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Three-dimensional elastic displacements induced by a dislocation of polygonal shape in anisotropic elastic crystals

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ABSTRACT

Dislocations and the elastic fields they induce in anisotropic elastic crystals are basic for understanding and modeling the mechanical properties of crystalline solids. Unlike previous solutions that provide the strain and/or stress fields induced by dislocation loops, in this paper, we develop, *for the first time*, an approach to solve the more fundamental problem—the anisotropic elastic dislocation displacement field. By applying the point-force Green's function for a three-dimensional anisotropic elastic material, the elastic displacement induced by a dislocation of polygonal shape is derived in terms of a simple line integral. It is shown that the singularities in the integrand of this integral are all removable. The proposed expression is applied to calculate the elastic displacements of dislocations of two different fundamental shapes, i.e. triangular and hexagonal. The results show that the displacement jump across the dislocation loop surface exactly equals the assigned Burgers vector, demonstrating that the proposed approach is accurate. The dislocation-induced displacement contours are also presented, which could be used as benchmarks for future numerical studies.

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1. Introduction

The presence of dislocations and induced elastic fields strongly influence the material properties of crystalline solids, such as the crystal growth (Rupert et al., 2009; Rajgarhia et al., 2009), the mechanical strength (Püschl, 2002; Kurzic, 2009) and other related physical properties (Bai et al., 2001; Gromov et al., 2010). The elastic fields induced by dislocations were widely studied in the past (Mura, 1963; Willis, 1970; Hirth and Lothe, 1982; Ting, 1996; Lubarda, 2003; Ghoniem and Han, 2005; Paynter and Nowell, 2005; Paynter and Hills, 2009). Generally, the elastic fields due to dislocation loops in three-dimensional (3D) homogeneous solids can be evaluated by the integrals of the point-force Green's function and its derivatives over the dislocation surfaces (Mura, 1963; Willis, 1970; Wang, 1996). These surface integrals for the stress field or strain field were reduced to the integrals along the dislocation line by means of Stokes' theorem (Mura, 1987). Moreover, Willis (1970) found the analytical expression of the stress field for a straight segment of a dislocation loop in an anisotropic solid. Gosling and Willis (1994) derived a line integral for the stresses due to an arbitrary dislocation in an isotropic half-space. Wang (1996) discussed the integral along curved segments and presented a derivation for

the stress field induced by a curved dislocation loop. Obviously, reducing the surface integral to a line integral, or even to an analytical expression, is advantageous computationally and provides more accurate results and insight. However, in general, reductions to line integrals or analytical expressions have been applied for predictions of the dislocation-induced stress and/or strain field only, but not for the associated displacement field. As for the latter, Lerma et al. (2003) obtained the displacement field due to a symmetrical prism dislocation in isotropic solids. Ghoniem and Sun (1999) presented a line integral for an arbitrarily shaped dislocation loop in an isotropic material.

The major difficulty in reducing the surface integral in the expression for the displacement field induced by dislocations in anisotropic materials to a line integral is that the Stokes' theorem cannot be utilized. The displacement integral expression does not satisfy the conditions that are required in applying the Stokes' theorem. To the best of our knowledge, no explicit result or line integral expression has been reported for the elastic displacement field produced by the dislocation loops in 3D generally anisotropic media. In this paper, a line integral (from 0 to π) expression for the elastic displacement field induced by a triangular dislocation is derived by using the point-force Green's function in the Stroh formalism. With this fundamental solution, the solution to an arbitrary polygonal dislocation can be constructed by the method of superposition. The influence of dislocation shape is included in the integrand.

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This paper is organized as follows. In the next section, we first describe the problem of interest in brief and then review some relevant expressions for the point-force Green's function and the displacement field due to a dislocation loop. In Section 3, a line integral expression for the displacement field is achieved by integrating the triple integrals for a triangular dislocation. A discussion on the singularity concludes this section. Next, in section 4, numerical examples are provided for some fundamental dislocation loop configurations. Here, the efficiency and accuracy of the derived displacement solution is demonstrated. Conclusions are drawn in the final section.

