Displacement Fields and Self-Energies of Circular and Polygonal Dislocation Loops in Homogeneous and Layered Anisotropic Solids

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Abstract

There are large classes of materials problems that involve the solutions of stress, displacement, and strain energy of dislocation loops in elastically anisotropic solids, including increasingly detailed investigations of the generation and evolution of irradiation induced defect clusters ranging in sizes from the micro- to meso-scopic length scales. Based on a two-dimensional Fourier transform and Stroh formalism that are ideal for homogeneous and layered anisotropic solids, we have developed robust and computationally efficient methods to calculate the displacement fields for circular and polygonal dislocation loops. Using the homogeneous nature of the Green tensor of order -1, we have shown that the displacement and stress fields of dislocation loops can be obtained by numerical quadrature of a line integral. In addition, it is shown that the sextuple integrals associated with the strain energy of loops can be represented by the product of a pre-factor containing elastic anisotropy effects and a universal term that is singular and equal to that for elastic isotropic case. Furthermore, we have found that the self-energy pre-factor of prismatic loops is identical to the effective modulus of normal contact, and the pre-factor of shear loops differs from the effective indentation modulus in shear by only a few percent. These results provide a convenient method for examining dislocation reaction energetic and efficient procedures for numerical computation of local displacements and stresses of dislocation loops, both of which play integral roles in quantitative defect analyses within combined experimental-theoretical investigations.

Keywords: dislocation loop, anisotropic elasticity, equivalence between dislocation and contact problems

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1. Introduction

Dislocations are fundamental building blocks in understanding the deformation and failure of crystalline materials by interactions among themselves, with other point defects such as solute atoms and vacancies, and with three-dimensional features such as precipitates, cracks, and internal interfaces [1]. With decreasing materials microstructure scales and applications under extreme conditions such as high temperature and irradiation, it is imperative for dislocation mechanics analysis to quantitatively examine anisotropic elastic interactions [2-4] and to address the roles of nanostructure features [5-7]. In many cases, analytical solutions are not available for applications that involve complex geometric features and dislocation evolution, so large scale computational investigations based on discrete dislocation dynamics have been routinely used in recent years [8-12]. Undoubtedly these calculations are slow because of the larger number of degrees of freedom and the computationally intensive evaluation of individual dislocation segments. The latter becomes more demanding for anisotropic elasticity analysis since closed-form solutions in real space exist only for the isotropic elastic case. Therefore, significant effort has been devoted to addressing the computational efficiency of dislocation dynamics in three-dimensional anisotropic, heterogeneous solids [8,12].

The other challenge in dislocation mechanics in three-dimensional anisotropic, heterogeneous solids is the calculation of displacement fields generated by defect clusters. In current dislocation dynamics simulations, stress fields are used in a linear superposition scheme, so that a boundary value problem without dislocations, but subjected to complex traction boundary conditions, is of the central interest. For stress field calculations, the computational cost can be reduced by taking advantage of the homogeneous nature of the Green tensor in Fourier space, such as the use of the fast multipole method [12]. Stress calculations require the evaluation of a line integral along dislocation segments, and displacement calculations are challenged by a surface integral over the dislocated area. When dealing with anisotropic elasticity in the absence of a closed-form solution in real space, Fourier transformation is required but it introduces another double integral. Complicating performance of the computations further is the fact that displacement fields are discontinuous (by a Burgers vector jump) over the dislocated surface. This is much harder to deal with than the stress singularity near the dislocation core, for which a cutoff radius can be introduced.

We comment also that two-dimensional defects such as cracks can be modeled based on the dislocation density, where the dislocation density field can be solved by differential-integral equations [13,14]. The integrands are essentially the displacement fields generated by unit dislocation segments. These problems suffer the same difficulties as the evaluation of displacement fields in dislocation mechanics, *i.e.*, the cumbersome evaluation of double or quadruple integrals with singular kernels. This method becomes computationally intractable for the study of randomly distributed cracks in three-dimensional solids.

While stress components are of central interest in the above mentioned dislocation dynamics computations as well as for defect interaction phenomena, displacement fields associated with dislocations are required to characterize dislocation distributions. For instance, the displacements introduced by the local rotations and elastic strains associated with dislocation loops can be used to compute diffraction contrast [15-17] for direct imaging of loops by both conventional and high-resolution electron microscopy. Similarly, the displacements form the basis for calculating diffuse x-ray diffraction-scattering cross-sections for dislocation loops. These cross-sections in turn make it possible to use x-ray diffuse scattering measurements to determine the loop size, their vacancy-interstitial type, and also the orientations of dislocation loops in neutron and ion-beam irradiated materials [18-21]. Diffuse scattering near Bragg reflections provide a non-destructive tool complementary to transmission electron microscopy (TEM) for studying small dislocation loops that are hard to resolve by direct imaging.

An example in which the determination of the orientations and sizes of small and large dislocation loops is required is in obtaining an experimental confirmation of the recently proposed mechanisms of Xu et al. [4] for the formation and growth of sessile $\langle 100 \rangle$ interstitial loops in irradiated bcc Fe and Fe-based alloys through reactions between glissile $\frac{1}{2}\langle 111 \rangle$ interstitial loops. The energy gain associated with such reactions (which interestingly do not obey the Burgers geometric relationship) is not large and the small size of interstitial loops in room temperature irradiated Fe samples hampers ambient temperature TEM studies of the evolution of loop orientations and sizes associated with the proposed mechanism. High-temperature *in situ* electron microscopy investigations of ion-irradiation in Fe have reported large, sessile $\langle 100 \rangle$ loops [22]. However, detailed confirmation of the proposed mechanism of Xu et al. [4] for the growth of sessile $\langle 100 \rangle$ loops by interaction of glissile $\frac{1}{2}\langle 111 \rangle$ loops at high temperature is just now in progress [23]. Because of the smaller sizes of the loops at room

temperature, x-ray diffuse scattering investigations based on numerically calculated displacement fields for $\langle 100 \rangle$ and $\frac{1}{2}\langle 111 \rangle$ dislocation loops in Fe can be used in conjunction with TEM for analyzing the dislocation loop orientations and evolution.

Yet another important application of three-dimensional anisotropic elastic analysis of dislocation loops is the dislocation energy [24]. For line dislocations, the two-dimensional elastic analysis gives rise to the following self-energy density:

$$W_{edge}^{line} = \frac{Eb_{edge}^2}{8\pi(1-\nu^2)} \ln\left(\frac{R}{\rho_0}\right), \quad W_{screw}^{line} = \frac{Eb_{screw}^2}{8\pi(1+\nu)} \ln\left(\frac{R}{\rho_0}\right), \quad (1)$$

where E is the Young's modulus, ν is Poisson's ratio, b_{edge} and b_{screw} are Burgers vectors, and ρ_0 and R are core and faraway cutoff radii, respectively. For dislocation loops with radius of a , the self-energies are

$$W_{prismatic}^{loop} = \frac{Eab_p^2}{4(1-\nu^2)} \left\{ \ln\left(\frac{4a}{\rho_0}\right) - 1 \right\}, \quad W_{shear}^{loop} = \frac{Eab_s^2(2-\nu)}{4(1-\nu^2)} \left\{ \ln\left(\frac{4a}{\rho_0}\right) - 2 \right\}, \quad (2)$$

again with a cutoff radius ρ_0 . The Burgers vectors for prismatic and shear loops are illustrated in Fig. 1 where the notations in [1] are adopted with $\boldsymbol{\varsigma}$ being the line sense. The pre-factors in the above equations depend on E and ν in different forms. Whether a dislocation reaction proceeds is usually determined by the comparison between the strain energies of the reactants and the end products. Furthermore, there are many engineering problems that require a self-energy representation based on anisotropic elasticity. Consider, for instance, the above mentioned formation of a sessile $\langle 100 \rangle$ interstitial loop from two glissile $\frac{1}{2}\langle 111 \rangle$ loops in bcc Fe [4], the misfit dislocations in layered heterostructure [7], the thermal fatigue behavior by dislocation activity in strained thin films [8], and the stability of dislocation loops in nano-pillars and nanowires [25], among many others.

In this paper, we develop a robust and computationally efficient method to evaluate the displacement fields generated by circular or polygonal dislocation loops in three-dimensional anisotropic, layered solids. The consideration of layered structures as well as homogeneous materials is motivated by the applications of interfacial dislocation loops in electronic materials, *e.g.*, [7]. The method is based on the Green tensor which is solved analytically in closed form in Fourier space. We focus on methods to reduce double, quadruple, and sextuple integrals to line integrals. And for cases in which such reductions are not feasible, we examine whether the

anisotropy dependence can be decoupled from these high-order integrals, so that self-energies can be analyzed easily by a separation-of-variables approach. Example calculations are given for various dislocation loop types on $\{100\}$ and $\{111\}$ planes of cubic crystals, as shown schematically in Fig. 1. Potential applications are discussed at the end of the paper.

2. Formulations Based on 3D Green Tensors in Layered Anisotropic Solids

2.1. General formulation

In three-dimensional space, the Green tensor is defined as the displacement fields caused by a point force loaded at the coordinate center. Applied displacement discontinuities are equivalent to the derivatives of the Green tensor. Therefore, for a dislocation loop on a surface with surface normal n_i and Burgers vector b_i , the displacement fields are [26-33]

$$u_m(\mathbf{x}') = -\int_A b_i c_{ijkl} G_{mk,l}(\mathbf{x}, \mathbf{x}') dA_j, \quad (3)$$

where c_{ijkl} are elastic constants, $dA_j = n_j dA$, and the integration and differentiation are conducted for $\mathbf{x} = (x_1, x_2, x_3)^T$, e.g., $G_{mk,l}(\mathbf{x}, \mathbf{x}') = \partial G_{mk} / \partial x_l$. The Green tensor $G_{ij}(\mathbf{x}, \mathbf{x}')$ is given at location $\mathbf{x}$ with the point force applied at $\mathbf{x}'$. Summation convention is assumed for repeated subscripts. Since we start from the Volterra formulation in Eq. (3), the strain and stress formulation requires the subtraction of a compatible displacement field, e.g., the eigenstrain formulation by Mura [44]. The displacement gradient consists of the elastic distortion β_{ji} and the plastic distortion β_{ji}^* [44],

$$u_{m,n} = \beta_{nm} + \beta_{nm}^* = -\int_A b_i c_{ijkl} \frac{\partial G_{mk,l}(\mathbf{x}, \mathbf{x}')}{\partial x'_n} dA_j. \quad (4)$$

The eigenstrain is given by the delta function, $\beta_{ji}^*(\mathbf{x}') = -b_i n_j \delta(\mathbf{x}_s - \mathbf{x}')$, where $\mathbf{x}_s$ are located on the slip zone. The stress tensor is obtained from Hooke's law as

$$\sigma_{ij}(\mathbf{x}') = c_{ijmn} \beta_{nm} = c_{ijmn} (u_{m,n} - \beta_{nm}^*). \quad (5)$$

Following Mura [44] and Bower [24], the strain energy of a dislocation loop is given by

$$W^{loop} = \frac{1}{2} \int_s \sigma_{ij}(\mathbf{x}') b_i dA'_j, \quad (6)$$

where the integration is over coordinates $\mathbf{x}'$. We also note that in a number of works by Lazar and co-authors [46-48], the displacement fields can be represented by the Burgers equation in

anisotropic elasticity, which and the corresponding stress and energy integrals have reduced dimension. However, our Green tensor is given in Fourier space, which facilitates the derivation from the above equations.

