Elastic Displacement and Stress Fields Induced by a Dislocation of Polygonal Shape in an Anisotropic Elastic Half-Space

The elastic displacement and stress fields due to a polygonal dislocation within an anisotropic homogeneous half-space are studied in this paper. Simple line integrals from 0 to π for the elastic fields are derived by applying the point-force Green's functions in the corresponding half-space. Notably, the geometry of the polygonal dislocation is included entirely in the integrand easing integration for any arbitrarily shaped dislocation. We apply the proposed method to a hexagonal shaped dislocation loop with Burgers vector along [1 1 0] lying on the crystallographic (1 1 1) slip plane within a half-space of a copper crystal. It is demonstrated numerically that the displacement jump condition on the dislocation loop surface and the traction-free condition on the surface of the half-space are both satisfied. On the free surface of the half-space, it is shown that the distributions of the hydrostatic stress (σ11 + σ22)/2 and pseudohydrostatic displacement (u1 + u2)/2 are both anti-symmetric, while the biaxial stress (σ11 − σ22)/2 and pseudobiaxial displacement (u1 − u2)/2 are both symmetric. [DOI: 10.1115/1.4005554]

Keywords: polygonal dislocation, displacement and stress fields, Green’s function, anisotropic half-space

1 Introduction

Misfit dislocations often emerge during the fabrication of metal crystals [1,2], ceramic [3] and some high-performance nanostructures, such as quantum dots [4] and quantum wells [5]. Generation of such dislocations is an energetically favorable way for the material to relieve the strain energy induced by an inherent lattice mismatch or thermal mismatch. An important element of the problem of stress fields produced by misfit dislocations is the presence of a free surface [6]. For this reason, straight dislocations including edge and screw dislocations near a free surface have been well investigated for isotropic solids [7–11] and even anisotropic solids [12,13]. Assuming a three-dimensional (3D) isotropic half-space, Bacon and Groves [14] presented a surface integral for the stresses induced by an arbitrary dislocation, and Gosling and Willis [6] a line integral expression (along the dislocation boundary) for the stresses due to an arbitrary shaped dislocation. Special cases such as an angular dislocations [15] and dislocations inside an anisotropic elliptical inclusion [16] were also studied. Some other theory/method including the stress coupled theory [17] and multiscale method [18] were recently utilized to study the response of dislocations.

The elastic fields due to dislocation loops in a 3D anisotropic half-space can be expressed by the integrals of the point-force Green’s function and its derivatives over the dislocation surfaces [6,18–20]. The point-force Green’s function for an anisotropic half-space is often separated into two parts: the full-space part and the image part [6,21,22]. The surface integral of the full-space Green’s function for the stress field can be reduced to a line integral using Stokes’ theorem [23], or even to an analytical expression in the case of straight dislocation line segments [24,25]. However, an explicit expression for the second part, that is, the stresses relating to the image part of Green’s function in the half-space, does not currently exist. In the study of the displacements due to dislocations, only the general surface integral over a dislocation loop has been derived where the point-force Green’s function lies in its integral [6,19]. Thus, a corresponding line integral expression for the image portion of the problem of a dislocation in an anisotropic 3D half-space is lacking. Reducing the surface integral to a line integral is crucial for efficient and accurate prediction of the dislocation-induced elastic fields. The major difficulty in reducing the surface integral to a line integral for the image displacement and stress fields due to dislocations in anisotropic materials is that Stokes’ theorem cannot be utilized.

In this paper, we use the point-force Green’s function in the Stroh formalism to derive line integrals (from 0 to π) for the elastic displacements and strains due to polygonal dislocations in an anisotropic 3D half-space. In these analytical line integrals, the influence of dislocation geometry on the displacement and strain fields is completely included in the integrands. This paper is organized as follows. In Sec. 2, some basic expressions for the displacements and stresses due to the dislocation loops and the point-force Green’s function are reviewed. In section 3, line integral expressions for the elastic field including displacements and strains are derived by integrating the generalized triple integrals over a triangular dislocation, the fundamental dislocation element from which any polygonal dislocation can be constructed. In Sec. 4, the proposed integral expressions are then applied to calculate the elastic displacement and stress fields due to a hexagonal dislocation in a half-space of a single crystal with a face centered cubic (fcc) crystal structure. Lastly, we end with some discussion and conclusions.