2. Problem description and some applicable formula in anisotropic elastic materials

Consider an arbitrarily shaped dislocation loop located in an elastic and anisotropic solid as shown in Fig. 1. The dislocation loop is denoted by the surface *S*. In order to describe the dislocation, the dislocation surface is divided into two adjacent surfaces: S^+ with its normal n^+ and S^- with its normal n^- . The upper surface S^+ slips by **b** relative to the lower surface S^- , i.e.

$$\boldsymbol{b} = \boldsymbol{u}^+ - \boldsymbol{u}^- \tag{1}$$

where **b** is called the Burgers vector. According to the Volterra formula (Volterra, 1907), the displacement field due to the dislocation loop can be expressed as

$$u_k(\boldsymbol{y}) = \int_{S} C_{ijml} G_{mk,l}(\boldsymbol{y}; \boldsymbol{x}) b_j n_i \mathrm{d}S \tag{2}$$

where C_{ijml} denotes the elastic stiffness tensor, n_i equal to n_i^- is the component of the normal vector of the dislocation surface. The Green's function $G_{mk}(\mathbf{y}; \mathbf{x})$ denotes the displacement in *m*-direction at the field point \mathbf{x} due to a point force in *k*-direction applied at the source point \mathbf{y} . By considering the corresponding relation between the eigenstrain and the dislocation Burgers vector, Mura (1963) obtained a similar expression for the displacement field due to a dislocation loop.

There are several ways to construct the point-force Green's function in 3D anisotropic materials (Wang, 1997; Ting and Lee, 1997; Ting, 2000; Pan and Yuan, 2000; Tonon et al., 2001). One well-known method is to apply the Fourier transform method



Fig. 1. Geometry of an arbitrarily shaped dislocation loop *S* in an anisotropic, elastic, and infinite space E^3 . The vector **b** denotes the Burgers vector of the dislocation, which is equal to the displacement jump across the dislocation surface. The vector \mathbf{n}^+ denotes the normal of the surface S^+ towards S^- , and $\mathbf{n}^- = -\mathbf{n}^+$.

(Mura, 1987). Consequently, the solution for the general anisotropic media often includes the 3D infinite integral associated with the inverse Fourier transform. With some mathematical manipulations, it can be shown that the inverse transform integral can be reduced to a line integral. Another method is the Radon transform (Tonon et al., 2001). Recalling Eq. (2), one can easily observe that, in general, the displacements due to dislocation loops are expressed in terms of triple integrals. In this paper, we will show how the triple integrals can be reduced to a line integral.

To this end, we first present the Green's function solutions in terms of the Stroh formalism. Consider a point force f applied at (0,0,d) in an anisotropic material. For brevity, bold symbols will be used for tensors and vectors. The main idea here is to divide the full space into two half spaces. One is in the domain with $x_3 > d$ and the other in $x_3 < d$. In each half space, the two-dimensional Fourier transforms

$$\tilde{u}_{k}(\xi_{1},\xi_{2},x_{3}) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} u_{k}(x_{1},x_{2},x_{3}) e^{i(x_{1}\xi_{1}+x_{2}\xi_{2})} dx_{1} dx_{2}$$
(3)

are applied. In the Fourier transformed domain, the equilibrium equation in the source-free domain is

$$C_{i\alpha k\beta}\xi_{\alpha}\xi_{\beta}\tilde{u}_{k} + i(C_{i\alpha k3} + C_{i3k\alpha})\xi_{\alpha}\tilde{u}_{k,3} - C_{i3k3}\tilde{u}_{k,33} = 0$$

$$\tag{4}$$

The general solution of Eq. (4) in Fourier transformed domain is

$$\tilde{\boldsymbol{u}}(\xi_1,\xi_2,\boldsymbol{x}_3) = \boldsymbol{a} \exp(-i \ p\eta \boldsymbol{x}_3) \tag{5}$$

where *p* and *a* satisfy the following Stroh eigenequation:

$$[\mathbf{Q} + p(\mathbf{R} + \mathbf{R}^T) + p^2 \mathbf{T}]\mathbf{a} = 0$$
(6)

with

$$\mathbf{Q}_{ij} = \mathbf{C}_{ikjs} \mathbf{n}_k \mathbf{n}_s, \quad \mathbf{R}_{ik} = \mathbf{C}_{ikjs} \mathbf{n}_k \mathbf{m}_s, \quad \mathbf{R}_{ik} = \mathbf{C}_{ikjs} \mathbf{n}_k \mathbf{m}_s$$

$$\mathbf{n} = [\cos\theta, \sin\theta, 0]^T, \quad \mathbf{m} = [0, 0, 1]^T, \quad \boldsymbol{\xi} = \eta \mathbf{n}$$
(7)

where the superscript '*T* denotes the transpose of the matrix. Suppose p_i , \boldsymbol{a}_i (i = 1,2,...,6) are the eigenvalues and the associated eigenvectors, respectively. We let

$$Im(p_i) > 0, \quad p_{i+3} = \bar{p}_i, \quad \bar{\boldsymbol{a}}_{i+3} = \bar{\boldsymbol{a}}_i, \quad (i = 1, 2, 3)$$

$$\boldsymbol{A} \equiv [\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3], \quad \boldsymbol{B} \equiv [\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3] \text{ with } \boldsymbol{b}_i = (\boldsymbol{R}^T + p_i \mathbf{T}) \boldsymbol{a}_i$$
(8)

where the symbol 'Im' and the over bar denote the imaginary part and the complex conjugate, respectively. There is no summation over the repeated index i in Eq. (8).