Since the Green's function is the elastic solution in an infinite anisotropic space subjected to a point force at the coordinate origin, the boundary value problem can only be solved analytically in closed form in Fourier space. For layered anisotropic solids as illustrated in Fig. 2, the solution can be obtained by the combination of the Stroh formalism and a two-dimensional Fourier transform in plane parallel to the interfaces of a layered solid [34-37]. For an arbitrary field of $\mathbf{t}(x_i)$, we define the Fourier transform by

$$\hat{\mathbf{t}}(\xi_1, \xi_2, x_3) = \frac{1}{2\pi} \iint \mathbf{t}(x_1, x_2, x_3) \exp(ix_1\xi_1 + ix_2\xi_2) dx_1 dx_2, \quad (7)$$

$$\mathbf{t}(x_1, x_2, x_3) = \frac{1}{2\pi} \iint \hat{\mathbf{t}}(\xi_1, \xi_2, x_3) \exp(-ix_1\xi_1 - ix_2\xi_2) d\xi_1 d\xi_2. \quad (8)$$

where the coordinates in reciprocal space are $(\xi_1, \xi_2) = \xi(h_1, h_2)$, ξ is the magnitude of the wavevector, and (h_1, h_2) is a unit vector.

In the plane spanned by x_3 and (ξ_1, ξ_2) , the plane-field solution can be obtained by the Stroh formalism [13]. This method has been applied earlier in contact problems [36,37], so only a brief summary is presented below. For each Fourier component, the general solution can be represented by three pairs of complex functions,

$$u_l = \sum_a A_{la} f_a(z_a) + \sum_a \bar{A}_{la} \bar{f}_a(\bar{z}_a), \quad (9)$$

where a bar on the top of a quantity denotes the complex conjugate, $f_1(z_1)$, $f_2(z_2)$, and $f_3(z_3)$ are three analytic functions to be determined from boundary conditions, and the three complex variables are $z_a = h_1 x_1 + h_2 x_2 + p_a x_3$, $a = 1, 2, 3$. The traction vector on any plane normal to the x_3 axis, $\mathbf{t} = (\sigma_{13}, \sigma_{23}, \sigma_{33})^T$, is given by

$$\sigma_{i3} = \sum_a L_{ia} f'_a(z_a) + \sum_a \bar{L}_{ia} \bar{f}'_a(\bar{z}_a), \quad (10)$$

where the three vectors L_{ia} are defined as $L_{ia} = (c_{i3l1} h_1 + c_{i3l2} h_2 + c_{i3l3} p_a) A_{la}$ with summation convention over a not being implied. Once the stiffness tensor c_{ijkl} is prescribed, for a given direction (h_1, h_2) , one can solve an eigenvalue problem numerically to obtain the eigenvalues p

and eigenvectors A_l . For brevity and to illustrate the algebraic structure, we write $p = h_3$. Furthermore, we use a positive definite Hermitian $\mathbf{B} = i\mathbf{A}\mathbf{L}^{-1}$ in our formulation.

We use the analytic continuation method in [13] to determine the three analytic functions $f_1(z_1)$, $f_2(z_2)$, $f_3(z_3)$ from boundary conditions. Define z^* as any complex variable of the form $z^* = h_1x_1 + h_2x_2 + qx_3$, where q is an arbitrary complex number with a positive imaginary part. On the plane $x_3 = 0$, the four complex variables, z_1 , z_2 , z_3 , z^* , all equal to $h_1x_1 + h_2x_2$, so that the traction vector and the displacement vector are

$$\mathbf{t} = \mathbf{L}\mathbf{f}'(h_\alpha x_\alpha) + \bar{\mathbf{L}}\bar{\mathbf{f}}'(h_\alpha x_\alpha), \quad (11)$$

$$\mathbf{u} = \mathbf{A}\mathbf{f}'(h_\alpha x_\alpha) + \bar{\mathbf{A}}\bar{\mathbf{f}}'(h_\alpha x_\alpha), \quad (12)$$

where we use the vector notation, $\mathbf{f}(z^*) = [f_1(z^*), f_2(z^*), f_3(z^*)]^T$.

By the principle of linear superposition, we need to find the solution of only one Fourier component:

$$\mathbf{t} = \bar{\mathbf{a}} \exp(i\xi_1 x_1 + i\xi_2 x_2) + \mathbf{a} \exp(-i\xi_1 x_1 - i\xi_2 x_2). \quad (13)$$

From Fig. 2, the displacement continuity and force balance on the plane of $x_3 = 0$ gives

$$\mathbf{u}^-(x_1, x_2) = \mathbf{u}^+(x_1, x_2), \quad (14)$$

$$\mathbf{t}^-(x_1, x_2) - \mathbf{t}^+(x_1, x_2) = \mathbf{t}_0 \delta(x_1) \delta(x_2), \quad (15)$$

where $\pm$ denotes $x_3 = 0^\pm$, respectively. The Fourier transform of the point force gives

$$\frac{1}{2\pi} \iint t_0 \delta(x_1) \delta(x_2) \exp(ix_1 \xi_1 + ix_2 \xi_2) dx_1 dx_2 = \frac{1}{2\pi} t_0. \quad (16)$$

Now if we consider only one Fourier component as in Eq. (13), we need to find analytic functions $\mathbf{f}(z^*)$ that both satisfy the traction boundary conditions (13), and vanishes (*i.e.*, $\mathbf{f}(z^*) \rightarrow 0$) as $x_3 \rightarrow \pm\infty$.

2.2. Green tensor in a homogeneous solid in Fig. 2(a)

For the lower half-space, $x_3 < 0$, inspection gives the solution

$$\mathbf{L}\mathbf{f}'(z^*) = \mathbf{a}_- \exp(-i\xi z^*), \quad (17)$$

where $\mathbf{a}_-$ is to be determined by the boundary conditions. The fact that q in $z^* = h_1 x_1 + h_2 x_2 + q x_3$ has positive imaginary part ensures that $f(z^*) \rightarrow 0$ as $x_3 \rightarrow -\infty$. From Eq. (17), after obtaining $f_1(z^*)$, $f_2(z^*)$, $f_3(z^*)$, we replace the variable to obtain $f_1(z_1)$, $f_2(z_2)$, $f_3(z_3)$, and calculate the displacement field from Eq. (9) and the stress field from Eq. (10). Therefore, we have

$$\mathbf{t} = \mathbf{L} \langle \exp(-i\xi p^* x_3) \rangle \mathbf{L}^{-1} \mathbf{a}_- \exp(-i\xi_\alpha x_\alpha) + conj., \quad (18)$$

$$\mathbf{u} = \frac{i}{\xi} \mathbf{A} \langle \exp(-i\xi p^* x_3) \rangle \mathbf{L}^{-1} \mathbf{a}_- \exp(-i\xi_\alpha x_\alpha) + conj., \quad (19)$$

where *conj.* denote the complex conjugate of the first term in the right hand sides of these equations. Since the three eigenvalues p_a do not allow an index representation, in the above equations, we have introduced a diagonal matrix representation by

$$\langle (..) \rangle = \begin{bmatrix} (..) \\ & (..) \\ & & (..) \end{bmatrix}. \quad (20)$$

Similarly, for the upper half-space, $x_3 > 0$, inspection gives the solution

$$\mathbf{L} \mathbf{f}'(z^*) = \mathbf{a}_+ \exp(i\xi z^*), \quad (21)$$

where the fact that q in $z^* = h_1 x_1 + h_2 x_2 + q x_3$ has positive imaginary part ensures that $f(z^*) \rightarrow 0$ as $x_3 \rightarrow +\infty$. And the analytic continuation gives rise to

$$\mathbf{t} = \mathbf{L} \langle \exp(i\xi p^* x_3) \rangle \mathbf{L}^{-1} \mathbf{a}_+ \exp(i\xi_\alpha x_\alpha) + conj. \quad (22)$$

$$\mathbf{u} = -\frac{i}{\xi} \mathbf{A} \langle \exp(i\xi p^* x_3) \rangle \mathbf{L}^{-1} \mathbf{a}_+ \exp(i\xi_\alpha x_\alpha) + conj. \quad (23)$$

The boundary conditions at $x_3 = 0$ for one Fourier component lead to

$$\mathbf{B} \mathbf{a}_- = -\bar{\mathbf{B}} \bar{\mathbf{a}}_+, \quad \mathbf{a}_- - \bar{\mathbf{a}}_+ = \frac{1}{2\pi} \mathbf{t}_0. \quad (24)$$

The displacement Green's function in Fourier space is therefore given in Eq. (19) for $x_3 < 0$ and Eq. (23) for $x_3 > 0$ with $\mathbf{a}^\pm$ given in Eq. (24), i.e.,

$$\hat{u}_i(\xi_1, \xi_2, x_3) = \begin{cases} \frac{1}{2\pi\xi} \bar{\mathbf{A}} \langle \exp(-i\xi \bar{p}_* x_3) \rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} \mathbf{t}_0, & x_3 > 0 \\ \frac{1}{2\pi\xi} \mathbf{A} \langle \exp(-i\xi p_* x_3) \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} \mathbf{t}_0, & x_3 < 0 \end{cases} \quad (25)$$

which is clearly homogeneous of degree -1.