2 Problem Description and Some Basic Formula

The problem is to predict the elastic field (displacements and stresses) due to a dislocation of polygonal shape with Burgers
the equilibrium equation is by a unit point force applied at an anisotropic material: the half-space, on the surface of the half-space (surfaces: surface discontinuity on S)

Green's functions, we first consider two independent systems in the global coordinate system (i.e., one part covers $x_3 = 0$ and the other 0 $\leq x_3 < d$) and apply the two-dimensional Fourier transforms to the system. In the Fourier space, the boundary conditions in Eq. (1) become

$$\left\{ \begin{array}{l} u_{1|_{x_3 = \infty}} = 0, \\ u_{i|_{x_3 = d}} - u_{i|_{x_3 = 0}} = \delta_{ij} b_j, \\ \sigma_{ij|_{x_3 = 0}} + \sigma_{ij|_{x_3 = d}} = 0 \end{array} \right. \quad (9)$$

where the displacement in the Fourier space is

$$\tilde{u}_k(\xi_1, \xi_2, x_3) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} u_{1}(x_1, x_2, x_3) e^{i(\xi_1 x_1 + \xi_2 x_2)} d\xi_1 d\xi_2 \quad (10)$$

The equilibrium equation in the Fourier domain in a source-free region is

$$C_{ij\beta\xi}\xi^2 \hat{u}_k + i(C_{ij33} + C_{ij22})\xi_s \hat{u}_k - C_{ij33} \hat{u}_k = 0 \quad (11)$$

The general solution of Eq. (11) can be expressed as

$$\tilde{u}(\xi_1, \xi_2, x_3) = \exp(-i \rho \xi_3) \quad (12)$$

where $\rho$ and $a$ are the eigenvalue and eigenvector of the Stroh eigenrelation (Ting, [21]), i.e.,

$$[Q + p(R + R^T)] \vec{a} = 0 \quad (13)$$

with

$$Q_{ij} = C_{ij\beta\xi} \xi_i \xi_j, \quad R_{ij} = C_{ij\beta\xi} \xi_i \xi_j, \quad T_{ij} = C_{ij\beta\xi}, \quad n = [\cos \theta, \sin \theta, 0]^T, \quad m = [0, 0, 1]^T, \quad \xi = \eta m \quad (14)$$
where the superscript \( 'T' \) indicates the matrix transpose. With the eigenvalues and the associated eigenvectors \( \rho_i \) and \( \mathbf{a}_i \) \((i = 1, 2, \ldots, 6)\), we let
\[
\text{Im}(\rho_i) > 0, \quad \rho_{i+3} = \bar{\rho}_i, \quad \mathbf{a}_{i+3} = \bar{\mathbf{a}}_i, \quad (i = 1, 2, 3)
\]
\[
\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3], \quad \mathbf{B} = [\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3] \text{ with } \mathbf{b}_i \equiv (\mathbf{R}^T + \rho_i \mathbf{T}) \mathbf{a}_i.
\]
(15)

where the symbol \( \text{‘Im’} \) and the overbar denote, respectively, the imaginary part and the complex conjugate of a complex variable. In this case, no summation is taken over the repeated index \( i \) in Eq. (15).

Making use of the displacement and traction conditions in Eq. (9), the elastic displacement vector in the transformed domain is found to be
\[
\mathbf{u} = \left\{ \begin{array}{ll}
-\frac{1}{2\pi^2} \int_0^\infty \int_0^\pi \mathbf{A} \mathbf{H}_1(\rho) \mathbf{A}^T \mathbf{f} + \mathbf{A} \mathbf{H}_2 \mathbf{A}^T \mathbf{f} \mathbf{e}^{-i \mathbf{h} \cdot \mathbf{d} \cos \theta} d\xi_1 d\xi_2, & x_3 > d \\
\frac{1}{2\pi^2} \int_0^\infty \int_0^\pi \mathbf{A} \mathbf{H}_1(\rho) \mathbf{A}^T \mathbf{f} - \mathbf{A} \mathbf{H}_2 \mathbf{A}^T \mathbf{f} \mathbf{e}^{-i \mathbf{h} \cdot \mathbf{d} \cos \theta} d\xi_1 d\xi_2, & 0 \leq x_3 < d
\end{array} \right.
\]
(16)