By considering the displacement continuity and the traction condition at $x_3 = d$, we finally get

$$\tilde{u}(\xi_1,\xi_2,\mathbf{x}_3) = \begin{cases} -i\eta^{-1}\overline{\mathbf{A}}\langle e^{-ip_*\eta(\mathbf{x}_3-d)}\rangle\overline{\mathbf{A}}^T \mathbf{f}, & \mathbf{x}_3 > d\\ i\eta^{-1}\mathbf{A}\langle e^{-ip_*\eta(\mathbf{x}_3-d)}\rangle\mathbf{A}^T \mathbf{f}, & \mathbf{x}_3 < d \end{cases}$$
(9)

where the symbol $\langle \cdot \rangle$ denotes the diagonal matrix. The subscript "*" represents 1, 2 and 3, which corresponds to the three diagonal elements.

By applying the Fourier inverse transform to Eq. (9), the pointforce Green's function displacement in the physical domain can be expressed as

$$\boldsymbol{u}(x_{1},x_{2},x_{3}) = \begin{cases} \frac{-i}{4\pi^{2}} \int \int \eta^{-1} \overline{\mathbf{A}} \langle e^{-ip_{*}\eta(x_{3}-d)} \rangle \overline{\mathbf{A}}^{T} \boldsymbol{f} e^{-i(x_{1}\xi_{1}+x_{2}\xi_{2})} d\xi_{1} d\xi_{2}, \ x_{3} > d \\ \frac{i}{4\pi^{2}} \int \int \eta^{-1} \mathbf{A} \langle e^{-ip_{*}\eta(x_{3}-d)} \rangle \mathbf{A}^{T} \boldsymbol{f} e^{-i(x_{1}\xi_{1}+x_{2}\xi_{2})} d\xi_{1} d\xi_{2}, \ x_{3} < d \end{cases}$$
(10)

Making use of the last expression in Eq. (7) and introducing a polar coordinate transform, we have

$$\xi_1 = \eta \cos \theta \tag{11}$$

$$\xi_2 = \eta \sin \theta \tag{11}$$

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Therefore, Eq. (10) becomes

$$\boldsymbol{u}(x_1, x_2, x_3) = \begin{cases} \frac{-i}{4\pi^2} \int_0^{2\pi} \mathrm{d}\theta \int_0^{\infty} \overline{\mathbf{A}} \langle \mathbf{e}^{-ip, \eta(x_3 - d)} \rangle \overline{\mathbf{A}}^T \mathbf{f} \mathbf{e}^{-i\eta(x_1 \cos\theta + x_2 \sin\theta)} \mathrm{d}\eta, & x_3 > d \\ \frac{i}{4\pi^2} \int_0^{2\pi} \mathrm{d}\theta \int_0^{\infty} \mathbf{A} \langle \mathbf{e}^{-ip, \eta(x_3 - d)} \rangle \mathbf{A}^T \mathbf{f} \mathbf{e}^{-i\eta(x_1 \cos\theta + x_2 \sin\theta)} \mathrm{d}\eta, & x_3 < d \end{cases}$$
(12)

Since the matrices A, A^T and their complex conjugates are independent of the radial integrating variable η , the integral with respect to η can be performed analytically, i.e.

$$\boldsymbol{u}(x_1, x_2, x_3) = \begin{cases} \frac{1}{2\pi^2} \int_0^{\pi} \overline{\mathbf{A}} \left\langle \frac{-1}{\overline{p_*}(x_3 - d) + x_1 \cos \theta + x_2 \sin \theta} \right\rangle \overline{\mathbf{A}}^T \boldsymbol{f} d\theta, & x_3 > d \\ \frac{1}{2\pi^2} \int_0^{\pi} \mathbf{A} \left\langle \frac{1}{p_*(x_3 - d) + x_1 \cos \theta + x_2 \sin \theta} \right\rangle \mathbf{A}^T \boldsymbol{f} d\theta, & x_3 < d \end{cases}$$
(13)

In writing Eq. (13), the periodical properties of the integrand have been used to reduce the upper limit of the integral from 2 π to π (Ting, 2000).