Another way to perform the analytic continuation is to use the continuity of the displacement across $x_3 = 0$ directly, which ensures the following relationship,

$$\mathbf{A} \mathbf{f}^+(z) = \bar{\mathbf{A}} \bar{\mathbf{f}}^-(z), \quad z \in \text{upper half space}, \quad (26)$$

from which analytic complex functions are obtained, given by,

$$\mathbf{f}^-(z) = \frac{i}{\xi} \mathbf{L}^{-1} \mathbf{a}_- \exp(-i\xi z), \quad z \in \text{lower half space}, \quad (27)$$

$$\mathbf{f}^+(z) = \mathbf{A}^{-1} \bar{\mathbf{A}} \frac{-i}{\xi} \bar{\mathbf{L}}^{-1} \bar{\mathbf{a}}_- \exp(i\xi z) = \frac{1}{\xi} \mathbf{A}^{-1} \bar{\mathbf{B}} \bar{\mathbf{a}}_- \exp(i\xi z). \quad (28)$$

Using the interface traction boundary condition, the same displacement fields will be obtained as in Eq. (25).

From the definition of Fourier transform and Eq. (25), we obtain the following Green tensor in Fourier space,

$$\hat{G}_{ij}(\xi_1, \xi_2, x_3) = \begin{cases} \frac{1}{2\pi\xi} \bar{\mathbf{A}} \langle \exp(-i\xi \bar{p}_* x_3) \rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1}, & x_3 > 0 \\ \frac{1}{2\pi\xi} \mathbf{A} \langle \exp(-i\xi p_* x_3) \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1}, & x_3 < 0 \end{cases} \quad (29)$$

where ij denotes the i -th displacement component caused by the j -th point force applied at the coordinate origin. Note that matrices $\mathbf{A}$ and $\mathbf{B}$ depend on elastic constants and ξ_α/ξ , which is the direction of the wavevector.

2.3. Green tensor in a bi-material in Fig. 2(b)

Consider the bi-material in Fig. 2(b), where the two materials extend to infinity at $x_3 = \pm\infty$, respectively. For the lower half space, we have

$$\mathbf{t} = \mathbf{L}_\Pi \langle \exp(-i\xi p_\Pi^* x_3) \rangle \mathbf{L}_\Pi^{-1} \mathbf{a}_- \exp(-i\xi_\alpha x_\alpha) + \text{conj.}, \quad (30)$$

$$\mathbf{u} = \frac{i}{\xi} \mathbf{A}_\Pi \langle \exp(-i\xi p_\Pi^* x_3) \rangle \mathbf{L}_\Pi^{-1} \mathbf{a}_- \exp(-i\xi_\alpha x_\alpha) + \text{conj.}, \quad (31)$$

and for the upper half space, we have

$$\mathbf{t} = \mathbf{L}_I \left\langle \exp(i\xi p_1^* x_3) \right\rangle \mathbf{L}_I^{-1} \mathbf{a}_+ \exp(i\xi_\alpha x_\alpha) + \text{conj}. \quad (32)$$

$$\mathbf{u} = -\frac{i}{\xi} \mathbf{A}_I \left\langle \exp(i\xi p_1^* x_3) \right\rangle \mathbf{L}_I^{-1} \mathbf{a}_+ \exp(i\xi_\alpha x_\alpha) + \text{conj}. \quad (33)$$

The boundary conditions at $x_3 = 0$ gives rise to $\mathbf{B}_\Pi \mathbf{a}_- = -\bar{\mathbf{B}}_I \bar{\mathbf{a}}_+$ and $\mathbf{a}_- - \bar{\mathbf{a}}_+ = \frac{1}{2\pi} \mathbf{t}_0$, so that

$$\mathbf{a}_- = \frac{1}{2\pi} \mathbf{B}_\Pi^{-1} (\mathbf{B}_\Pi^{-1} + \bar{\mathbf{B}}_I^{-1})^{-1} \mathbf{t}_0, \quad \bar{\mathbf{a}}_+ = -\frac{1}{2\pi} \bar{\mathbf{B}}_I^{-1} (\mathbf{B}_\Pi^{-1} + \bar{\mathbf{B}}_I^{-1})^{-1} \mathbf{t}_0. \quad (34)$$

A straightforward derivation gives rise to the following Green tensor,

$$\hat{G}_{ij}(\xi_1, \xi_2, x_3) = \begin{cases} \frac{1}{2\pi\xi} \bar{\mathbf{A}}_I \left\langle \exp(-i\xi \bar{p}_1^* x_3) \right\rangle \bar{\mathbf{A}}_I^{-1} (\mathbf{B}_\Pi^{-1} + \bar{\mathbf{B}}_I^{-1})^{-1}, & x_3 > 0 \\ \frac{1}{2\pi\xi} \mathbf{A}_\Pi \left\langle \exp(-i\xi p_\Pi^* x_3) \right\rangle \mathbf{A}_\Pi^{-1} (\mathbf{B}_\Pi^{-1} + \bar{\mathbf{B}}_I^{-1})^{-1}, & x_3 < 0 \end{cases} \quad (35)$$

2.4. Green tensor in a tri-material in Fig. 2(c)

As a representative example of multilayered structure, we consider the tri-material example in Fig. 2(c), in which an interface layer (Material II) is sandwiched between Material I and Material III. When the lower half space is made of a film (Material II) on substrate (Material III), the use of the analytic continuation technique leads to the following general solution:

$$\mathbf{L}_\Pi \mathbf{f}'_\Pi(z^*) = \mathbf{P} \exp(-i\xi z^*) + \mathbf{Q} \exp(i\xi z^*), \quad (36)$$

$$\mathbf{A}_\Pi \mathbf{f}_\Pi(z^*) = \frac{\mathbf{B}_\Pi \mathbf{P}}{\xi} \exp(-i\xi z^*) - \frac{\mathbf{B}_\Pi \mathbf{Q}}{\xi} \exp(i\xi z^*), \quad (37)$$

where $\mathbf{P}$ and $\mathbf{Q}$ are two unknown vectors to be determined from boundary conditions. The displacement and traction fields can be evaluated from Eqs. (9) and (10), giving

$$\mathbf{u}_\Pi = \frac{\bar{\mathbf{B}}_\Pi \bar{\mathbf{T}}_\Pi^{-1} \bar{\mathbf{P}} - \mathbf{B}_\Pi \mathbf{T}_\Pi^+ \mathbf{Q}}{\xi} \exp(i\xi_1 x_1 + i\xi_2 x_2) + \frac{\mathbf{B}_\Pi \mathbf{T}_\Pi^- \mathbf{P} - \bar{\mathbf{B}}_\Pi \bar{\mathbf{T}}_\Pi^+ \bar{\mathbf{Q}}}{\xi} \exp(-i\xi_1 x_1 - i\xi_2 x_2), \quad (38)$$

$$\mathbf{t}_\Pi = (\bar{\mathbf{T}}_\Pi^- \bar{\mathbf{P}} + \mathbf{T}_\Pi^+ \mathbf{Q}) \exp(i\xi_1 x_1 + i\xi_2 x_2) + (\mathbf{T}_\Pi^- \mathbf{P} + \bar{\mathbf{T}}_\Pi^+ \bar{\mathbf{Q}}) \exp(-i\xi_1 x_1 - i\xi_2 x_2), \quad (39)$$

where the dimensionless matrices $\mathbf{T}_{\text{II}}^{\pm}$ are $T_{\text{II},lj}^{\pm} = \sum_{a=1}^3 L_{\text{II},la} L_{\text{II},aj}^{-1} \exp(\pm i\xi p_{\text{II},a} x_3)$. The unknown vectors

$\mathbf{P}$ and $\mathbf{Q}$ are obtained from the boundary condition, $\mathbf{P} + \bar{\mathbf{Q}} = \mathbf{a}_-$ at $x_3 = 0$ from Eq. (13), and the continuity condition at the materials II/III interface ($x_3 = -d$),

$$\mathbf{B}_{\text{II}} \mathbf{C}_{\text{II}}^- \mathbf{P} - \bar{\mathbf{B}}_{\text{II}} \bar{\mathbf{C}}_{\text{II}}^+ \bar{\mathbf{Q}} = \mathbf{B}_{\text{III}} (\mathbf{C}_{\text{II}}^- \mathbf{P} + \bar{\mathbf{C}}_{\text{II}}^- \bar{\mathbf{Q}}). \quad (40)$$

where $\mathbf{C}_{\text{II}}^{\pm} = \mathbf{T}_{\text{II}}^{\pm} \big|_{x_3=-d}$. Consequently,

$$\begin{pmatrix} \mathbf{P} \\ \bar{\mathbf{Q}} \end{pmatrix} = \begin{pmatrix} [(\mathbf{B}_{\text{II}} - \mathbf{B}_{\text{III}}) \mathbf{C}_{\text{II}}^- + (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{III}}) \bar{\mathbf{C}}_{\text{II}}^+]^{-1} (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{III}}) \bar{\mathbf{C}}_{\text{II}}^+ \mathbf{a}_- \\ \left\{ \mathbf{I} - [(\mathbf{B}_{\text{II}} - \mathbf{B}_{\text{III}}) \mathbf{C}_{\text{II}}^- + (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{III}}) \bar{\mathbf{C}}_{\text{II}}^+]^{-1} (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{III}}) \bar{\mathbf{C}}_{\text{II}}^+ \right\} \mathbf{a}_- \end{pmatrix}. \quad (41)$$