To best manipulate the double integrals, the polar coordinate system is introduced. As seen below, this transformation allows integration over the radial variable to be carried out exactly. From Eq. (14), we have
\[
\xi_1 = \eta \cos \theta; \quad \xi_2 = \eta \sin \theta
\]
(19)

which converts Eq. (18) to
\[
\mathbf{u} = \left\{ \begin{array}{ll}
-\frac{1}{2\pi^2} \int_0^\infty \int_0^\pi \mathbf{A} \mathbf{Q}_1(\rho) \mathbf{A}^T \mathbf{f} \mathbf{e}^{-i \mathbf{h} \cdot \mathbf{d} \cos \theta} d\eta, & x_3 > d \\
\frac{1}{2\pi^2} \int_0^\infty \int_0^\pi \mathbf{A} \mathbf{Q}_1(\rho) \mathbf{A}^T \mathbf{f} \mathbf{e}^{-i \mathbf{h} \cdot \mathbf{d} \cos \theta} d\eta, & 0 \leq x_3 < d
\end{array} \right.
\]
(20)

Since \( \mathbf{A} \) and \( \mathbf{B} \) are independent of \( \eta \), the integral over \( \eta \) can be carried out exactly. With this, the displacement vector can be finally expressed as
\[
\mathbf{u}(x) = \left\{ \begin{array}{ll}
\frac{1}{2\pi^2} \int_0^\infty \int_0^\pi \mathbf{A} \mathbf{Q}_1(\rho) \mathbf{A}^T \mathbf{f} d\eta, & x_3 > d \\
\frac{1}{2\pi^2} \int_0^\infty \int_0^\pi \mathbf{A} \mathbf{Q}_1(\rho) \mathbf{A}^T \mathbf{f} d\eta, & 0 \leq x_3 < d
\end{array} \right.
\]
(21)

where
\[
[\mathbf{Q}_1(\rho)]_{ij} = \frac{\delta_{ij}}{\rho_i(x_3 - d) + x_1 \cos \theta + x_2 \sin \theta}
\]
(22)

\[
[\mathbf{Q}_2]_{ij} = \frac{\delta_{ij}}{\rho_i x_1 - \rho_i d + x_1 \cos \theta + x_2 \sin \theta}
\]
(23)

If the point-force vector \( \mathbf{f} \) is applied at a general point \( y \), the expression for the displacement vector in Eq. (21) remains the same, while Eq. (22) should be modified to
\[
[\mathbf{Q}_1(\rho)]_{ij} = \frac{\delta_{ij}}{\rho_i(x_3 - y_3) + (x_1 - y_1) \cos \theta + (x_2 - y_2) \sin \theta}
\]
(24)

It is observed that the Green’s function solution for the displacement contains two parts. The first part corresponds to the Green’s function in the full space, while the second part is the image one, which is induced by the free surface of the half-space. Notably, the full-space part of the Green’s function depends only on material properties. In what follows, we will use this expression to derive the elastic fields due to a dislocation of polygonal shape in a general homogeneous, elastically anisotropic 3D half-space.

3 The Elastic Fields Induced by a Dislocation of Polygonal Shape

A triangular shape serves as the fundamental unit for any polygon. An arbitrary polygonal surface can always be approximated by a summation of triangular elements. Therefore, the solution of a dislocation of polygonal shape can then be obtained from the solution of a dislocation of triangular shape via the method of
Consider the triangular dislocation shown in Fig. 2. Let the maximum value of \( x_3 \) on the dislocation loop be \( x_{3\text{max}} \) and the minimum \( x_3 \) be \( x_{3\text{min}} \). Substituting Eq. (24) into Eq. (8) gives the following expression for the displacement induced by a triangular dislocation.