Therefore, the Green's function matrix due to a point force applied at y is

$$\boldsymbol{G}(\boldsymbol{y};\boldsymbol{x}) = \begin{cases} \frac{-1}{2\pi^2} \int_0^{\pi} \overline{\mathbf{A}} \mathbf{H}(\bar{p}_*,\boldsymbol{y}) \overline{\mathbf{A}}^T \mathrm{d}\theta, & x_3 > d \\ \frac{1}{2\pi^2} \int_0^{\pi} \mathbf{A} \mathbf{H}(p_*,\boldsymbol{y}) \mathbf{A}^T \mathrm{d}\theta, & x_3 < d \end{cases}$$
(14)

with

$$H_{ij}(p_*, \mathbf{y}) = \frac{\delta_{ij}}{p_i(x_3 - d) + (x_1 - y_1)\cos\theta + (x_2 - y_2)\sin\theta}$$
(15)

where there is no summation over the repeated index *i*. Substituting Eq. (14) into Eq. (2), one can easily find that the displacement field induced by dislocation loops actually involves a triple integral. For the stress or strain field, by means of the Stokes' theorem, the integration over the dislocation surface can be reduced to a line integral along the boundary of the dislocation loop. However, the expression of the displacement field prevents us from making use of Stokes' theorem.

3. The displacement field induced by polygonal dislocations

A triangular element can be regarded as a fundamental unit for constructing any arbitrary shaped polygon dislocation surface. A polygon dislocation can be built using a combination of two or more triangles, possibly differing in size. (A set that involves the least number of triangles is clearly optimal.) This fact implies that once we solve the displacement field for a single triangular dislocation, the displacement field due to a polygonal dislocation can be obtained by superposition of the fields of its component triangles. It is interesting to note that the triangular dislocation itself can be used to model the macroscopic plastic flow (McKellar et al., 2003).

We consider a triangular dislocation as shown in Fig. 2. We assume that the maximum and minimum values for x_3 on the dislocation loop are x_{3max} and x_{3min} . Substituting Eq. (14) into Eq. (2), we obtain the displacement field induced by a triangular dislocation, i.e.

$$u_{k}^{\Delta}(\boldsymbol{y}) = \begin{cases} \frac{-1}{2\pi^{2}} \int_{0}^{\pi} \mathrm{d}\theta \int_{\Delta} C_{ijml} [\bar{\boldsymbol{\mathsf{A}}}\boldsymbol{\mathsf{H}}(\bar{p}_{*},\boldsymbol{y})\boldsymbol{\mathsf{A}}^{T}]_{mk,l} b_{j} n_{i} \mathrm{d}S(\boldsymbol{x}), & y_{3} > x_{3\max} \\ \frac{1}{2\pi^{2}} \int_{0}^{\pi} \mathrm{d}\theta \int_{\Delta} C_{ijml} [\bar{\boldsymbol{\mathsf{A}}}\boldsymbol{\mathsf{H}}(p_{*},\boldsymbol{y})\boldsymbol{\mathsf{A}}^{T}]_{mk,l} b_{j} n_{i} \mathrm{d}S(\boldsymbol{x}), & y_{3} < x_{3\min} \end{cases}$$
(16)

Since the eigenvector matrix A is independent of the integral variable over the dislocation surface, Eq. (16) can be written as:

.

$$u_{k}^{\Delta}(\mathbf{y}) = \begin{cases} \frac{-1}{2\pi^{2}} \int_{0}^{\pi} \left[C_{ijml} b_{j} n_{i} \overline{A}_{mt} A_{sk}^{T} \int_{\Delta} H(\bar{p}_{*}, \mathbf{y})_{ts, x_{l}} dS(\mathbf{x}) \right] d\theta, & y_{3} > x_{3 \max} \\ \frac{-1}{2\pi^{2}} \int_{0}^{\pi} \left[C_{ijml} b_{j} n_{i} A_{mt} A_{sk}^{T} \int_{\Delta} H(p_{*}, \mathbf{y})_{ts, x_{l}} dS(\mathbf{x}) \right] d\theta, & y_{3} > x_{3 \min} \end{cases}$$
(17)



Fig. 2. Geometry of a triangular dislocation with corners P_1 , P_2 , P_3 with respect to the global coordinate system ($\mathbf{0}$; x_1, x_2, x_3) and local coordinate system (\mathbf{x}_0 ; ξ_1, ξ_2, ξ_3) where $h = \xi_2(P_1)$, $l_1 = -\xi_1(P_2)$, $l_2 = \xi_1(P_3)$. Obviously, l_1 and l_2 can be negative.