The boundary conditions at $x_3 = 0$ gives rise to $\mathbf{Y}_{\text{II,III}} \mathbf{a}_- = -\bar{\mathbf{B}}_{\text{I}} \bar{\mathbf{a}}_+$ and $\mathbf{a}_- - \bar{\mathbf{a}}_+ = \frac{1}{2\pi} \mathbf{t}_0$, so

that we obtain

$$\mathbf{a}_- = \frac{1}{2\pi} \mathbf{Y}_{\text{II,III}}^{-1} (\mathbf{Y}_{\text{II,III}}^{-1} + \bar{\mathbf{B}}_{\text{I}}^{-1})^{-1} \mathbf{t}_0, \quad \bar{\mathbf{a}}_+ = -\frac{1}{2\pi} \bar{\mathbf{B}}_{\text{I}}^{-1} (\mathbf{Y}_{\text{II,III}}^{-1} + \bar{\mathbf{B}}_{\text{I}}^{-1})^{-1} \mathbf{t}_0, \quad (42)$$

where $\mathbf{Y}_{\text{II,III}} = -\bar{\mathbf{B}}_{\text{II}} + (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{II}}) [(\mathbf{B}_{\text{II}} - \mathbf{B}_{\text{III}}) \mathbf{C}_{\text{II}}^- + (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{III}}) \bar{\mathbf{C}}_{\text{II}}^+]^{-1} (\bar{\mathbf{B}}_{\text{II}} + \mathbf{B}_{\text{III}}) \bar{\mathbf{C}}_{\text{II}}^+$ [35]. Thus the Green tensor is

$$\hat{G}_{ij}(\xi_1, \xi_2, x_3) = \frac{1}{2\pi\xi} \bar{\mathbf{A}}_{\text{I}} \langle \exp(-i\xi \bar{p}_1^* x_3) \rangle \bar{\mathbf{A}}_{\text{I}}^{-1} (\mathbf{Y}_{\text{II,III}}^{-1} + \bar{\mathbf{B}}_{\text{I}}^{-1})^{-1}, \quad x_3 > 0. \quad (43)$$

The representations for $-d < x_3 < 0$ and $x_3 < -d$ are quite lengthy, since the matrices of $\mathbf{P}$, $\mathbf{Q}$, $\mathbf{B}_{\text{II}}$, and $\mathbf{T}_{\text{II}}^{\pm}$ are all involved in Eqs. (37) and (38), and the matrices of $\mathbf{P}$, $\mathbf{Q}$, $\mathbf{B}_{\text{III}}$, and

$T_{\text{III},lj}^{\pm} = \sum_{a=1}^3 L_{\text{III},la} L_{\text{III},aj}^{-1} \exp(\pm i\xi p_{\text{III},a} x_3)$ are involved for expressions in material III. We also note that

stress components in multilayer thin films have been solved by essentially the equivalent method in [49], but the displacement Green tensor is of our interests in this work.

3. Displacements of Circular Dislocation Loops in Anisotropic Solids

All the Green tensors in Fourier space have the same mathematical structure. That is, they are homogeneous of degree -1 with a separate dependence on wavenumber ξ and wavevector direction, $\theta = \tan^{-1}(h_2/h_1)$. The dependence on x_3 (that does not contribute to the two-

dimensional Fourier transform) is through the diagonal matrix $\langle \exp(-i\xi p^* x_3) \rangle$ and the matrix $\mathbf{Y}_{\text{II,III}}$ in Eq. (43). Consequently, we adopt the Green tensor in a homogeneous solid in Eq. (29) for the following derivations; the use of Eqs. (35) and (43) will be essentially the same.

From Eq. (29), the Green tensor in real space is

$$G_{ij}(x_1, x_2, x_3) = \frac{1}{2\pi} \iint \hat{G}_{ij}(\xi_1, \xi_2, x_3) \exp(-i\xi_1 x_1 - i\xi_2 x_2) d\xi_1 d\xi_2$$

$$= \begin{cases} \frac{1}{4\pi^2} \iint \frac{1}{\xi} \bar{\mathbf{A}} \langle \exp(-i\xi \bar{p}_* x_3) \rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} \exp(-i\xi_1 x_1 - i\xi_2 x_2) d\xi_1 d\xi_2, & x_3 > 0 \\ \frac{1}{4\pi^2} \iint \frac{1}{\xi} \mathbf{A} \langle \exp(-i\xi p_* x_3) \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} \exp(-i\xi_1 x_1 - i\xi_2 x_2) d\xi_1 d\xi_2, & x_3 < 0 \end{cases} \quad (44)$$

Noting that $\mathbf{A}$ and $\mathbf{B}$ are functions of θ only, we have

$$G_{ij}(x_1, x_2, x_3) = \begin{cases} \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^\infty \bar{\mathbf{A}} \langle \exp(-i\xi \bar{p}_* x_3) \rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} e^{-i\xi(x_1 \cos \theta + x_2 \sin \theta)} d\xi, & x_3 > 0 \\ \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^\infty \mathbf{A} \langle \exp(-i\xi p_* x_3) \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} e^{-i\xi(x_1 \cos \theta + x_2 \sin \theta)} d\xi, & x_3 < 0 \end{cases} \quad (45)$$

$$= \begin{cases} \frac{1}{4\pi^2} \int_0^{2\pi} \bar{\mathbf{A}} \left\langle \frac{-i}{x_1 \cos \theta + x_2 \sin \theta + \bar{p}_* x_3} \right\rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & x_3 > 0 \\ \frac{1}{4\pi^2} \int_0^{2\pi} \mathbf{A} \left\langle \frac{-i}{x_1 \cos \theta + x_2 \sin \theta + p_* x_3} \right\rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & x_3 < 0 \end{cases}$$

To see the algebraic structure, we write $(h_1^*, h_2^*, h_3^*) = (\cos \theta, \sin \theta, p^*)$. The integrand in Eq. (3)

requires the evaluation of $G_{mk,l}(\mathbf{x}, \mathbf{x}')$, given by

$$\frac{\partial \mathbf{G}(\mathbf{x}, \mathbf{x}')}{\partial x_m} = \begin{cases} \frac{1}{4\pi^2} \int_0^{2\pi} \bar{\mathbf{A}} \left\langle \frac{i\bar{h}_m^*}{[(x_1 - x'_1) \cos \theta + (x_2 - x'_2) \sin \theta + \bar{p}_* (x_3 - x'_3)]^2} \right\rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & x_3 > x'_3 \\ \frac{1}{4\pi^2} \int_0^{2\pi} \mathbf{A} \left\langle \frac{i h_m^*}{[(x_1 - x'_1) \cos \theta + (x_2 - x'_2) \sin \theta + p_* (x_3 - x'_3)]^2} \right\rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & x_3 < x'_3 \end{cases} \quad (46)$$

Substituting the above equation into Eq. (3), the numerical evaluation of the resulting triple integral is obviously very time consuming. Thus we first integrate the diagonal matrix in

Eq. (46) over the dislocated surface in Fig. 1, so that the following scalar operations will be encountered,

$$\int_0^{2\pi} \dots d\theta \int_A \frac{1}{\left[(x_1 - x'_1) \cos \theta + (x_2 - x'_2) \sin \theta + p_*(x_3 - x'_3) \right]^2} dA. \quad (47)$$

An analytical treatment of the above surface integral can be found in Appendix B. Consequently, we obtain

$$\int_A \frac{\partial \mathbf{G}(\mathbf{x}, \mathbf{x}')}{\partial x_m} dA = \begin{cases} \frac{1}{4\pi^2} \int_0^{2\pi} i\bar{\mathbf{A}} \left\langle \bar{h}_m^* \left[-2\pi + \frac{2i\bar{s}_*}{\sqrt{1-\bar{s}_*^2}} \tan^{-1} \left(\frac{iy\bar{s}_*}{\sqrt{1-\bar{s}_*^2} \sqrt{1-y^2}} \right) \right]_{y=-1}^{y=1} \right\rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & 0 > x'_3 \\ \frac{1}{4\pi^2} \int_0^{2\pi} i\mathbf{A} \left\langle h_m^* \left[-2\pi + \frac{2is_*}{\sqrt{1-s_*^2}} \tan^{-1} \left(\frac{iy s_*}{\sqrt{1-s_*^2} \sqrt{1-y^2}} \right) \right]_{y=-1}^{y=1} \right\rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & 0 < x'_3 \end{cases}, \quad (48)$$

with $s_* = (x'_1 \cos \theta + x'_2 \sin \theta + p_* x'_3)/a$ and $\bar{s}_* = (x'_1 \cos \theta + x'_2 \sin \theta + \bar{p}_* x'_3)/a$. From the above equation, the triple integral formulation is converted to a line integral performed over the wavevector direction, $\theta = \tan^{-1}(\xi_2/\xi_1)$, in the Fourier space. The integrand of the line integral is singular. We use the adaptive Simpson method to evaluate this, and it is found that a quadrature tolerance of 10^{-4} near $x_3 = 0$ gives acceptable results. The quadrature speed can be accelerated by tabulating matrices $\mathbf{A}$ and $\mathbf{B}$ with respect to (h_1, h_2) or equivalently over θ . Or since the form of singularity in Eq. (48) is known, we can use weighted quadrature method such as the Chebyshev-Gauss quadrature. An alternative way that does not need the tabulation of matrices $\mathbf{A}$ and $\mathbf{B}$ can be achieved by taking advantage of the closed-form representation of Green tensor in three-dimensional Fourier space (as opposed to the two-dimensional Fourier transform in Section 2), as discussed in Appendix C.

As shown in Fig. 1, we consider dislocation loops on $\{100\}$ and $\{111\}$ planes of cubic crystals. The crystallographic orientations will only affect the Stroh matrices $\mathbf{A}$ and $\mathbf{B}$. The prismatic and shear components will be calculated separately. As an example, consider the prismatic dislocation loop in Fig. 1 and evaluate only u_3 , so that $b_3 = -b$, $n_3 = 1$, and $dA_3 = dA$. Eq. (3) can be written as

$$\begin{aligned}
u_3(x'_1, x'_2, x'_3) &= b \int_A c_{33kl} G_{3k,l}(\mathbf{x}, \mathbf{x}') dA \\
&= b \int_A dA \left[c_{3311} G_{31,1} + c_{3321} G_{32,1} + c_{3331} G_{33,1} + c_{3312} G_{31,2} + c_{3322} G_{32,2} \right. \\
&\quad \left. + c_{3332} G_{33,2} + c_{3313} G_{31,3} + c_{3323} G_{32,3} + c_{3333} G_{33,3} \right]
\end{aligned} \tag{49}$$

Note that the elastic constants c_{ijkl} are given in the local coordinates.