Comparing Eq. (27) to Eq. (30), we observe that the denominators in the integrands of \( J_2 \) and \( D_2 \) can be, respectively, degenerated to those in \( J_1 \) and \( D_1 \) by letting \( p_3 = p_i \). Thus, we only need to analyze integrals \( J_2 \) and \( D_2 \). Moreover, since the numerators of the integrands in the expressions of \( J_2 \) and \( D_2 \) are independent of \( x \), their integrals are simply the power functions of \(-2 \) and \(-3 \). The power order is determined by the derivative order applied to the Green’s displacement function. For the \((n-1)\)th-order derivative, the power order is \( n \). Accordingly, the kernel integral on the triangular dislocation is generally

\[
F_{(n)}^\Delta(p^*, q^*) = \int_\Delta \frac{dS(x)}{[h(p^*) \cdot x - h(q^*) \cdot y]^n}
\]

superposition. With this in mind, we first derive the solution induced by a dislocation of triangular shape. Because of the importance of this solution, we will denote the associated quantities by a superscript triangle symbol.
where \( p^* \) and \( q^* \) can be assigned to different eigenvalues. It is important to note that in Eqs. (26), (29) and (31), the influence of the triangular shape of the dislocation on the displacements and strains induced by the dislocation is mainly contained in the integral, Eq. (31). Therefore the function \( F_n^h \) can be appropriately named the \( n \)-th order shape factor. When \( n = 2 \), \( F_2^h \) is the shape factor for the displacement, and when \( n = 3 \), it is the shape factor for the corresponding strain.

In order to carry out the area integration in Eq. (31), the local coordinate system \((P_i; \xi_1, \xi_2, \xi_3)\) with the base vectors \( \xi_i^0 \) \((i = 1,2,3)\) shown in Fig. 2 is introduced. The base vectors in the corresponding global coordinate system \((O; x_1, x_2, x_3)\) are \( x_i^0 \) \((i = 1,2,3)\). The transformation matrix between the local and global systems is therefore

\[
D_{ij} = x_i^0 \cdot \xi_j^0
\]  

(32)

The integral in Eq. (31) is then rewritten as

\[
F_n^h(p^*, q^*) = \int_0^1 d \xi ^2 _1 \int_{-1}^{1} d \xi _1 \int_0^1 \frac{d \xi _2}{h} \left[ f_1(p^*, q^*) \xi_1 + f_2(p^*, q^*) \xi_2 + f_3(p^*, q^*) \right]^n
\]  

(33)

where

\[
f_1(p^*, q^*) = D_{i3} h_i(p^*), \quad \alpha = 1, 2
\]  

(34)

\[
f_3(p^*, q^*) = h_i(p^*) p_{i3} - h_i(q^*) y_i
\]  

(35)

Integration of Eq. (33) for \( n = 2 \) and \( 3 \) gives

\[
F_2^h(p^*, q^*) = \left( \frac{1}{f_1} \ln f_1 + f_2 - \frac{1}{f_1} \ln f_3 + f_2 \right)
\]  

(36)

\[
F_3^h(p^*, q^*) = \frac{2}{h_2} \left( f_1 + f_2 \right) \left( f_2 + f_3 \right) \left( f_3 + f_2 \right)
\]  

(37)

For a polygonal dislocation constructed by \( N \) distinct (nonoverlapping) triangles, the shape factors are

\[
F_n(p^*, q^*) = \sum_{n=1}^{N} F_n^h(p^*, q^*)
\]  

(38)

Using Eqs. (26), (29) and (38), we finally obtain the following displacement field due to the polygonal dislocation,

\[
u_p(y) = \begin{cases} 
- \frac{1}{2 \pi^2} \int_0^y \left[ C_{ijkl} h_i h_j A_{kl} \left( A_{kl} D_{1il} (p_1) + A_{kl} D_{2il} \right) \right] d \theta, & y_3 > x_3 \max \\
1 \frac{1}{2 \pi^2} \int_0^y \left[ C_{ijkl} h_i h_j A_{kl} \left( A_{kl} D_{1il} (p_1) - A_{kl} D_{2il} \right) \right] d \theta, & y_3 < x_3 \min 
\end{cases}
\]  

(39)

where

\[
D_{1il} (p_1) = - \delta_{il} h_i(p_1) F_2(p_1, p_1)
\]  

\[
D_{2il} = - (B^{-1} B)_l h_i(p_1) F_2(p_1, p_1)
\]  

(40)

The corresponding strain field is

\[
u_{u,p}(y) = \begin{cases} 
- \frac{1}{2 \pi^2} \int_0^y \left[ C_{ijkl} h_i h_j A_{kl} \left( A_{kl} J_{1ilp} (p_1) + A_{kl} J_{2ilp} \right) \right] d \theta, & y_3 > x_3 \max \\
1 \frac{1}{2 \pi^2} \int_0^y \left[ C_{ijkl} h_i h_j A_{kl} \left( A_{kl} J_{1ilp} (p_1) - A_{kl} J_{2ilp} \right) \right] d \theta, & y_3 < x_3 \min 
\end{cases}
\]  