By applying Eq. (15), the surface integral involved in Eq. (17) becomes

$$\begin{cases} \int_{\Delta} H(\bar{p}_{*}, \boldsymbol{y})_{ts, \boldsymbol{x}_{l}} dS(\boldsymbol{x}) = \int_{\Delta} \frac{-\delta_{ts} h_{l}(\bar{p}_{t})}{|\mathbf{h}(\bar{p}_{t})\cdot(\boldsymbol{x}-\boldsymbol{y})|^{2}} dS(\boldsymbol{x}) \\ \int_{\Delta} H(p_{*}, \boldsymbol{y})_{ts, \boldsymbol{x}_{l}} dS(\boldsymbol{x}) = \int_{\Delta} \frac{-\delta_{ts} h_{l}(p_{t})}{|\mathbf{h}(p_{t})\cdot(\boldsymbol{x}-\boldsymbol{y})|^{2}} dS(\boldsymbol{x}) \end{cases}$$
(18)

where there is no summation over the repeated index t, and the vector h is defined as

$$\boldsymbol{h}(\boldsymbol{p}) = [\cos\theta, \sin\theta, \boldsymbol{p}]^{T}$$
(19)

Since the numerators of the integrands in Eq. (18) are independent of **x**, their integrals are simply power functions (to the power of -2). Since the two integrals in Eq. (18) have a similar mathematical form, the kernel integral on the triangular dislocation can be expressed as:

$$F_2(\boldsymbol{y},\theta) = \int_{\Delta} \frac{\mathrm{d}S(\boldsymbol{x})}{\left[\boldsymbol{h}(\boldsymbol{p}) \cdot (\boldsymbol{x} - \boldsymbol{y})\right]^2}$$
(20)

where *p* can be assigned to different eigenvalues. In order to carry out the area integration over a flat triangle in Eq. (20), a local coordinate system (\mathbf{x}_0 : ξ_1, ξ_2, ξ_3) with the base vectors $\xi_i^0(i = 1, 2, 3)$ is introduced as shown in Fig. 2. The base vectors of the global coordinate system ($\mathbf{0}$: x_1, x_2, x_3) are $x_i^0(i = 1, 2, 3)$. Thus, the transformation matrix between the two systems is (super 0 denotes the base vector)

$$D_{ij} = \boldsymbol{x}_i^0 \cdot \boldsymbol{\xi}_j^0 \tag{21}$$

Therefore, the relation between the global and local coordinates is

$$[\boldsymbol{x} - \boldsymbol{x}_0] = [\mathbf{D}][\boldsymbol{\xi}] \tag{22}$$

Then, the integration in Eq. (20) becomes

$$F_{2}(\mathbf{y},\theta) = \int_{0}^{h} d\xi_{2} \int_{-l_{1}+l_{1}\xi_{2}/h}^{l_{2}-l_{2}\xi_{2}/h} d\xi_{1} \\ \times \frac{1}{\left[f_{1}(\mathbf{y},\theta)\xi_{1}+f_{2}(\mathbf{y},\theta)\xi_{2}+f_{3}(\mathbf{y},\theta)\right]^{2}}$$
(23)

where

$$f_{\alpha}(\mathbf{y},\theta) = D_{k\alpha}h_{k}(p), \quad \alpha = 1,2$$

$$f_{3}(\mathbf{y},\theta) = (\mathbf{x}_{0k} - \mathbf{y}_{k})h_{k}(p)$$
(24)
(25)

The results are

$$F_2(y,\theta) = \frac{1}{f_1} \left(\frac{1}{f_2 + f_1 l_1^*} \ln \frac{f_3^* + f_2}{f_3^* - f_1 l_1^*} - \frac{1}{f_2 - f_1 l_2^*} \ln \frac{f_3^* + f_2}{f_3^* + f_1 l_2^*} \right)$$
(26)

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with

$$l_1^* = l_1/h, \quad l_2^* = l_2/h, \quad f_3^* = f_3/h$$
(27)

Thus, we have obtained the exact solution for the integral H over an arbitrary triangular dislocation. Substituting these analytical results to Eq. (17), we have then successfully reduced the original triple integrals of the displacements into a simple line integral from 0 to π .

Before analyzing the displacement field, we will need to address three possible singularities in Eq. (26) associated with

1)
$$f_2 + f_1 l_1^* = 0$$
; 2) $f_2 - f_1 l_2^* = 0$; 3) $f_1 = 0$ (28)

These singularities are independent of the field point y, but dependent on the integration variable θ . This implies that they could influence the numerical results at any field point y. For this reason we examine their characteristics below.