Three types of prismatic dislocation loops are compared in Fig. 3, including isotropic elasticity with $\nu=0.3$, and Cu $\{100\}$ and $\{111\}$ planes. The isotropic elasticity corresponds to a degenerate case in the Stroh formalism [13], with three repeated eigenvalues $p=i$ where $i = \sqrt{-1}$. A small perturbation of the elastic constants actually removes this degeneracy, and the resulting calculation reproduces the analytical solution in Hirth and Lothe [1] as summarized in Appendix A. The elastic constants of copper are $c_{11}=1.69 \times 10^{11}$ Pa, $c_{12}=1.22 \times 10^{11}$ Pa, and $c_{44}=0.755 \times 10^{11}$ Pa. Contour plots of the loop-normal displacement, u_3 , are given in the plane that is orthogonal to the dislocation plane and cuts through the loop center. In the geometric setup in Fig. 1, this gives rise to (x_1, x_3) plane at $x_2=0$. Displacement u_3 along the x_3 direction is plotted in Fig. 4 for a number of cases of interest including circular loops for both Fe and Cu, loops on $\{111\}$ and $\{100\}$ planes, and for triangular and hexagonal shaped loops. Across the dislocated plane at $x_3=0^\pm$, the displacement jumps by a Burgers vector of b_p , so that a peak value of $b_p/2$ can be found in all the plots in Fig. 3, and a discontinuity of $\pm b_p/2$ in Fig. 4. The general features of these mesh plots are similar but we note that the slopes are governed by the degree of elastic anisotropy. For example, the displacements for a Cu $\{111\}$ prismatic loop can be seen in Fig. 3(c), and more clearly Fig. 4(a), to extend further along the x_3 direction, because the $\langle 111 \rangle$ direction in Cu is the least compliant. Results for Fe in Fig. 4(b) have the same features as those for Cu in Fig. 4(a) since these two materials have similar ratios for c_{12}/c_{11} and in both cases, $c_{12} + 2c_{44} > c_{11}$ (*i.e.*, an anisotropy measure).

For the loop geometries in Fig. 1, we compute the resulting u_1 and u_3 fields for α -Fe as shown in Figs. 5 and 6. The elastic constants for Fe are $c_{11}=2.29 \times 10^{11}$ Pa, $c_{12}=1.34 \times 10^{11}$ Pa, and $c_{44}=1.15 \times 10^{11}$ Pa. The prismatic loop produces a discontinuity in u_3 as shown by the right column in Fig. 5, and the shear loop leads to a discontinuity in u_1 as shown by the left column in

Fig. 6. Note that in Fig. 5, $b_3 = b_p$, which is opposite to Figs. 3 and 4, so that the displacement signs are flipped in the plots in Fig. 5. Similar to the Cu {111} case, Fig. 5(f) for Fe shows that the displacement u_3 extends farther than other cases. The gradients in the x_3 direction (*i.e.*, slopes in the loop normal direction) in these plots play a critical role in numerical diffuse scattering simulations and the interpretation of diffuse scattering measurements. This is because the linear falloffs in the x_3 direction correspond to regions of constant elastic strain ε_{33} and, hence, to the so-called “local Bragg” diffuse scattering [18,19,38]. Comprised of Bragg scattering from local regions with constant strain (*i.e.*, constant lattice parameter), this scattering appears near the Bragg peak at distances proportional to ε_{33} but outside the Huang diffuse scattering [39,40] that diverges at the Bragg peak. Since the Burgers vector of a loop is independent of size while the spatial extent of the displacement field scales inversely with the radius, local Bragg diffuse scattering contains loop size and vacancy-interstitial-type information [18,19,38]. On the other hand, no significant difference of the decay length for the shear displacement u_1 in Figs. 5(a), 5(c), and 5(e) can be found. The bottom panels in Figs. 5 and 6 demonstrate an asymmetry in u_1 in the positive and negative x_1 directions as a result of the 3-fold symmetry, because the dislocation loop normal is in the $\langle 111 \rangle$ direction and the in-plane $[11\bar{2}]$ and $[\bar{1}\bar{1}2]$ directions (*i.e.*, $\pm x_1$ directions) are not symmetric.

In view of the central importance of the loop normal elastic strains, we now examine ε_{33} for Fe {100} and Fe {111} interstitial loops more closely. For the sake of clarity, the presentation of the formulation of the strain tensor is deferred to Section 5 where the formulation of both the stress tensor and the self-energy are presented. The jumps (or change in sign) of the displacements in the dislocated area can be observed easily in Figs. 5 and 6. The strains and stresses associated with the displacements are actually continuous on the dislocated plane (see the slopes of the curves in Fig. 4 at $x_3 = 0$), but they diverge near the dislocation core so a cutoff of $0.2a$ is introduced in the calculations in Fig. 7. We note also that although strains are dimensionless, for generality our calculations use the displacements in units of the Burgers vector and the spatial coordinates in units of the loop radius. Accordingly, the strains plotted in Fig. 7 are in the form of $\varepsilon_{33}a/b_p$. These contour plots emphasize that the geometric features, *e.g.*, a more protruded strain distribution for the Fe {111} than for the Fe {100} interstitial loop

case along the center line $(x_1, x_2) = (0, 0)$ is a direct consequence of the characteristics of the displacement fields shown in Figs. 5(d) and 5(f). Moreover, there is a direct correspondence between the slopes of the displacements plotted in Fig. 4(b) for Fe $\{111\}$ and $\{100\}$ loops. We note in Fig. 4(b) that the slopes of the displacements for loops of all orientations and elasticity are similar out to $0.3a \sim 0.4a$, at which point the displacements for the various cases increase to different, but relatively constant slopes out to about $1.0a$. The small inner (light green) contours and the following dark green bands in Fig. 7 correspond to the regions with the lower and higher slopes, respectively. Now, since $7/8$ of the volume of a sphere is outside half the radius, the spherical volume inscribing the dislocation loops will be dominated by the ε_{33} strains in the second contour in Fig. 7.

4. Displacements of Triangular and Polygonal Dislocation Loops in Anisotropic Solids

The integral in this case is performed over a triangular area. Following Chu et al. [32,33], we transform the global coordinates to local coordinates attached to the triangle as illustrated in Fig. 8(a). Derivations in Appendix B lead to the following line integral,

$$\int_A \frac{\partial \mathbf{G}(\mathbf{x}, \mathbf{x}')}{\partial x_m} dA = \begin{cases} \frac{1}{4\pi^2} \int_0^{2\pi} i\bar{\mathbf{A}} \left\langle \frac{1}{h_m^* f_1} \left[\frac{1}{f_2 + f_1 l_1^*} \ln \frac{\bar{f}_3^* + f_2}{\bar{f}_3^* - f_1 l_1^*} - \frac{1}{f_2 - f_1 l_2^*} \ln \frac{\bar{f}_3^* + f_2}{\bar{f}_3^* + f_1 l_2^*} \right] \right\rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & 0 > x'_3 \\ \frac{1}{4\pi^2} \int_0^{2\pi} i\mathbf{A} \left\langle \frac{1}{h_m^* f_1} \left[\frac{1}{f_2 + f_1 l_1^*} \ln \frac{f_3^* + f_2}{f_3^* - f_1 l_1^*} - \frac{1}{f_2 - f_1 l_2^*} \ln \frac{f_3^* + f_2}{f_3^* + f_1 l_2^*} \right] \right\rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & 0 < x'_3 \end{cases} \quad (50)$$

Interestingly, it is found that the numerical quadrature of Eq. (50) for a triangular loop is much more challenging than that of Eq. (48) for a circular loop. A mechanistic explanation is given below. An analogous problem is the calculation of the stress intensity factor of a circular crack as opposed to a polygonal crack by Bower and Ortiz [14]. The stress singularity at the crack root is described by the stress intensity factor, and the stress intensity factor itself diverges at the sharp corners along the crack periphery. This issue does not arise for circular dislocation loops. Practically, it is found that the quadrature tolerance of Eq. (50) has to be at least one order of magnitude (occasionally two orders of magnitude) smaller than that of Eq. (48). As pointed out by Bower and Ortiz [14], a small fillet at the sharp corner will reduce the singularity of the stress intensity factor. However, the solution of triangular dislocation loop is intended to simulate dislocation segments in a general dislocation dynamics simulation, so rounding the sharp corner

is not in the plan. A better solution is to document the asymptotic fields near the sharp corner as a function of the angle and the directions of the two segments that form the sharp corner.

We compare in Fig. 8(b) three dislocation loop geometries (*i.e.*, circular, triangular, and hexagonal shapes) with the same surface area. The loop-normal displacement along the x_3 axis in Fig. 4 shows essentially no difference for these three types of dislocation loops. Contour and mesh plots of u_3 are given in Fig. 9 for the triangular dislocation loop, and in Fig. 10 for circular and hexagonal loops. Again it is demonstrated that the elastic deformation fields near a dislocation loop are governed primarily by the elastic anisotropy, and depend only secondarily on the shape of the dislocation loop. In other words, the loop shape only affects the displacement and strain fields very close to the loop, but the diffuse scattering is primarily governed by the $0.4a \sim 1.0a$ region. This observation is of practical importance in connection with numerical diffuse scattering simulations, because it means that the diffraction patterns for circular and polygonal dislocation loops will not exhibit noticeable differences. It is the above discussed slope of the displacement field in Fig. 4 (which is governed by the slip system and the elastic anisotropy) and the dislocation loop size that determine the diffuse scattering. Accordingly, the information contained in Figs. 4, 7, and 10 make it possible to perform detailed characterizations of dislocation loops using local-Bragg diffuse scattering measurements, essentially independent of the shape of the loops. Our synergistic experimental-theoretical studies along this line will be reported in a future work.

