fields produce zero average volume dilatations both for the cylinder and the sphere.

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INTRODUCTION

In the immediate neighborhood of a point defect in a crystalline solid, atomic positions are altered relative to the normal lattice positions. Beyond some distance from the defect, probably only a few interatomic distances, the elastic displacements can be represented by an elastic strain field in a continuous medium. This strain field can be thought of as arising from highly localized body forces acting in opposing pairs. Such a pair of forces is called an elastic double force.^{1,2,3} Three equal double forces, orthogonal to one another and acting at a point $r = 0$ in an elastically isotropic medium, will produce the spherically symmetrical displacement field

$$(1) \quad \vec{u}(\vec{r}) = c \vec{r}/r^3$$

in an infinite medium. As an example where the medium is not isotropic, Mann et al.⁴ have calculated the complicated displacement field produced by three equal double forces in an infinite crystal of copper. If the medium is isotropic, Love¹ gives the general displacements produced by double forces along a given axis. Three orthogonal double forces of unequal strength will produce a more general displacement field that possesses non-radial displacements as well, and the surfaces of constant displacement become ellipsoids rather than spheres.

In addition to the problem of determining displacements produced in an infinite medium, Eshelby⁵ has emphasized the importance of meeting the boundary conditions at the surface of a finite object. These boundary conditions are met by introducing image stresses which in turn produce their corresponding image displacement fields in the object. Thus the total displacement field, $\vec{u}^d$, produced by a defect in a finite object is given by

$$(2) \quad \vec{u}^d = \vec{u}^\infty + \vec{u}^I$$

where $\vec{u}^\infty$ is the displacement field in an infinite medium and $\vec{u}^I$ results from image forces on the object's surface. Eshelby's discussion was limited to volume change calculations, so details of the displacement field could be avoided. In other cases these details are needed. For example, the electrical resistivity arising from point defects is in part a consequence of the elastic strains which displace atoms from their normal positions. Also, the interaction energy and forces acting between point defects are in part a consequence of the displacement field, including image displacements.

Huntington and Johnson⁶ (referred to as HJ hereafter) have considered the effect of image forces on the distortion of a sphere by an anisotropic defect at the center of the sphere. As shown below, their defect is essentially equivalent to a single double force. It is the purpose of this paper to extend their work to an elastically isotropic sphere and cylinder having a distribution of single axis double-force throughout the volume of the object.

METHOD OF CALCULATION

Consider a defect characterized by a double force acting along the z-axis at the origin. The force per unit volume, as defined by Love,¹ can be written in vector notation as:

$$(3) \quad \vec{f}^d = \lim_{h \rightarrow 0} \underline{i}_3 \frac{P}{h} [\delta(\vec{r}) - \delta(\vec{r} + \underline{i}_3 h)] = -\underline{i}_3 P \frac{\partial}{\partial x_3} \delta(\vec{r})$$

where $\underline{i}_3$ is a unit vector along the z-axis, $\delta(\vec{r})$ is the three dimensional Dirac delta function, h is the small separation of the points at which the point forces are applied, and P is the double force strength. The corresponding displacement field in an infinite isotropic medium is

$$(4) \quad \vec{u}_i^\infty = \frac{C \underline{i}_r}{3 r^2} + \frac{D \underline{i}_r}{r^2} (3 \cos^2 \theta - 1) - \frac{C}{r^2} \underline{i}_\theta \sin \theta \cos \theta$$

where $C = -P/4\pi(\lambda + 2\mu)$, μ and λ are the shear and Lamé elastic constants for isotropic media, $D = C(5\mu + 3\lambda)/6\mu$, θ is the polar angle relative to the z-axis, $\underline{i}_r$ is a unit radial vector and $\underline{i}_\theta$ is a unit vector perpendicular to $\underline{i}_r$ in the direction of increasing θ . This definition of C is identical with that of HJ, though they omitted the spherically symmetric first term which was of no interest to them. Thus the displacement field considered by HJ is the spherically asymmetric part of the field produced by a single double-force.

