A distributed-dislocation method for generalized eigenstrain problems

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Abstract

In this work, a numerical method for finding the elastic fields of inclusions in an infinite solid with arbitrary eigenstrains is presented. The method is valid, under isotropic elasticity assumptions, for an inclusion and a surrounding matrix of equal elastic constants. The method is general in the sense that it works for any particle or inclusion of arbitrary shape and any eigenstrains. In other words, the method is applicable to any misfit profile along the particle-matrix interface. And since the method is numerical in nature, it is capable of calculating the elastic fields inside and outside the inclusion; something that is not easily attainable using analytical techniques restricted further to simple particle geometry and misfit profiles. The main idea behind the method is that the continuous misfit region between the particle and matrix is discretized into local misfit regions consisting of dislocation loops. From the principle of linear superposition, the elastic fields at a material point in the continuum are simply those obtained by summing the fields of all dislocation loops involved in the approximation process. The results indicate very good agreement with analytical solutions and better convergence with increasing loop density. Such a method has valuable application in recent advances in dislocation dynamics modeling.

1 Introduction

Eigenstrain is the generic name given by Mura [1] to such strains as misfit strains, thermal strains, phase transformation, and initial strains.
among others. Here our emphasis will be on volume misfit strains. The problem is illustrated in Figure 1, which shows a misfit particle of arbitrary shape fitted into a smaller volume cavity in an infinite elastic matrix. The misfit region between the particle and the surrounding matrix is denoted by $\delta(\theta)$, where $\delta(\theta)$ is not constant in general along the interface.

In the field of micromechanics it is often desirable to quantify the elastic fields generated by the presence of such misfit particles. These fields are sought for both inside the particle and for the matrix material. The ideal situation would be to be able to analytically derive the mentioned fields for particles of any geometric shape and of any distribution of the misfit along the interface where the elastic constants of the particle may differ from those of the host matrix. But this is not usually the case. Analytical solutions are typically derived for simplified particle geometries as well as for well-described or behaved misfit distributions.

One example of such derivations was demonstrated by Teodosiu [2] who solved the boundary-value problem (BVP) of a spherical misfit particle of uniform radial misfit and of different elastic properties than those of the matrix. The main disadvantage of the BVP method is that every time the geometry of the problem changes, the solution must be recreated. Of course, the analytical solution for an infinite cylindrical particle with constant or uniform misfit can also be deduced as a special case from more advanced analytical solutions. For example, it can be deduced from the solution for an ellipsoidal particle presented by Eshelby [3], among others, using the eigenstrain method. Mura [1] presents an excellent treatise of the eigenstrain method for solving particle problems, including misfit situations. However, once again, every time the problem geometry changes, the solution must be re-formulated, and the eigenstrains are typically restricted to simple analytical functions.
Below, we present a distributed-dislocation method for numerically solving particle misfit problems of any geometry and any misfit distribution along the interface. Here the state of continuous misfit region along the particle-matrix interface is replaced by a distribution of local misfits. Each local misfit region is represented by a prismatic interstitial dislocation loop. As the dislocation loop density increases, i.e. the number of loops increases and the size of each decrease, the numerical solution converges to the analytical solution. Here the Burgers vector of each loop corresponds to the local amount of misfit between the particle and the matrix. Due to its numerical nature, the method can be used to quantify the elastic fields of a particle of any geometry and any misfit distribution.

In order to better explain our numerical method we illustrate it with two of the simplest cases of misfit particles. The first will be the two-dimensional case of an infinitely long misfit cylindrical particle where the surrounding matrix is infinite. We then present the simplest existing three-dimensional case. This is the case of a spherical misfit particle where again the surrounding matrix is infinitely large.

To illustrate the present numerical method we consider for simplicity the case where $G = G'$ and $\nu = \nu'$ (where $G$ is the shear modulus and $\nu$ is Poisson’s ratio). Here the primed quantities represent those of the particle material.