(41)

where

\[
J_{1ilp} (p_1) = -2 \delta_{il} h_i(p_1) h_j(p_1) F_3(p_1, p_1)
\]  

\[
J_{2ilp} = - (B^{-1} B)_l h_i(p_1) h_j(p_1) F_3(p_1, p_1)
\]  

(42)

The solutions presented here have two outstanding features. First, the generalized triple integrals for dislocation-induced displacements and strains have been reduced to a more mathematically convenient form of line integrals. Second, in either integral, Eq. (39) or integral, Eq. (41), the solution includes both the contribution from the full-space and image parts in the integrals for the strains when \( y_3 \in (x_3 \min, x_3 \max) \). Let us consider the contribution of the image part first. Based on the Green’s function in Eq. (24), it can easily be seen that the image part is continuous, signifying that the contribution of the image part in the integral for the strain is the same as that in Eq. (41). The contribution of the full-space part in the strain, however, is dealt with in a different way. The strategy in this case is to transform the integral of the full-space part to a new coordinate system and carry out the integral under this system. In this new coordinate system, the \( x_3 \)-axis is designated as the normal of the dislocation surface. This gives \( x_3 \max = x_3 \min \). On the dislocation surface, allowing the contribution of full-space part at any point in the full space to be evaluated by following the same procedure as that in Eq. (41). Accordingly, the derived formula will have the same form as the contribution of the full-space part in Eq. (41). In this treatment all material and geometrical properties, such as...
Fig. 3  Geometry of a regular hexagon dislocation where (O; x1, x2, x3) is the global coordinate system and (P0; n1, n2, n3) the local dislocation coordinate system

\[ C_{ijkl}, b_i, n_i \] and the positions of the vertex of the polygons must also be transformed to the new coordinate system. After obtaining the contribution of the full-space part under the new coordinates, then it is desirable to transform them back to the original global coordinates. This general approach also can be used to evaluate the dislocation-induced displacement field.

4 Numerical Examples

In this section, the displacements and stress fields induced by a hexagonal shaped dislocation lying within a half-space of a copper single crystal are analyzed by the new line-integral expressions derived in the present work. In face-centered cubic (fcc) crystals like copper, dislocation glide occurs along the \([1 1 1]\) slip planes in the \([1 1 0]\) slip direction. Without loss of generality, the hexagonal dislocation with the side length \(a\) in the present problem is placed on the \([1 1 0]\) slip plane and its Burgers vector \(b\) is parallel to \([1 1 0]\) within this plane (Fig. 3). The distance between the center of the hexagonal dislocation and the free surface of the half-space is \(4a\). Figure 3 shows the relationship between the local dislocation coordinates \((\eta; i = 1, 2, 3)\) and the global coordinates \((x_i; i = 1, 2, 3)\) as well as the locations of the four points A, B, C, D in our numerical calculation. For convenience, the displacements and stresses are normalized according to

\[
\begin{align*}
\tilde{u}_i &= u_i/b \\
\tilde{\sigma}_{ij} &= a \frac{\sigma_{ij}}{\sigma_{max}} \equiv \frac{\sigma_{ij}}{\sigma_{max}}
\end{align*}
\]

where \(\sigma_{max} = C_{11}\) is used to normalize the stress and \(b\) is the magnitude of the Burgers vector \(b\). The local and global coordinates are normalized to

\[
\begin{align*}
\tilde{\eta}_i &= \eta_i/a \\
\tilde{x}_i &= x_i/a
\end{align*}
\]

Numerical results for this problem are provided in Table 1 and Figs. 4–12, and are discussed next.