5. Self-Energy of Dislocation Loops in Anisotropic Solids

The elastic energies (or energy densities) in Eqs. (1) and (2) are often used to determine whether a dislocation reaction is feasible. A question that arises naturally is whether these energy representations remain the same for elastically anisotropic materials and what will be the pre-factors that replace the terms involving elastic constants. For a line dislocation, the representation is straightforward, given by [13]

$$W^{line} = \frac{1}{2\pi} \mathbf{b}^T (\mathbf{B} + \bar{\mathbf{B}})^{-1} \mathbf{b} \ln \frac{R}{\rho_0}, \quad (51)$$

or for a bi-material,

$$W^{line} = \frac{1}{2\pi} \mathbf{b}^T (\mathbf{B}_I + \bar{\mathbf{B}}_{II})^{-1} \mathbf{b} \ln \frac{R}{\rho_0}. \quad (52)$$

To find the self-energy of a dislocation loop lying on the (x_1, x_2) plane in Eq. (6), the evaluation of stress tensor in Eq. (5) involves the evaluation of $\partial G_{mk,l}(\mathbf{x}, \mathbf{x}')/\partial x'_n$. We note that the Green tensor has the property, $\mathbf{G}(\mathbf{x}, \mathbf{x}') = \mathbf{G}(\mathbf{x} - \mathbf{x}')$, as can be seen from example in Eq. (45).

Consequently, $\frac{\partial^2 G_{mk}(\mathbf{x}, \mathbf{x}')}{\partial x_i \partial x'_n} = -\frac{\partial^2 G_{mk}(\mathbf{x}, \mathbf{x}')}{\partial x_i \partial x_n}$, and the dislocation self-energy requires the following quantities:

$$\begin{aligned} & \frac{\partial^2 \mathbf{G}(\mathbf{x}, \mathbf{x}')}{\partial x_i \partial x_j} \\ &= \begin{cases} \frac{1}{4\pi^2} \int_0^{2\pi} \bar{\mathbf{A}} \left\langle \frac{-2ih_i^* h_j^*}{[(x_1 - x'_1) \cos \theta + (x_2 - x'_2) \sin \theta + \bar{p}_s(x_3 - x'_3)]^3} \right\rangle \bar{\mathbf{A}}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & x_3 > x'_3 \\ \frac{1}{4\pi^2} \int_0^{2\pi} \mathbf{A} \left\langle \frac{-2ih_i^* h_j^*}{[(x_1 - x'_1) \cos \theta + (x_2 - x'_2) \sin \theta + p_s(x_3 - x'_3)]^3} \right\rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, & x_3 < x'_3 \end{cases} \quad (53) \end{aligned}$$

To evaluate the strain energy as in Eq. (6), we need to perform a double integral of Eq. (53) over (x'_1, x'_2) . The resulting calculations will be very challenging because of the triple integral and also the presence of singular kernels. Noting that the stress is continuous at $x'_3 = 0$ and using the auxiliary integrals in Appendix B, we find that the triple integral can be converted into the product of a pre-factor (line integral) and a singular integral (double integral), given by

$$\begin{aligned} & \iint_{A'} \left[\int_A \frac{\partial^2 \mathbf{G}(\mathbf{x}, \mathbf{x}')}{\partial x_i \partial x_j} dA \right] dx'_1 dx'_2 \\ &= \frac{1}{4\pi^2} \int_0^{2\pi} \left\{ \mathbf{A} \langle 8ih_i^* h_j^* \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} \right\} \times \\ & \quad \left\{ \int_{\beta=0}^{2\pi} \int_{r'=0}^{1-\rho_0} \left[r'^2 \cos(\beta - \theta) I_4(r' \cos(\beta - \theta)) \right] dr' d\beta \right\} d\theta \\ &= \frac{1}{4\pi^2} \left\{ \int_0^{2\pi} \mathbf{A} \langle 8ih_i^* h_j^* \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta \right\} \times \\ & \quad \int_{\beta=0}^{2\pi} \int_{r'=0}^{1-\rho_0} \left[r'^2 \cos(\beta) I_4(r' \cos(\beta)) \right] dr' d\beta \quad (54) \\ &= \frac{1}{4\pi^2} \mathbf{E}^{ij} (c_{pq}/c_{11}, \mathbf{n}, \mathbf{b}) J_{\text{singular}} \end{aligned}$$

where the dependence on slip systems and elastic anisotropy is lumped into $\mathbf{E}^{ij}(c_{pq}/c_{11}, \mathbf{n}, \mathbf{b})$,

$$\mathbf{E}^{ij} (c_{pq}/c_{11}, \mathbf{n}, \mathbf{b}) = \int_0^{2\pi} \mathbf{A} \langle 8ih_i^* h_j^* \rangle \mathbf{A}^{-1} (\mathbf{B}^{-1} + \bar{\mathbf{B}}^{-1})^{-1} d\theta, \quad (55)$$

and the singular integral J_{singular} does not depend on the crystallography,

$$\begin{aligned} J_{\text{singular}} &= \int_{\beta=0}^{2\pi} \int_{r'=0}^{1-\rho_0} \left[r'^2 \cos(\beta) I_4(r' \cos(\beta)) \right] dr' d\beta \\ &= \int_{\beta=0}^{2\pi} \int_{r'=0}^{1-\rho_0} \left\{ r'^2 \cos \beta \left[\frac{\tan \phi}{2 \left[(r' \cos \beta)^2 - 1 \right] \left[(r' \cos \beta)^2 (1 + \tan^2 \phi) - 1 \right]} + \right. \right. \\ &\quad \left. \left. \frac{\tan^{-1} \left(r' \cos \beta \tan \phi / \sqrt{(r' \cos \beta)^2 - 1} \right)}{2 r' \cos \beta \left[(r' \cos \beta)^2 - 1 \right]^{3/2}} \right] \right\}_{\phi=(\pi/2)^-} dr' d\beta \end{aligned} \quad (56)$$

The function $I_4(\dots)$ is given in Eq. (84). Since the above results are derived for arbitrary elastic anisotropy, we note that J_{singular} remains the same for isotropic and anisotropic elasticity. Therefore, the strain energies in Eq. (2) remain unchanged for anisotropic elasticity with the only change being the pre-factors.

Note that Fig. 7 plots the strain component, ε_{33} , given by

$$\varepsilon_{33} = \frac{\partial u_3(\mathbf{x}')}{\partial x'_3} = - \int_A b_i c_{ijkl} \frac{\partial}{\partial x'_3} [G_{3k,l}(\mathbf{x}, \mathbf{x}')] dA_j, \quad (57)$$

which can be easily evaluated in a similar procedure as that of deriving Eq. (54). However, Eq. (54) uses $x'_3 = 0$; here we need to use the full result in Eq. (85) for numerical evaluations.

As an example, considering a prismatic dislocation loop on (001) plane with $b_3 = -b_p$ and $dA_3 = dA$, we can simplify the above equation as

$$\begin{aligned} W_{\text{prismatic}}^{\text{loop}} &= \frac{1}{2} \int_S \sigma_{ij}(\mathbf{x}') b_i n_j dA' = \frac{1}{2} \int_S \sigma_{33}(\mathbf{x}') b_3 n_3 dA' \\ &= \frac{1}{2} b_p^2 \int_A \int_{A'} \left[c_{11}^2 G_{33,33} + c_{12}^2 (G_{11,11} + G_{12,12} + G_{21,21} + G_{22,22}) \right. \\ &\quad \left. + c_{12} c_{11} (G_{13,13} + G_{23,23} + G_{31,31} + G_{32,32}) \right] dA' dA \end{aligned} \quad (58)$$

Write $\mathbf{E}^{ij} = \{E_{mij}^{\text{eff}}\}$, and we can define the following pre-factor for the prismatic dislocation loop,

$$\begin{aligned}
E_{prismatic} = & c_{12}c_{12}E_{1111}^{eff} + c_{12}c_{12}E_{1212}^{eff} + c_{12}c_{11}E_{1313}^{eff} \\
& + c_{12}c_{12}E_{2121}^{eff} + c_{12}c_{12}E_{2222}^{eff} + c_{12}c_{11}E_{2323}^{eff} \cdot \\
& + c_{11}c_{12}E_{3131}^{eff} + c_{11}c_{12}E_{3232}^{eff} + c_{11}c_{11}E_{3333}^{eff}
\end{aligned} \tag{59}$$

A similar representation for a shear dislocation loop with $b_1 = b_s$ and $dA_3 = dA$ gives

$$E_{shear} = -c_{44}^2 \left(E_{1133}^{eff} + E_{1313}^{eff} + E_{3131}^{eff} + E_{3311}^{eff} \right). \tag{60}$$

The modulus-related pre-factors for strain energies of prismatic and shear dislocation loops can be found in Bower [24] for isotropic elasticity, as given in Eq. (2). We have used these solutions to validate our approach, by numerically proving

$$E_{prismatic} \propto E/(1-\nu^2), \quad E_{shear} \propto E(2-\nu)/(1-\nu^2). \tag{61}$$

Now consider cubic crystals, which can be described by two parameters,

$$\eta = c_{12}/c_{11}, \quad \chi = \frac{c_{12} + 2c_{44}}{c_{11}} - 1, \tag{62}$$

with the restrictions of $-0.5 < \eta < 1$ and $\eta - 1 < \chi < \infty$. When $\chi = 0$, the material is isotropic and the Young's modulus and Poisson's ratio are

$$E = c_{11} \frac{(1-\eta)(1+2\eta)}{1+\eta}, \quad \nu = \frac{\eta}{1+\eta}. \tag{63}$$

And the corresponding $E_{prismatic}$ and E_{shear} will be normalized by

$$\tilde{E}_{prismatic}^{dislocation\ loop} = \frac{E_{prismatic}}{E_{prismatic}(\chi=0)}, \quad \tilde{E}_{shear}^{dislocation\ loop} = \frac{E_{shear}}{E_{shear}(\chi=0)}. \tag{64}$$

The normalized self-energy factors for prismatic and shear dislocation loops are presented in Fig. 11 with respect to χ for three values of η . The representative case of Cu is also marked.

The results in Fig. 11 are similar to the dependence of the effective indentation moduli on η and χ . As proved recently [36,41], the indentation stiffness is proportional to the square root of the contact area and an effective indentation modulus, which can be evaluated from a flat-ended punch contact problem. For isotropic elasticity, the normal and tangential effective moduli are

$$E_{eff} = \frac{E}{1-\nu^2}, \quad G_{eff} = \frac{\mu}{2-\nu} = \frac{E}{2(1+\nu)(2-\nu)}. \tag{65}$$

The effective normal modulus is identical to the energy pre-factor of a prismatic dislocation loop, while the effective shear modulus differs by a factor of $\left[(1+\nu)(1-\nu^2)\right]^{-1}$.