Consider a closed surface S filled with an elastically isotropic medium containing n defects per unit volume. If S is surrounded by an infinite extent of the same medium free of defects, then one can find the displacement on and outside of S by considering the defects as body

forces as in (3) or displacement field sources as in (4). If n is everywhere uniform within S , then one can find (using Gauss' theorem) the average surface stress acting on S due to the volume forces which cancel one another inside of S .

$$\begin{aligned}
 (5) \quad n \int \vec{f}^d d\text{vol} &= -\underline{i}_3 P n \int \frac{\partial}{\partial x_3} \delta(\vec{r}) d\text{vol} \\
 &= -\underline{i}_3 P n \int_S (\underline{i}_3 \cdot \underline{i}_n) dS
 \end{aligned}$$

where $\underline{i}_n$ is normal to S . Thus a body surrounded by an elastic medium and uniformly filled with n double force defects per unit volume has a force per unit area $-n P(\underline{i}_3 \cdot \underline{i}_n) \underline{i}_3$ acting on its surface. This is a generalization of Eshelby's result⁵ for the spherically symmetric point defect. Following Eshelby, one can imagine applying minus this force at every point of the surface S to reduce the strains to zero, scraping away the surrounding medium, and then releasing the surface which now has the surface force acting. The resultant distortion, $\vec{u}^d$, will be that produced by the defects in the finite object bounded by S , and includes the image effects. This procedure does not isolate the image distortions from those produced by the defects alone when S is in an infinite medium.

When the defects are not uniformly distributed or when it is desirable to separate the image force effects, one can find the average displacement within and on S by taking the displacement from a volume element dv as given by $n \vec{u}_1^\infty dv$ where $\vec{u}_1^\infty$ is given by eqn. (4) and n may vary with position. From this calculation one can find $\vec{u}^\infty$ and thereby $\vec{u}^I$ from the relation $\vec{u}^d = \vec{u}^I + \vec{u}^\infty$ where $\vec{u}^d$ is found by the method of the previous paragraph. This is the procedure used in the following discussions.

A. Spherical Objects

If the sphere of radius R is uniformly filled with defects, the resultant distortion is that produced by a surface force given by equation 5 corresponding to surface stresses:

$$(6) \quad \sigma_{rr} = -(mP/3) - (mP/3)(3\cos^2\theta - 1), \quad \sigma_{r\theta} = mP\sin\theta\cos\theta$$

where σ_{rr} has been written in the form of a constant radial stress plus one which gives no net volume change. Application of these stresses to an isotropic elastic sphere produces a total distortion for $r \leq R$ given by

$$(7) \quad \vec{u}^d(r, \theta) = \frac{4\pi m c r}{9} \cdot \left(\frac{6\mu + 3\lambda}{2\mu + 3\lambda} \right) \hat{i}_r + \frac{4\pi m c r}{3} \left(\frac{2\mu + \lambda}{2\mu} \right) \cdot \left[\begin{array}{l} (3\cos^2\theta - 1) \hat{i}_r \\ -3\cos\theta\sin\theta \hat{i}_\theta \end{array} \right]$$

The first term of (7) results from the spherically symmetric first term of (4), and the factor in parenthesis is the same as Eshelby's factor γ . This displacement term is N times that of a single spherically symmetric defect at the center of S . The second term of eqn. (7), which gives no volume change, is not simply related to the distortion of a defect located at the center of the sphere.

Inside of S eqn. (7) must be used with care, however, for that portion of $\vec{u}^d$ arising from image forces is slowly varying while $\vec{u}^\infty$, arising from a superposition of $\vec{u}_1^\infty$, is subject to large fluctuations. In particular Eshelby has noted that the spherically symmetrical part of $\vec{u}^I$ has a constant dilatation while the dilatation from the corresponding part of $\vec{u}_1^\infty$ is zero except at the defects themselves. The second term of $\vec{u}^d$ has zero dilatation inside of S , but the dilatation of the single defect

displacement $\vec{u}_1^\infty$ is given by $Cr^{-3}(3 \cos^2 \theta - 1)$. Here the fluctuating displacement field has a dilatation, but the total field does not.

It would, therefore, be desirable to calculate $\vec{u}^I$ and $\vec{u}^\infty$ separately.