For the first case, Eq. (26) can be written equivalently as

$$F_{2}(y,\theta) = \frac{1}{f_{1}} \left[\frac{1}{f_{2} + f_{1}l_{1}^{*}} \ln \left(1 + \frac{f_{1}l_{1}^{*} + f_{2}}{-f_{1}l_{1}^{*} + f_{3}^{*}} \right) - \frac{1}{f_{2} - f_{1}l_{2}^{*}} \ln \frac{f_{2} + f_{3}^{*}}{f_{1}l_{2}^{*} + f_{3}^{*}} \right]$$
(29)

When $f_2 + f_1 l_1^* \rightarrow 0$, according to the Taylor series expansion, we have

$$F_{2}(y,\theta) = \frac{1}{f_{1}} \left\{ \frac{1}{f_{3}^{*} - f_{1}l_{1}^{*}} \sum_{n=1}^{\infty} \frac{1}{n} \left(-\frac{f_{1}l_{1}^{*} + f_{2}}{f_{3}^{*} - f_{1}l_{1}^{*}} \right)^{n-1} - \frac{1}{f_{2} - f_{1}l_{2}^{*}} \ln \frac{f_{2} + f_{3}^{*}}{f_{1}l_{2}^{*} + f_{3}^{*}} \right\}$$
(30)

Similarly, for the second case, i.e. $f_2 - f_1 l_2^* \rightarrow 0$, we have

$$F_{2}(y,\theta) = \frac{1}{f_{1}} \left\{ \frac{1}{f_{2} + f_{1}l_{1}^{*}} \ln\left(\frac{f_{2} + f_{3}^{*}}{-f_{1}l_{1}^{*} + f_{3}^{*}}\right) - \frac{1}{f_{1}l_{2}^{*} + f_{3}^{*}} \sum_{n=1}^{\infty} \frac{1}{n} \left(-\frac{f_{2} - f_{1}l_{2}^{*}}{f_{1}l_{2}^{*} + f_{3}^{*}}\right)^{n-1} \right\}$$
(31)

For the third case, i.e., $f_1 \rightarrow 0$, Eq. (26) can be rewritten as

$$F_{2}(\boldsymbol{y},\theta) = \frac{l_{1}^{*} \ln \frac{I_{2}^{*}+I_{1}I_{2}^{*}}{f_{3}^{*}+f_{2}^{*}} + l_{2}^{*} \ln \frac{I_{2}^{*}-I_{1}I_{1}^{*}}{f_{3}^{*}+f_{2}^{*}} + \frac{f_{2}}{f_{1}} \ln \left(1 + \frac{f_{1}I_{1}^{*}+f_{1}I_{2}^{*}}{f_{3}^{*}-f_{1}I_{1}^{*}}\right)}{(f_{2} + f_{1}I_{1}^{*})(f_{2} - f_{1}I_{2}^{*})}$$
(32)

When $f_1 \rightarrow 0$, by mean of the series expansion, we have

$$F_{2}(y,\theta) = \frac{1}{(f_{2} + f_{1}l_{1}^{*})(f_{2} - f_{1}l_{2}^{*})} \begin{cases} l_{1}^{*} \ln \frac{f_{3}^{*} + f_{1}l_{2}^{*}}{f_{3}^{*} + f_{2}} + l_{2}^{*} \ln \frac{f_{3}^{*} - f_{1}l_{1}^{*}}{f_{3}^{*} + f_{2}} \\ + \frac{f_{2}(l_{1}^{*} + l_{2}^{*})}{f_{3}^{*} - f_{1}l_{1}^{*}} \sum_{n=1}^{\infty} \left[\frac{f_{1}(l_{1}^{*} + l_{2}^{*})}{f_{3}^{*} - f_{1}l_{1}^{*}} \right]^{n-1} \end{cases}$$
(33)

Therefore, all three singularities are removable. Other singularities, such as $f_3^* + f_2 \rightarrow 0$, $f_3^* - f_1 l_1^* \rightarrow 0$ and $f_3^* + f_1 l_2^* \rightarrow 0$ are possible, but because these only occur at special points, they will not be discussed in this paper.

It should be emphasized that Eq. (16) and the subsequent equations are not suitable for a field point **y** with coordinate components $y_3 \in (x_{3\min}, x_{3\max})$. To deal with this problem, we divide the triangular dislocation with corners P_1 , P_2 and P_3 into two parts (Fig. 3): One is $x_3 < y_3$, i.e. $\Delta P_4P_1P_5$; the other is $x_3 > y_3$, i.e. the quadrangle $P_1P_4P_5P_3$, where P_4 and P_5 are the points of the intersection of the triangular dislocation and the plane $x_3 = y_3$. For the quadrangular part, it can be divided into two sub-triangles. Therefore, when $y_3 \in (x_{3\min}, x_{3\max})$, the original triangular dislocation can be divided into three sub-triangles. (When $y_3 = x_3(P_1)$, there are only two sub-triangles.) For each sub-triangle, we can use Eq. (16) and related formulae.

As mentioned earlier, any arbitrary polygonal dislocation can be represented as a combination of triangles. Thus the displacement field of the polygonal dislocation is obtained by superposing the results of the triangular dislocations that constitute the polygonal dislocation.