2 Cylindrical misfit particle

The problem is depicted in Figure 2, which shows the cross-section of an infinitely long misfit particle, of radius $r_m$, placed into a smaller size hole within an infinite matrix ($R = \infty$). The radial misfit between the particle and the hole is denoted as $\delta$. In this figure, the particle and hole are shown to be perfect cylinders with uniform $\delta$ along the interface. The misfit region between the particle and the matrix is approximated with an enclosed polygon (e.g. see Figure 2). Each side of the polygon stands for a local misfit region. This local misfit representation is facilitated by considering the face of each side to be a prismatic dislocation loop (i.e., one whose burgers vector $b$ is pointed normal to its habit plane). The dislocation loop in this case is rectangular and is composed of four edge dislocation segments (two of them at $z=\pm\infty$, Figure 2). A prismatic dislocation loop is simply a layer of matter inserted in a surrounding matrix (Hirth and Lothe [4], Hull and Bacon [5]).

Figure 2 also shows an oblique view of a section of the enclosed polygon. Each side has a Burgers vector normal to its face. The dislocation segments at the end of the infinite prism do not contribute to the state of elastic deformation in the material. Figure 3 shows a cross-section of the infinitely long prism (normal to its axis), with each prismatic dislocation loop being represented by two oppositely signed, infinite edge dislocations.

The elastic fields (displacement, strain and stress) at a field point $P(x,y)$ are numerically found to be, from the principle of linear superposition, the summation of the elastic fields due to the edge dislocations in Figure 3.
Figure 2: Cylindrical particle of radius $r_0$ inside a cylindrical shell of radius $R$. The amount of misfit is denoted by $\delta$. The particle-matrix interface can be approximated with a polygonal prism. An oblique view of a section of the polygon is also shown.

Figure 3: A cross-section of the polygonal prism in Figure 2. Each dislocation loop is represented by two oppositely signed infinite edge dislocations. Point P is a material point that can reside inside or outside the particle. Also shown is a dislocation $i$ whose Burgers vector is decomposed into $x$ and $y$ components.
Note here that the Burgers vector of each dislocation $i$, $b^i$, can be decomposed into two components: a glide component $b^i_x$, and a climb component $b^i_y$. The terminology for the glide and climb components has been defined by Weertman [6]. As explained above, the displacement ($u_x$ and $u_y$) and stress ($\sigma_{xx}$, $\sigma_{xy}$, and $\sigma_{yy}$) fields at a material or field point will then be given by eqn (1) and eqn (2), respectively.

\[
\begin{align*}
 u_x &= \sum_{i=1}^{2N} u^i_x, \quad u_y = \sum_{i=1}^{2N} u^i_y \\
 \sigma_{xx} &= \sum_{i=1}^{2N} \sigma_{xx}^i, \quad \sigma_{xy} = \sum_{i=1}^{2N} \sigma_{xy}^i, \quad \sigma_{yy} = \sum_{i=1}^{2N} \sigma_{yy}^i, \quad \sigma_{zz} = \sum_{i=1}^{2N} \sigma_{zz}^i
\end{align*}
\] (1)

Notice that for $N$ sides of the polygon, $2N$ edge dislocations exist (see Figure 3) and hence the $2N$ summation limit in eqns (1) and (2).

The stresses and displacements at $(x,y)$ due to a single infinite edge dislocation $i$ located at $(x^i, y^i)$ with a Burgers vector $b^i = b^i_x + b^i_y$ are given by (Weertman [6]) eqns (3) and (4), respectively.

\[
\begin{align*}
 \sigma_{xx}^i &= \frac{Gb^i_x}{2\pi(1-\nu)} \frac{(y - y^i)(3(x - x^i)^2 + (y - y^i)^2)}{((x - x^i)^2 + (y - y^i)^2)^2} + \frac{Gb^i_y}{2\pi(1-\nu)} \frac{(x - x^i)((x - x^i)^2 - (y - y^i)^2)}{((x - x^i)^2 + (y - y^i)^2)^2} \\
 \sigma_{yy}^i &= \frac{Gb^i_y}{2\pi(1-\nu)} \frac{(y - y^i)((x - x^i)^2 - (y - y^i)^2)}{((x - x^i)^2 + (y - y^i)^2)^2} + \frac{Gb^i_x}{2\pi(1-\nu)} \frac{(x - x^i)(3(y - y^i)^2 + (x - x^i)^2)}{((x - x^i)^2 + (y - y^i)^2)^2} \\
 \sigma_{xy}^i &= \frac{Gb^i_y}{2\pi(1-\nu)} \frac{(x - x^i)((x - x^i)^2 - (y - y^i)^2)}{((x - x^i)^2 + (y - y^i)^2)^2} + \frac{Gb^i_x}{2\pi(1-\nu)} \frac{(y - y^i)((x - x^i)^2 - (y - y^i)^2)}{((x - x^i)^2 + (y - y^i)^2)^2} \\
 \sigma_{zz}^i &= \nu(\sigma_{xx}^i + \sigma_{yy}^i)
\end{align*}
\] (3)