4.1 Validation on Boundary Conditions. The correctness of the proposed solution is first evaluated by checking the displacement discontinuity condition across the dislocation surface \(S\) and the traction-free boundary condition on the free surface of the half-space. For the former, the displacement jump between the upper \(S^+\) and lower \(S^-\) surfaces of the dislocation should equal the Burgers vector \(b\). The displacements at the four different points \(A = (0, 0, 0), B = (0.5, 0.4, 0), C = (-0.6, 0.3, 0)\) and \(D = (0, -0.7, 0)\) on the dislocation surface are calculated in the local \(\eta_i (i = 1, 2, 3)\) coordinates (Fig. 3). Specifically, the adjacent points on opposing sides of the dislocation surface associated with each one are \(A^+ = (0, 0, \pm \eta_3), B^+ = (0.5, 0.4, \pm \eta_3), C^+ = (-0.6, 0.3, \pm \eta_3)\) and \(D^+ = (0, -0.7, \pm \eta_3)\), where these coordinates have

\[
\begin{align*}
A^+ &= (0, 0, \pm \eta_3), B^+ = (0.5, 0.4, \pm \eta_3), C^+ = (-0.6, 0.3, \pm \eta_3), D^+ = (0, -0.7, \pm \eta_3) \text{ where } \eta_3 = 10^{-7}.
\end{align*}
\]

<table>
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<th>(u_1)</th>
<th>(u_2)</th>
<th>(u_3)</th>
<th>(\Delta u_1)</th>
<th>(\Delta u_2)</th>
<th>(\Delta u_3)</th>
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<td>0.95624814 \times 10^{-7}</td>
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<tr>
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<td>0.99763493</td>
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<td>&lt;10^{-10}</td>
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<tr>
<td>(B^-)</td>
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<tr>
<td>(C^+)</td>
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<td>&lt;10^{-9}</td>
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<tr>
<td>(C^-)</td>
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</tr>
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</table>

Note: \(A^+ = (0, 0, \pm \eta_3), B^+ = (0.5, 0.4, \pm \eta_3), C^+ = (-0.6, 0.3, \pm \eta_3), D^+ = (0, -0.7, \pm \eta_3)\) where \(\eta_3 = 10^{-7}\).
Fig. 5 Contour map of the normalized local displacement component $u_2/b$ in local coordinates $\eta_1/a$ and $\eta_2/a$ induced by a regular hexagonal dislocation, where $b$ is the magnitude of the Burgers vector.

Fig. 6 Contour map of the normalized local displacement component $u_3/b$ in local coordinates $\eta_1/a$ and $\eta_2/a$ induced by a regular hexagonal dislocation, where $b$ is the magnitude of the Burgers vector.

Fig. 7 Contour map of $(s_{11}+s_{22})/2$ normalized according to Eq. (43) in global coordinates, where the coordinates are normalized by the side length $a$ of the hexagonal dislocation with Burgers vector of magnitude $b$.

Fig. 8 Contour map of $(s_{11}-s_{22})/2$ normalized according to Eq. (43) in global coordinates, where the coordinates are normalized by the side length $a$ of the hexagonal dislocation with Burgers vector of magnitude $b$.

Fig. 9 Contour map of the normalized stress component $s_{12}$ (normalized according to Eq. (43)) in global coordinates, normalized by the side length $a$ of the hexagonal dislocation with Burgers vector of magnitude $b$.

Fig. 10 Contour map of the normalized displacement $(u_1+u_2)/2b$ in the normalized global coordinates $x_1/a$ and $x_2/a$ induced by a regular hexagonal dislocation with Burgers vector of magnitude $b$. 

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been normalized by \( a \) and \( t_3 = 10^{-7} \). The numerical results are listed in Table 1, and are compared to the given Burgers vector along the local \( g \)-direction. They clearly show that the displacement jump at these four points nearly coincide with the Burgers vector with a relative error in the displacement along \( g \) being below 0.5%. We mention that more accurate results can be obtained by increasing the Gaussian points for the line integral from 0 to \( \pi \), and/or by further subdividing the triangles into more regular ones. The displacements along the \( g_2 \)- and \( g_1 \)-directions are extremely small (below \( 10^{-8} \)), which is to be expected since there is no slip along the \( g_2 \)- and \( g_1 \)-directions.

We have also randomly selected some points on the surface of the half-space in order to calculate the stress. It is shown that the magnitudes of the normalized tractions on the surface of the half-space are all below \( 10^{-5} \). Therefore, the traction-free condition is also satisfied.