To effect this separation, we consider a spherical shell of radius ρ and thickness $d\rho$. Limiting ourselves to radially symmetric variations in n , we permit n to vary only with ρ . By integrating $n\vec{u}_1^\infty dv$ over the entire shell, we find that $d\vec{u}^\infty = 0$ for the points inside of the spherical shell. For $r \geq \rho$,

$$(8) \quad d\vec{u}^\infty(r, \theta) = \delta N \cdot \vec{u}_1^\infty - \frac{\delta N \rho^2 (3D - C)}{3r^4} \left[(3 \cos^2 \theta - 1) \hat{i}_r + 2 \sin \theta \cos \theta \hat{i}_\theta \right]$$

where $\delta N = 4 \pi \rho^2 d\rho n(\rho)$. The first term is the result of assuming all the defects at the center of the shell; the second term represents the sizable "correction" which such a viewpoint requires.

To find the displacement $\vec{u}^\infty$, we integrate eqn. (8) from $\rho = 0$ to $\rho = r$ and obtain directly

$$(9) \quad \vec{u}^\infty = \frac{4\pi m \mu C}{3} \left[\frac{1}{3} \hat{i}_r + \left(\frac{8\mu + 3\lambda}{15\mu} \right) \left((3 \cos^2 \theta - 1) \hat{i}_r - 3 \cos \theta \sin \theta \hat{i}_\theta \right) \right]$$

By subtraction from eqn. (7) this result gives

$$(10) \quad \vec{u}^I = \frac{4\pi m \mu C}{3} \left[\frac{4\mu}{3(2\mu + 3\lambda)} \hat{i}_r + \left(\frac{14\mu + 9\lambda}{30\mu} \right) \left((3 \cos^2 \theta - 1) \hat{i}_r - 3 \cos \theta \sin \theta \hat{i}_\theta \right) \right]$$

The first terms of (9) and (10) give the spherically symmetric part of the displacements. It is of special interest to note that the dilatation of the remaining terms is zero in both cases.

B. Cylindrical Objects

Consider an elastically isotropic cylinder of length L and radius a whose axis coincides with the z -axis of a cylindrical coordinate system (r, ϕ, z) . Distributed uniformly through the cylinder are n defects per unit volume, each defect being characterized by a double force P acting along an axis ξ which makes an angle θ relative to the z -axis as shown in Fig. 1. Noting that $\underline{i}_n = \underline{i}_0$ over the surface $r = a$ and $\underline{i}_n = \pm \underline{i}_z$ over the ends of the cylinder, we find from eqn. (5) that the following surface stresses are acting:

over the surface, $r = a$

$$(11) \quad \begin{aligned} \sigma_{rr} &= -n P \sin^2 \theta \cos^2 \phi \\ \sigma_{r\phi} &= n P \sin^2 \theta \sin \phi \cos \phi \\ \sigma_{rz} &= -n P \sin \theta \cos \theta \cos \phi \end{aligned}$$

and on the ends, $z = \pm L/2$

$$(12) \quad \begin{aligned} \sigma_{zz} &= \mp n P \cos^2 \theta \\ \sigma_{z\phi} &= \pm n P \cos \theta \sin \theta \sin \phi \\ \sigma_{zr} &= \mp n P \cos \theta \sin \theta \cos \phi \end{aligned}$$

where $\mp$ signs refer to the ends at $\pm L/2$ respectively. The last two end stresses produce no net torque or force on the ends, and their effects will be felt only near the ends of the cylinder. Assuming L is sufficiently great, we ignore these end effects and consider the cylinder as acted upon by the three stresses of eqn. (11) plus σ_{zz} of eqn. (12).