\[
\begin{align*}
 u_x^i &= \frac{b^i_x}{2\pi} \left[ \tan^{-1} \left( \frac{y - y^i}{x - x^i} \right) + \frac{1}{2(1-\nu)} \frac{(x - x^i)(y - y^i)}{(x - x^i)^2 + (y - y^i)^2} \right] \\
 &+ \frac{b^i_y}{2\pi} \left[ \frac{(1-2\nu)}{2(1-\nu)} \ln \frac{\sqrt{(x - x^i)^2 + (y - y^i)^2}}{r_e} + \frac{1}{2(1-\nu)} \frac{(y - y^i)^2}{(x - x^i)^2 + (y - y^i)^2} \right]
\end{align*}
\] (4)
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\[ u_j^i = \frac{b_j^i}{2\pi} \left[ -\frac{1-2\nu}{2(1-\nu)} \ln \frac{\sqrt{(x-x')^2 + (y-y')^2}}{r_c} + \frac{1}{2(1-\nu)} \frac{(y-y')^2}{(x-x')^2 + (y-y')^2} \right] + \frac{b_j^i}{2\pi} \left[ \tan^{-1} \left( \frac{y-y'}{x-x'} \right) - \frac{1}{2(1-\nu)} \frac{(x-x')(y-y')}{(x-x')^2 + (y-y')^2} \right] \]

In the above equations, \( r_c \) is a cut-off or dislocation core radius taken here equal to the magnitude of one Burgers vector, \( b \), in our numerical examples presented below.

In Figure 4, \( \sigma_{xx} \) is plotted along the \( x \)-axis for \( \nu = 0.3 \) and \( r_o = 100b \). The figure shows different curves each corresponding to a given dislocation loop density (the loop densities used are 4, 5, 6, 8 10, 15, 20, 30, 40, 100, and 200 loops, represented by the increasing dash size in Figure 4). We note in Figure 4 that, for any given loop density, as the distance from the particle increases the numerical solution approaches the analytical solution (in solid line). For points relatively close to the particle (i.e. at \( x=100b \)), the numerical solution is only accurate for relatively large dislocation densities. Overall, the numerical solution converges to the analytical one as the loop (or mesh) density increases. Similar figures were obtained for other stress and displacement components.

![Figure 4: \( \sigma_{xx}/G \) vs \( x \) along the \( x \)-axis (for \( y = 0 \)). \( x \) is in units of \( b \), Burgers vector magnitude. The solid line is the analytical solution. The dashed lines are for the numerical solution. The larger the dash size, the denser the dislocation loop density (4, 5, 6, 8 10, 15, 20, 30, and 40 loops). Here, \( \nu = 0.3 \) and \( r_o = 100b \).](image-url)
3 Spherical misfit particle

The misfit region between the particle and the matrix is approximated via a random triangular-element mesh discretizing the interface. Three of the meshes utilized in our calculations are shown in Figure 5. The mesh was generated using the pre-processor of the finite-element software ANSYS 5.7. Each element in the mesh represents a local misfit region. Again, we consider each element to be a prismatic dislocation loop. Each dislocation loop in this case is triangular and thus composed of three dislocation segments.

Figure 6 shows a close-up view of a generic prismatic dislocation loop. It is composed of three linear dislocation segments (AB, BC and CA) of edge character. The line sense of the dislocation line is indicated with the ξ vectors. The Burgers vector magnitude b is set equal to the radial misfit δ between the particle and matrix. Point P(x,y,z) in the figure is simply a material or field point at which the elastic fields (displacement, strain, and stress) due to the nearby dislocation loop are felt. The strength of the fields at P is a direct function of the relative distance between P and the loop.

The elastic fields (e.g. stress) at a field point due to the particle are numerically found to be, from the principle of linear superposition, the summation of the elastic fields due to all the dislocation loops in Figure 5. Note here that the Burgers vector of each dislocation i, b′, is generally composed of three components: \( b_x^i \), \( b_y^i \), and \( b_z^i \). The direction of b′ in the computations is simply found by taking the cross product of two dislocation segments of a loop (e.g. segment AB crossed with BC).