Fig. 3. Partition of a triangular dislocation into three sub-triangles, when the coordinate component y_3 of the field point y is located between the x_{3min} and x_{3max} . P_4 and P_5 are points lying along the intersection line of the dislocation loop and the plane $x_3 = y_3$. When $y_3 = x_3(P_1)$, there are only two sub-triangles in the partition.

4. Numerical examples

In this section, the derived line integral expression is used to calculate the displacement field induced by triangular and hexagonal dislocations in a copper crystal.

4.1. Displacement field from a triangular dislocation loop in a copper crystal

Copper has a face-centered cubic (fcc) crystal structure. Dislocations in copper glide easily on the {1 1 1} planes of highest atomic density in the close packed $\langle 110 \rangle$ direction. As an example, consider a dislocation loop modeled as a regular triangle with side length *a* lying in the (1 1 1) slip plane (Fig. 4). The displacement jump across the upper S⁺ and lower S⁻ surfaces bounded by the dislocation is equal to its Burgers vector **b**. We define a local orthogonal coordinate system (ξ_1, ξ_2, ξ_3), where ξ_3 is parallel to the slip plane normal [1 1 1] and ξ_1 coincides with the slip direction [-1 1 0].

We first check our line integral expression by applying it to predict the displacement jump for any point lying within the slipped region of this dislocation. Fig. 4 shows the positions of the four points *A*, *B*, *C* and *D* chosen for this calculation. Because the dislocated surface is discontinuous, it is necessary to calculate the dis-



Fig. 4. Geometry of a regular triangular dislocation with corners P_1 , P_2 , P_3 in local coordinates (\mathbf{x}_0 ; ξ_1 , ξ_2 , ξ_3) and the selected points *A*, *B*, *C*, *D* within the slipped region of the dislocation plane.

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Numerical results of the displacement jumps across the dislocation plane at points *A*, *B*, *C*, and *D*. All data are in the local coordinates and are normalized by the Burgers vector magnitude *b*. The superscript "+" and subscript "-" denote, respectively, the points on the upper and lower surfaces of the dislocation.

Field points	<i>u</i> ₁	<i>u</i> ₂	<i>u</i> ₃	Δu_1	Δu_2	Δu_3
A^+	0.50097566	0.00000000	0.00000000	0.99823045	0.00000000	0.00000000
A^-	-0.49725479	0.0000000	0.0000000			
B^+	0.50038775	0.0000000	0.00000000	0.99881769	0.00000000	0.00000000
B^{-}	-0.49842994	0.0000000	0.0000000			
C^+	0.49986823	0.00018151	0.03156048	0.99858703	-0.0000015	0.0000002
C-	-0.49871880	0.00018166	0.03156046			
D^{+}	0.49687362	-0.00254462	0.07911198	0.99658039	-0.00016644	0.0000025
D^{-}	-0.49970677	-0.00237818	0.07911173			

placements at these points on both the upper and lower surfaces, denoted as A^{\pm} , B^{\pm} , C^{\pm} and D^{\pm} . For instance, $A^{\pm} = (\xi_{A1}, \xi_{A2}, \pm \xi_3)$, with ξ_3 being very small (i.e., $\xi_3 = 10^{-5}$). The numerical results are listed in Table 1, where the displacements are normalized by the magnitude of the Burgers value *b*. Table 1 shows that the displacement

jump at the four points almost coincide with the Burgers vector. The relative error of the displacement along ξ_1 is below 0.2% at the points *A*, *B* and *C*, and below 0.4% at the point *D*. Due to the symmetry, the displacements at *A* and *B* along ξ_2 and ξ_3 are zero. The numerical results at points *A* and *B* are below 10^{-16} . Thus, the accuracy of the proposed method is demonstrated.



Fig. 5. Contour map of the normalized local displacement component u_1/b in local coordinates ξ_1/b and ξ_2/b induced by a triangular dislocation with the Burgers vector magnitude *b*. The normalized side length of the triangle is a/b.



Fig. 6. Contour map of the normalized local displacement component u_2/b in local coordinates ξ_1/b and ξ_2/b induced by a triangular dislocation with the Burgers vector magnitude *b*. The normalized side length of the triangle is a/b.

Fig. 7. Contour map of the normalized local displacement component u_3/b in local coordinates ξ_1/b and ξ_2/b induced by a triangular dislocation with the Burgers vector magnitude *b*. The normalized side length of the triangle is a/b.

Fig. 8. Geometry of a regular hexagonal dislocation, which is divided into four subtriangular dislocations, where the ξ_1 -axis points to $[-1 \ 1 \ 0]$ and ξ_2 -axis points to $[-1 \ -1 \ 2]$.