These four surface stress boundary conditions can be met using solutions of the isotropic elastic equation having a constant dilatation throughout the cylinder. Thus the x , y , and z components of the displacement are harmonic functions. Expressed in cylindrical coordinates, one

finds for the total displacement field, if $r \leq a$,

$$\begin{aligned}
 u_r^d &= \frac{A\lambda}{3(3\lambda+2\mu)} + \frac{A\lambda}{6\mu} (3\sin^2\theta \cos^2\phi - 1) \\
 (13) \quad u_z^d &= \frac{AZ}{3(3\lambda+2\mu)} + \frac{A}{6\mu} \left\{ (3\cos^2\theta - 1)z + 6\lambda \sin\theta \cos\theta \cos\phi \right\} \\
 u_\phi^d &= -\frac{A\lambda}{2\mu} \sin^2\theta \cos\phi \sin\phi
 \end{aligned}$$

where $A = 4\pi n c(\lambda + 2\mu)$.

To separate $\vec{u}^I$ from this total displacement field, $\vec{u}^\infty$ was calculated at point Q of Fig. 1 by direct integration and use then was made of the relation $\vec{u}^d = \vec{u}^I + \vec{u}^\infty$. The result of integrating over a long cylindrical shell of radius ρ and thickness $d\rho$ with a density of defects $n(\rho)$ gives $d\vec{u}^\infty = 0$ if $r < \rho$, while for $r \geq \rho$

$$\begin{aligned}
 du_r^\infty &= \frac{\delta q \cdot c}{\lambda} \left\{ \frac{2}{3} + \left(\frac{\lambda + \mu}{\mu} \right) \sin^2\theta \cos 2\phi \left(1 - \frac{\rho^2}{r^2} \right) + \frac{2}{3} (3\sin^2\theta \cos^2\phi - 1) \right\} \\
 du_z^\infty &= \frac{4\delta q \cdot c}{\lambda} \left(\frac{2\mu + \lambda}{\mu} \right) \cos\theta \sin\theta \cos\phi \\
 (14) \quad du_\phi^\infty &= -\frac{\delta q \cdot c}{\lambda} \sin^2\theta \sin 2\phi \left\{ 1 + \left(\frac{\lambda + \mu}{\mu} \right) \frac{\rho^2}{r^2} \right\}
 \end{aligned}$$

where ϕ and θ are defined in Fig. 1, $\delta q = 2\pi\rho n(\rho)d\rho$ is the number of defects per unit length of cylindrical shell and the first term in $d\vec{u}_r^\infty$ is the only displacement resulting from the spherically symmetric part

of eqn. (4). Taking $n(\rho)$ as a constant, one finds that inside the cylinder at a distance $r \leq a$ from its axis

$$\begin{aligned}
 u_r^\infty &= \frac{2\pi n \rho c}{3} + 2\pi n \rho c \left\{ \left(\frac{3\mu + \lambda}{2\mu} \right) \sin^2 \theta \cos^2 \phi - \left(\frac{\lambda + \mu}{4\mu} \right) \sin^2 \theta - \frac{1}{3} \right\} \\
 u_z^\infty &= 2\pi n \rho c \left(\frac{4\mu + 2\lambda}{3\mu} \right) \cos \theta \sin \theta \cos \phi \\
 u_\phi^\infty &= -2\pi n \rho c \left(\frac{3\mu + \lambda}{2\mu} \right) \sin \phi \cos \phi
 \end{aligned}
 \tag{15}$$

where the first term of u_r^∞ arises from the spherically symmetric displacement field. Contrary to the spherical case, the non-spherically symmetric displacements of eqn. (15) do not give a zero dilation within the cylinder. One finds for Δ^∞ , the dilatation,

$$\Delta^\infty = \frac{4\pi n c}{3} + \frac{2\pi n c}{3} (1 - 3 \cos^2 \theta)
 \tag{16}$$

We obtain from Eq. (13) the result $\Delta^d = 4\pi n c (\lambda + 2\mu) / (3\lambda + 2\mu)$, so we find, using $\Delta^d = \Delta^I + \Delta^\infty$, that

$$\Delta^I = \frac{4\pi n c}{3} \frac{4\mu}{(3\lambda + 2\mu)} - \frac{2\pi n c}{3} (1 - 3 \cos^2 \theta)
 \tag{17}$$

The second terms of (16) and (17) give the non-spherically symmetric contributions which just cancel in producing Δ^d , the total dilatation.