Based on the above, the stresses at a material or field point P are given by:

\[
\sigma_{ij}^{\text{particle}} = \sum_{k=1}^{N} \sigma_{ij}^{k}
\]

(5)

where the short hand index notation has been employed (i.e., \( \sigma_{ij}^{k} \) represents the \( ij^{th} \) component of stress due to dislocation loop k). Notice that N here represents the total number of elements or dislocation loops.

Moreover, since each triangular dislocation loop k (Figure 6, for example) is composed of three dislocation segments, the stress field due to such loop is also given by another superposition process. It is the sum of the stress fields due to each of the segments. More specifically, the stress field is given by:

\[
\sigma_{ij}^{\text{loop}} = \sigma_{ij}^{AB} + \sigma_{ij}^{BC} + \sigma_{ij}^{CA}
\]

(6)

To find the stress field due to a straight dislocation segment of an arbitrary Burgers vector and line sense and under the assumption of isotropic linear elastic materials, two literature sources are often used: [4,7]. The first reference
Figure 5: Surface-meshed spheres with 106, 202, and 302 triangular elements or dislocation loops. The sphere radius is $r_o$.

gives the stress field in terms of local or body-fixed coordinate system that is attached to the segment itself. The second reference gives the stress field (based on [8]) with respect to a global or arbitrary coordinate system. Although both methods are equivalent, the first one requires a second-order transformation for the stress tensor and hence more careful coding to avoid errors.

In this work, we’ve used the stress field of a dislocation segment following [7]. For completeness, according to this method, the stress field $\sigma_{ij}^{AB}(r)$ due to a segment such as AB shown in Figure 7, where $r(x,y,z)$ is the position vector of point P, is given by:

$$\sigma_{ij}^{AB}(r) = \sigma_{ij}(r)|_{r'=r_A} - \sigma_{ij}(r)|_{r'=r_B},$$

(7)

, where

$$\sigma_{ij}(r) = \frac{G}{\pi Y^2} \left[ \begin{bmatrix} b \xi Y \end{bmatrix}_j - \frac{1}{(1-\nu)} \begin{bmatrix} b \xi Y \end{bmatrix}_j - \frac{b}{2(1-\nu)} \left[ \begin{bmatrix} \xi \end{bmatrix}_j + \frac{2}{Y^2} \left[ \begin{bmatrix} \xi \end{bmatrix}_j + \frac{L}{R} \begin{bmatrix} \xi \end{bmatrix}_j \right] \right] \right]$$

(8)

In the last equations, $b$ is the Burgers vector of the segment, $\xi$ is its line sense, $\delta_{ij}$ is Kronecker delta, $r_A'$ and $r_B'$ are the position vectors of the segment’s end points. Other quantities are:

$$R = r - r', \quad L' = R \cdot \xi, \quad Y = R + R \xi, \quad \rho = R \cdot L' \xi$$

(9)

$$(a,b,c) = (a \times b) \cdot c$$

$$[abc]_j = \frac{1}{2} \left( (a \times b)_j c_j + (a \times b)_j c_j \right)$$

(10)

The notations ( ) and [ ] represent, respectively, the scalar-triple-product and a symmetric-tensor-operator.
Figure 6: A triangular prismatic dislocation loop composed of three line segments AB, BC, and AC, following the dislocation line sense.

Figure 7: A schematic of a dislocation line segment AB and some of the parameters used in Equations (7-10).

Figure 8: A plot of $\sigma_{yy}/G$ vs $x$ along the $x$-axis, outside a spherical particle.
In Figure 8, $\sigma_{xy}$ is plotted along the x-axis for $\nu = 0.3$ and $r_o = 100b$. The figure shows different curves each corresponding to a given dislocation loop density (the loop densities used are 76, 106, 146, 202, 302, 402, 812, and 1048 loops, represented by the increasing dash size in Figure 8). Like in the cylindrical case, in Figure 8 we note that as the number of loops is increased the numerical solution approaches the analytical solution (in solid line). Again, for points relatively close to the particle (i.e. at $x = 100b$), the numerical solution is only accurate for relatively large dislocation loop densities. Similar figures were obtained for other stress components.

References