The contour maps for the normalized displacements u_1 , u_2 , and u_3 in the local coordinates (ξ_1, ξ_2, ξ_3) due to the triangle dislocation are shown in Figs. 5–7 respectively. In these figures, the plane is $\xi_3 = 0.01a$, and the local coordinates ξ_1 and ξ_2 are both normalized by *b*.

As shown in Fig. 5, the displacement component u_1 is symmetric, as expected from the loop geometry with respect to the crystal structure. It is observed that, except for the upper region, the displacement u_1 in the ξ_1 -direction is positive, and that its values inside the dislocation triangle are much larger than those outside. In fact, Table 1 shows that the latter tends to 0.5, as $\xi_3 \rightarrow 0$. The high density of contour lines at the dislocation boundary region implies that the strain and stress fields in the boundary region are quite large and may even have singularities. This phenomenon is consistent with analytical formula for the stress field given in (Willis, 1970; Wang, 1996).

Shown in Figs. 6,7 are the u_2 and u_3 displacement distributions in the ξ_{2^-} and ξ_3 -directions. Note that both distributions are asymmetric about the ξ_2 -axis. The displacements inside the dislocation region have the same order of magnitude compared to those outside, which is quite different from the results shown in Fig. 5 where they differ by two-orders of magnitude. At the base of the triangle, the transition between the contours is smooth, and therefore the strain component $u_{2,2}$ in the local coordinates is continuous at this edge.

4.2. Displacement field from a hexagonal dislocation loop in a copper crystal

We consider now a dislocation loop in the shape of a regular hexagon, which lies on the $(1 \ 1 \ 1)$ slip plane, as illustrated in Fig. 8. As before, the Burgers vector **b** lies along $[-1 \ 1 \ 0]$. The length of each side of the hexagon is *a*. The distributions for the three displacements u_1 , u_2 , and u_3 on the plane $\xi_3 = 0.1a$ are shown in Figs. 9–11, respectively. It is observed in Fig. 9 that the u_1 distribution is symmetric about the ξ_1 - and ξ_2 -axes. On the other hand, as shown in Figs. 10,11, the distributions of u_2 and u_3 are asymmetric about the ξ_2 -axis. These characteristics are consistent with the combined symmetric condition of the crystal property, the dislocation geometry and the direction of the Burgers vector. Note from Fig. 9 that u_1 reaches its peak value at the center $(\xi_1, \xi_2, \xi_3) = (0, 0, 0.1a)$ and decreases with increasing distance away from the center. This reduction occurs more rapidly at the bound-

Fig. 9. Distribution of the normalized local displacement u_1/b on the plane $\xi_3 = 0.1a$ in the local coordinates ξ_1/b and ξ_2/b induced by a hexagonal dislocation with the Burgers vector magnitude *b*. The normalized side length of the hexagon is a/b.

Fig. 10. Distribution of the normalized local displacement u_2/b on the plane $\xi_3 = 0.1a$ in the local coordinates ξ_1/b and ξ_2/b induced by a hexagonal dislocation with the Burgers vector magnitude *b*. The normalized side length of the hexagon is a/b.

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Fig. 11. Distribution of the normalized local displacement u_3/b on the plane $\xi_3 = 0.1a$ in the local coordinates ξ_1/b and ξ_2/b induced by a hexagonal dislocation with the Burgers vector magnitude b. The normalized side length of the hexagon is a/b.

ary region than elsewhere. On the contrary, u_2 and u_3 are nearly zero in the center region and peak on the left and right boundaries.

5. Conclusions

In this paper, a line integral expression for the three-dimensional, anisotropic elastic displacement field induced by polygonal dislocations is presented. It is derived using the associated Green's function in the Stroh formalism. The influence of the shape of the polygon dislocation on the elastic displacements is included entirely in the integrand. Based on the proposed approach, the displacement field induced by a dislocation in the shape of a triangle is calculated. Since a dislocation loop of any arbitrary polygon shape can be constructed from a triangle, the present solution for a triangle is fundamental. Via superposition, the displacement field for any polygon dislocation can be obtained. The proposed line integral expression is applied to calculate the displacement field of a triangular dislocation and a hexagonal dislocation (constructed using four triangles). We use the former to demonstrate the accuracy of the method by comparing the calculated displacement jump across the dislocation surface with the given Burgers vector. Our numerical results also show that near and at the boundary region, there is a large gradient in the u_1 displacement distribution, which indicates, at the very least, a large strain field and possibly a strain concentration. To sum, the line integral form provides a computationally efficient method to calculate displacement fields in three-dimensions induced by polygon dislocation(s) contained in an elastically anisotropic solid.

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