### 4.2 Displacement Field on the Dislocation Plane

For demonstration, displacements and stresses on the local plane \( \eta_1 = 0.1a \) are calculated. Figures 4–6 show the distributions of the normalized displacements \( u_1 \), \( u_2 \) and \( u_3 \), respectively, in the local coordinate system. As shown in Fig. 4, the distribution of the displacement \( u_1 \) is symmetric about the local axis \( g_2 \), while the distribution of displacements \( u_2 \) and \( u_3 \) in Figs. 5–6 are anti-symmetric. It should be noted that the symmetric or anti-symmetric characteristics of the induced fields strongly depend on the Burgers vector. In our examples, the Burgers vector is assumed to be along the \([1 1 0]\) direction. If, for instance, the Burgers vector is assumed to be along the local \( g_2 \)-axis, i.e., the \([1 1 2]\) direction, then the displacement \( u_2 \) will be symmetric about \( g_2 \), while the displacement \( u_1 \) becomes anti-symmetric. It should be also noted that the magnitude of the displacement \( u_1 \) at the center of the dislocation is nearly two orders of magnitude larger than others, except for near the corners of the hexagon.

### 4.3 Displacement and Stress Fields on the Free Surface

As mentioned in Sec. 4.1, our calculations using the present method verify that \( \sigma_{13} \), \( \sigma_{23} \) and \( \sigma_{33} \) on the free surface of the half-space are close to zero. The distributions of the remaining stress components on the free surface of the half-space in global coordinates are presented in Figs. 7–9. While both the \( \sigma_{11} \) and \( \sigma_{22} \) distributions are asymmetrical, the distributions of the hydrostatic stress \( \sigma_0 = (\sigma_{11} + \sigma_{22})/2 \) (Fig. 7) and biaxial stress \( \sigma_b = (\sigma_{11} - \sigma_{22})/2 \) (Fig. 8) possess obvious symmetry characteristics about the global line \( x_3 = x_1 \). The former is anti-symmetric and the latter is symmetric.

The distribution of \( \sigma_{12} \) (Fig. 9) in global coordinates is also anti-symmetric about \( x_2 = x_1 \).

Similar to the stresses, the distributions of the individual displacement components \( u_1 \) and \( u_2 \) in the global coordinates do not exhibit any particular symmetry property. However, the distribution of \( u_4 = (u_1 + u_2)/2 \), called the pseudohydrostatic displacement, and the distribution of \( u_6 = (u_1 - u_2)/2 \), the pseudobiaxial displacement, possess anti-symmetric and symmetric properties, respectively, as shown in Figs. 10–11. The \( u_1 \) distribution on the free surface shown in Fig. 12 is anti-symmetric about the line \( x_3 = x_1 \) and reaches its peak value around the points \((x_1, x_3) = (1, -3)\) and \((-3, 2)\) on the free surface \((x_3 = 0)\).

### 5 Discussions and Conclusions

In this paper, explicit expressions of the elastic displacement and stress fields due to an arbitrary dislocation loop in an anisotropic homogenous half-space are derived in terms of simple line integrals (from 0 to \( \pi \)). In the proposed integrals the influence of the shape of the polygonal dislocation on the elastic displacement and stress fields are all analytically contained in the integrand. Reduction from a surface integral to a line integral greatly improves the efficiency and accuracy on the calculation of the dislocation-induced elastic fields.

Based on the proposed method, the displacement and stress fields due to a hexagonal dislocation in a half-space of a copper crystal are obtained. Both the validity and precision of the method are well demonstrated by comparing the calculated displacement jump at the dislocation surface to the given Burgers vector and by checking the traction-free boundary condition on the free surface of the half-space. Results are also presented for the displacements and stresses on the global free surface of the half-space. These results could serve as benchmarks for numerical studies (utilizing, for instance, the finite element method) of similar dislocation problems in anisotropic crystals. The observed symmetric and anti-symmetric features of the elastic field distributions can provide insight when analyzing the influence and behavior of misfit dislocations present near free surfaces.

We mention that while the proposed unified integral interval (0, \( \pi \)) is more convenient to carry out and is furthermore independent of the loop shape, special numerical schemes are needed for handling the situation where the dislocation loop intersects with the free surface of the half space [26,27]. For example, the self-energy of an elliptic dislocation loop was derived in anisotropic elastic media and further corrected for one-dimensional core/shell nanowires by combining the boundary element method [26]. This solution was successfully in predicting the critical shell thickness corresponding to the defect-free core/shell nanowires [26].
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References