We now examine the relationship between the self-energy pre-factors and the indentation moduli for the general case of any anisotropic solid. The normalized self-energy pre-factors in Eq. (64) can be compared to the normalized effective moduli, defined by

$$\tilde{E}_{normal}^{contact} = \frac{E_{eff}}{E_{eff}(\chi=0)}, \quad \tilde{E}_{shear}^{contact} = \frac{G_{eff}}{G_{eff}(\chi=0)}. \quad (66)$$

For the normal/prismatic components, $\tilde{E}_{prismatic}^{dislocation\ loop} = \tilde{E}_{normal}^{contact}$, so that $\tilde{E}_{normal}^{contact}$ is not drawn in Fig. 11(a) for clarity. For the shear components, $\tilde{E}_{shear}^{dislocation\ loop}$ and $\tilde{E}_{shear}^{contact}$ almost collapse onto each other in Fig. 11(b), with a difference of only a few percent. Therefore, $\tilde{E}_{shear}^{dislocation\ loop} \approx \tilde{E}_{shear}^{contact}$. These results are general and not fortuitous. Both the self-energy pre-factor and the effective indentation modulus are computed from a line integral with the integrand depending on the Stroh matrices **A** and **B** against θ , *e.g.*, in Eq. (55). The diagonal terms of the tensorial integrands have the same mathematical structures, so that $\tilde{E}_{prismatic}^{dislocation\ loop} = \tilde{E}_{normal}^{contact}$; however, the off-diagonal terms differ so $\tilde{E}_{shear}^{dislocation\ loop} \approx \tilde{E}_{shear}^{contact}$. Considering the above discussion, we can rewrite Eq. (2) as

$$W_{prismatic}^{loop} = \frac{1}{4} E_{eff} a b_p^2 \left\{ \ln \left(\frac{4a}{\rho_0} \right) - 1 \right\}, \quad (67)$$

$$W_{shear}^{loop} \approx \frac{1}{4} G_{eff} a b_s^2 \frac{2(2+\eta)^2}{(1+\eta)} \left\{ \ln \left(\frac{4a}{\rho_0} \right) - 2 \right\}, \quad (68)$$

with indentation moduli, E_{eff} and G_{eff} , given by the line integrals in [36].

Care should be exercised in the choice of the cutoff radius in Eq. (2) and in $J_{singular}$ of Eq. (56); they are taken as constants in these representations. There are many ways to smear out the stress singularity at the dislocation core, such as the self-consistent approach by Cai et al. [42], the use of Peierls model in [43], and the use of gradient elasticity by Lazar and co-works [47,48]. In the Peierls model, the core size can be determined by balancing the dislocation interaction and the energy penalty (*i.e.*, the gamma potential as a function of the registry of the two conforming atomic planes). The dislocation interaction depends on the elastic anisotropy through the Green tensor kernel in the integral equations. It is the same Green tensor as in Eqs. (29) and

(35). Just as in the procedure for deriving the separation of variables in Eq. (54), it is anticipated that the same energy pre-factor, $\mathbf{E}^{ij}(c_{pq}/c_{11}, \mathbf{n}, \mathbf{b})$, will remain valid for non-singular Peierls dislocation loops in anisotropic solids.

The above finding can be applied to study the dislocation reactions. As discussed in Introduction, in α -Fe, Xu et al. [4] has proposed the reaction of two $\langle 111 \rangle$ interstitial loops transforming into a single $\langle 001 \rangle$ interstitial loop,

$$\frac{1}{2}[111] + \frac{1}{2}[\bar{1}\bar{1}\bar{1}] = [100]. \quad (69)$$

Comparing the strain energies for the two sides, we get

$$2 \times E_{prismatic}^{(111)} a_{\langle 111 \rangle} b_{\langle 111 \rangle}^2 \rightarrow E_{prismatic}^{(100)} a_{\langle 100 \rangle} b_{\langle 100 \rangle}^2, \quad (70)$$

where the Burgers vector $b_{\langle 111 \rangle}$ is $\sqrt{3}/2$ times the lattice constant, $b_{\langle 100 \rangle}$ equals to the lattice constant, and interstitial number conservation leads to $a_{\langle 100 \rangle} = \sqrt{2}a_{\langle 111 \rangle}$. The self-energy pre-factor for α -Fe is plotted in the standard triangle of the inverse pole figure in Fig. 12. These data correspond to a 15% energy reduction for the reaction in Eq. (69).

6. Conclusions

We have developed analytical representations of the displacement fields and self-energies of prismatic and shear loops in homogeneous and layered anisotropic solids. The major findings of this work are:

- Using the Green tensor in Fourier space, the quadruple integral required to evaluate the displacement fields of dislocation loops can be converted to a line integral with singular integrands. Displacement singularities (*i.e.*, jump by the Burgers vector) can be easily handled by weighted quadrature, but the geometric singularity related to the corners of polygonal dislocation loop causes excessive computational effort. It is proposed that asymptotic calculations at these corners will significantly expedite the numerical calculations.
- The displacement fields for dislocation loops are governed primarily by the elastic anisotropy and depend less strongly on the shape of dislocation loops. This suggests that scattering cross-sections calculated for the analysis of diffuse scattering measurements can be performed for circular dislocation loops to a good approximation.

- The sextuple integral associated with the self-energy of dislocation loops can be transformed into the product of a double integral (that is singular, requires a cutoff radius, and does not depend on elastic anisotropy) and a non-singular line integral (that is determined by the elastic anisotropy and the slip system). The latter is proportional to the self-energy pre-factors of dislocation loops.
- For any materials, the self-energy pre-factor of prismatic dislocation loop and the normal indentation stiffness are identical. For isotropic elastic materials, the self-energy pre-factor of shear dislocation loops and the shear contact stiffness differ by a factor that depends on ν . For cubic crystals, the normalized self-energy pre-factor of shear dislocation loops and normalized shear contact stiffness (as both are normalized by the values at $\chi = 0$) are practically the same with a difference of at most a few percent.

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Appendix A: Isotropic elasticity solution

Consider a circular dislocation loop of radius a lying on the (x_1, x_2) plane at $x_3 = 0$ with its center located at the coordinate origin. The stress formulation is a line integral, while the displacement is based on a double integral [1], given by

$$u_m(\mathbf{r}) = -\frac{1}{8\pi\mu} \int_A \left[\left(\lambda b_j \frac{\partial}{\partial x'_m} \nabla'^2 R dA_j + \mu b_m \frac{\partial}{\partial x'_j} \nabla'^2 R dA_j + \mu b_i \frac{\partial}{\partial x'_i} \nabla'^2 R dA_m \right) - \frac{\lambda + \mu}{\lambda + 2\mu} \left(\lambda b_j \frac{\partial^3 R}{\partial x'_m \partial^2 x'_k} dA_j + 2\mu b_i \frac{\partial^3 R}{\partial x'_m \partial x'_i \partial x'_j} dA_j \right) \right] \quad (71)$$

It involves surface integrals and singularities because of the displacement jump over the dislocated plane. That is, integrations at $x_3 = 0^\pm$ are different. In the above equation, the Lamé constants are

$$\frac{\lambda}{\mu} = \frac{2\nu}{1-2\nu}, \quad \frac{\lambda + \mu}{\lambda + 2\mu} = \frac{1}{2(1-\nu)}, \quad (72)$$

$R = \sqrt{(x'_1 - x_1)^2 + (x'_2 - x_2)^2 + (x'_3 - x_3)^2}$, ε_{ijk} is the permutation tensor, δ_{ij} is Kronecker delta, and the integrand involves terms like R^{-m} with m being positive integers.

Appendix B: Some integrals encountered in the stress and displacement derivations

The two-dimensional inverse Fourier transformation in Eq. (45) encounters the following integral,

$$\begin{aligned} & \int_0^\infty \exp[-i\xi(x_1 \cos \theta + x_2 \sin \theta + p_* x_3)] d\xi \\ &= \left\{ \frac{i}{(x_1 \cos \theta + x_2 \sin \theta + p_* x_3)} \exp[-i\xi(x_1 \cos \theta + x_2 \sin \theta + p_* x_3)] \right\} \bigg|_{\xi=0}^\infty \\ &= \frac{-i}{x_1 \cos \theta + x_2 \sin \theta + p_* x_3} \end{aligned} \quad (73)$$

which is to be further integrated over the dislocated surface, given by

$$I_1 = \int_A \frac{1}{[(x_1 - x'_1) \cos \theta + (x_2 - x'_2) \sin \theta + p_* (x_3 - x'_3)]^2} dA. \quad (74)$$

Integral I_1 can be first converted to polar coordinates and then back to rectangular ones:

$$I_1 = \int_{-\theta}^{2\pi-\theta} \int_0^a \frac{r}{[r \cos \phi - x'_1 \cos \theta - x'_2 \sin \theta - p_* x'_3]^2} dr d\phi = \int_{-1}^1 dy \int_{-\sqrt{1-y^2}}^{\sqrt{1-y^2}} \frac{1}{(x - t^*)^2} dx \quad (75)$$

with $t^* = (x'_1 \cos \theta + x'_2 \sin \theta + p_* x'_3)/a$. The result is singular when $t^* = 1$, as given by

$$I_1 = -2\pi + \frac{2it^*}{\sqrt{1-t^{*2}}} \tan^{-1} \left(\frac{iyt^*}{\sqrt{1-t^{*2}} \sqrt{1-y^2}} \right) \bigg|_{y=-1}^{y=1} \quad (76)$$

Note that in the above derivation, the complex analytic function $\ln(z)$ is encountered. An appropriate domain of definition of $\ln(z)$ is the z -plane cut along the negative real axis. Thus

$$\ln(y - i\sqrt{1-y^2}) \bigg|_{y=-1^+} = -\pi i.$$

We now repeat the surface integral of I_1 over a triangular dislocation loop. Following [32,33], we transform coordinates (x_1, x_2) to (ζ_1, ζ_2) from the new origin at point P_o and two basis vectors,

$$\mathbf{e}_1^\zeta = \frac{\mathbf{x}_{P_3} - \mathbf{x}_{P_o}}{|\mathbf{x}_{P_3} - \mathbf{x}_{P_o}|}, \quad \mathbf{e}_2^\zeta = \frac{\mathbf{x}_{P_1} - \mathbf{x}_{P_o}}{|\mathbf{x}_{P_1} - \mathbf{x}_{P_o}|}. \quad (77)$$