DISCUSSION

The principle results of these calculations apply to an elastically isotropic sphere or cylinder uniformly filled with aligned defects each of which is characterized by a single double force. Total displacement fields are given by eqns. (7) and (13) for the sphere and cylinder respectively. While the results are limited to isotropic media, they should apply quite closely to defects in Tungsten metal and give an analytical basis for comparison with any future results for anisotropic media.

Equations (7) and (13) are the results for defects each having a single double force. For defects characterized by three orthogonal double forces, one can rotate the axes and superpose the results given here. For the special case of two of the double forces having equal strengths, say $C_1 = C_2 \neq C_3$, one can use the results as given here by replacing C with $C_1 + C_2 + C_3$ in the spherically symmetric terms and replacing C with $C_3 - C_1$ in the remaining terms.

In the case of anisotropic defects, there is special interest in the energy of interaction between the defect and an applied stress.³ As Eshelby has shown,² one can obtain this interaction energy, W , in two ways:

$$(18) \quad W = \int_S \vec{u}^d \cdot \vec{\sigma}^e \cdot d\vec{S}$$

$$(19) \quad W = - \int \vec{f}^d \cdot \vec{u}^e dvol$$

where $\vec{u}^d$ and $\vec{u}^e$ are displacements produced by the defect and by the external stress respectively, $\vec{\sigma}^e$ is the external stress tensor acting on the closed

surface S , and $\vec{f}^d$ is the double force which results in $\vec{u}^d$. In using eqn. (18) $\vec{u}^d$ must include image displacements; for non-uniform external stresses this approach may be simplest. When the external stress produces a uniform strain, however, eqn. (19) becomes more convenient because image displacements are irrelevant and the interaction energy per defect is independent of location within the object. Inserting $\vec{f}^d$ from eqn. (3) in eqn. (19) we find

$$(20) \quad W = N P \epsilon_{zz}^e$$

where N is the number of defects and ϵ_{zz}^e is the externally induced strain along the z -axis. By noting that the HJ displacement is that of a double force and using the shear stresses considered by those authors, one finds their results for W directly from eqn. (20) when $N = 1$ and P is expressed as $-4\pi(\lambda + 2\mu)C$.

Nowick and Heller³ have introduced a λ -tensor in discussing the interaction energy W . They write

$$(21) \quad \lambda_{ij} = \frac{1}{v_0} \frac{\partial \epsilon_{ij}^d}{\partial n}$$

where v_0 is the atomic volume, ϵ_{ij}^d is the total defect strain tensor, and n is the concentration of aligned defects. Note that the necessity of including image strains makes λ shape dependent. One can use eqns. (7) and (13) directly to determine the λ tensors for double force defects in spherical and cylindrical coordinates respectively. As an example, for the uniformly filled sphere using coordinates (r, θ, ϕ) we have

$$(22) \quad \bar{\lambda} = \left(\frac{2\kappa a}{2\kappa + 3\lambda} \right) \bar{E} + \begin{pmatrix} ah_{\theta} & -3ag_{\theta} & 0 \\ -3ag_{\theta} & a(1-h_{\theta}) & 0 \\ 0 & 0 & -a \end{pmatrix}$$

where $a = 2\pi C(\lambda + 2\mu)/9\mu v_o$, $h_{\theta} = 3 \cos^2 \theta - 1$, $g_{\theta} = \cos \theta \sin \theta$, and $\bar{E}$ is the identity matrix. $\bar{\lambda}$ is written in two parts: the first part arising from the spherically symmetric displacement field, the second part from the assymmetric field.

CONCLUSIONS

1. The total and the image elastic displacement fields were found for elastically isotropic spheres and cylinders containing a distribution of defects each characterized by a double force. By superposition the results can be applied to defects having three orthogonal double forces of unequal strength.
2. The results permit direct evaluation of the λ tensor, introduced by Nowick and Heller,³ for the sphere and cylinder.
3. Recognition that the displacement field of Huntington and Johnson⁶ arises from a double force enables one to derive their defect-external stress interaction energies directly.

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Fig. 1. Coordinates for cylindrical case. $\vec{\xi}$ denotes axis of double force.