The tensor transformation matrix is then

$$\mathbf{Q} = \begin{bmatrix} e_1^\zeta|_1 & e_1^\zeta|_2 \\ e_2^\zeta|_1 & e_2^\zeta|_2 \end{bmatrix}, \quad \zeta = \mathbf{Q}(\mathbf{x} - \mathbf{x}_{P_o}). \quad (78)$$

The surface integral becomes

$$\begin{aligned} I_2 &= \int_A \frac{1}{[(x_1 - x'_1)\cos\theta + (x_2 - x'_2)\sin\theta - p_*x'_3]^2} dx_1 dx_2 \\ &= \int_0^h d\zeta_2 \int_{-l_1+l_1\zeta_2/h}^{l_2-l_2\zeta_2/h} \frac{1}{[f_1(\theta)\zeta_1 + f_2(\theta)\zeta_2 + f_3^*(\mathbf{x},\theta)]^2} d\zeta_1 \end{aligned} \quad (79)$$

where $f_1(\theta) = Q_{11}^{-1}\cos\theta + Q_{21}^{-1}\sin\theta$, $f_2(\theta) = Q_{12}^{-1}\cos\theta + Q_{22}^{-1}\sin\theta$, and

$$f_3^*(\mathbf{x},\theta) = x_1^{P_o}\cos\theta + x_2^{P_o}\sin\theta - t^*. \quad (80)$$

Our integrals are the same as those in [32,33], so that

$$I_2 = \frac{1}{f_1} \left[\frac{1}{f_2 + f_1 l_1^*} \ln \frac{f_3^* + f_2}{f_3^* - f_1 l_1^*} - \frac{1}{f_2 - f_1 l_2^*} \ln \frac{f_3^* + f_2}{f_3^* + f_1 l_2^*} \right], \quad (81)$$

where $l_1^* = l_1/h$, $l_2^* = l_2/h$, and $f_3^* = f_3/h$.

Next we determine the stress components, which require a derivative of the above integrals. The stress-related integral is

$$I_3 = \int_A \frac{1}{[(x_1 - x'_1)\cos\theta + (x_2 - x'_2)\sin\theta + p_*(x_3 - x'_3)]^3} dA \quad (82)$$

Again the conversion to polar coordinates and then back to rectangular coordinates gives rise to

$$I_3 = \int_{-\theta}^{2\pi-\theta} \int_0^a \frac{r}{[r\cos\phi - x'_1\cos\theta - x'_2\sin\theta - p_*x'_3]^3} dr d\phi = \frac{1}{a} \int_{-1}^1 dy \int_{-\sqrt{1-y^2}}^{\sqrt{1-y^2}} \frac{1}{(x-t^*)^3} dx \quad (83)$$

with $t^* = (x'_1\cos\theta + x'_2\sin\theta + p_*x'_3)/a$. The result is singular only when $t^* = 1$. Further derivation of the above equation requires the following integral,

$$\begin{aligned}
I_4(t^*) &= \int_0^{\pi/2} \frac{\cos^2 \phi}{(t^{*2} - \cos^2 \phi)^2} d\phi \\
&= \left[\frac{\tan \phi}{2(t^{*2} - 1)(t^{*2} \tan^2 \phi + t^{*2} - 1)} + \frac{1}{2t^*(t^{*2} - 1)^{3/2}} \tan^{-1} \left(\frac{t^*}{\sqrt{t^{*2} - 1}} \tan \phi \right) \right]_{\phi=0}^{\phi=\pi/2} \\
&= \left[\frac{\tan \phi}{2(t^{*2} - 1)(t^{*2} \tan^2 \phi + t^{*2} - 1)} + \frac{1}{2t^*(t^{*2} - 1)^{3/2}} \tan^{-1} \left(\frac{t^*}{\sqrt{t^{*2} - 1}} \tan \phi \right) \right]_{\phi=(\pi/2)^-}
\end{aligned} \tag{84}$$

We note that the singularity (when $t^* = 1$) corresponds to the case that (x'_1, x'_2) lies on the dislocation loop. This case requires a cutoff radius of $t^* = 1 - \rho_0$. Also, in the above, $\tan(\phi)$ diverges at $\phi = \pi/2$, but the result converges if we take $\phi = (\pi/2)^-$. Therefore,

$$\begin{aligned}
I_3 &= -\frac{4}{a} t^* I_4 = -\frac{4}{a} t^* \int_0^{\pi/2} \frac{\cos^2 \phi}{(t^{*2} - \cos^2 \phi)^2} d\phi \\
&= -\frac{4}{a} t^* \left[\frac{\tan \phi}{2(t^{*2} - 1)(t^{*2} \tan^2 \phi + t^{*2} - 1)} + \frac{1}{2t^*(t^{*2} - 1)^{3/2}} \tan^{-1} \left(\frac{t^*}{\sqrt{t^{*2} - 1}} \tan \phi \right) \right]_{\phi=(\pi/2)^-}
\end{aligned} \tag{85}$$

Appendix C: Fully closed-form Green tensor in 3D Fourier transform

It should be noted that for numerical diffuse-scattering cross-section calculations, a typical volume of $\sim 250,000$ atoms pose great challenges in the numerical quadrature performance. In this work, numerical quadrature of many nearly singular integrals is performed by the adaptive Simpson method, which requires many integrations points of variable θ . Our formulation has the advantage of separating this angular variable from others, so that numerical quadrature can be expedited by tabulating matrices **A** and **B**.

An alternative method can be used if the Green tensor can be written in fully closed form in three-dimensional Fourier space, such as for cubic materials and transversely isotropic materials [27-30, 50, 51]. To compare to our two-dimensional Fourier transform method in Section 2, the three-dimensional Fourier transform method in Ohr [29, 30] is summarized as below. Using the Fourier transform of $\hat{f}(\mathbf{k}) = \int f(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{x}$, the Green tensor in Fourier space

is given in closed form with respect to the cube axes as $\hat{G}_{mn}(\mathbf{k}) = \frac{\hat{g}_{mn}(\mathbf{\kappa})}{k^2}$, and $\hat{g}_{mn}(\mathbf{\kappa})$ does not depend on the magnitude of wavevector,

$$\hat{g}_{mn}(\mathbf{\kappa}) = \frac{\delta_{mn}}{D_m} - (c_{12} + c_{44}) \frac{\kappa_m \kappa_n}{D_m D_n D}, \quad (86)$$

where $\kappa_i = k_i/k$, $D_i = c_{44} + \mathcal{G}\kappa_i^2$, $D = 1 + (c_{12} + c_{44}) \left(\frac{\kappa_1^2}{D_1} + \frac{\kappa_2^2}{D_2} + \frac{\kappa_3^2}{D_3} \right)$, and $\mathcal{G} = c_{11} - c_{12} - 2c_{44}$ [28].

Clearly no summation is implied over repeated indices in this equation.

Using the inverse Fourier transformation, one can evaluate the integration over k explicitly and that over the zenith angle ϕ in $\mathbf{k}$ -space by the Chebyshev-Gauss quadrature [29]. Therefore the results are written as a line integral over the azimuth angle θ as

$$u_m(r) = -\frac{a}{4\pi N|z|} \int_0^{2\pi} \left[\sum_{n=1}^N (\mathbf{\kappa}_n \cdot \mathbf{r}) F_m(\mathbf{\kappa}_n) \right] d\theta, \quad (87)$$

where $\mathbf{\kappa}_n = \frac{1}{\sqrt{1+t_n^2}} (\cos \theta, \sin \theta, t_n)^T$, $t_n = \frac{d_1 + d_2}{2} + \frac{d_1 - d_2}{2} \cos \left[\frac{(2n-1)\pi}{2N} \right]$, a is the radius of the

circular dislocation loop, and d_1 and d_2 are given by $-\frac{x \cos \theta + y \sin \theta \pm 1}{z}$ and $d_1 > d_2$. Using

the configuration in Fig. 1 (*i.e.*, considering only $\mathbf{b} = (b_1, 0, b_3)^T$ and $dS_3 = dS$), the term $F_m(\mathbf{\kappa})$ in Eq. (87) is given by

$$F_m(\mathbf{\kappa}) = (b_3 c_{33jn} + b_1 c_{13jn}) \kappa_j \hat{g}_{nm}. \quad (88)$$

These calculations produce a high accuracy for total Chebyshev-Gauss integration points of about 100.

Note that the Green tensor is given in closed form only in the crystallographic axes X_i . The transformation matrix from X_i to x_j requires a transformation matrix $\mathbf{Q}$. While details of the method used were not provided in [29], our procedure is that, with a given vector $\mathbf{\kappa}$, we transform it back to X_i coordinates, so that $\mathbf{\kappa}^* = \mathbf{Q}^T \mathbf{\kappa}$. Now in the crystallographic X_i coordinates, $\hat{g}_{mn}^*$ are given in Eq. (86) as a function of $\mathbf{\kappa}^*$. The tensor transformation thus gives $\hat{\mathbf{g}} = \mathbf{Q} \hat{\mathbf{g}}^* \mathbf{Q}^T$. Our method in Section 2 and the method here give identical results, with roughly the same level of performance if the matrices $\mathbf{A}$ and $\mathbf{B}$ have been tabulated *a priori*.

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Figure Captions

- Figure 1 Orientations and geometric conventions for dislocation loops on $\{001\}$ and $\{111\}$ planes.
- Figure 2 Geometric conventions used in the Green's function analysis for a homogeneous, bi-layer, and multi-layer material. A point force, $\mathbf{t}_0$, is applied at the coordinate origin. The two-dimensional Fourier transform will be performed on (x_1, x_2) coordinates. The solutions will be used to analyze dislocation loops lying on the $x_3 = 0$ plane.
- Figure 3 Comparisons of the normalized displacement, u_3/b_p , at $x_2 = 0$ caused by a prismatic loop in (a) isotropic elastic solid, (b) Cu $\{100\}$ plane, and (c) Cu $\{111\}$ plane.
- Figure 4 (a) Comparisons of the loop normal displacements of circular prismatic loops on Cu $\{100\}$ and $\{111\}$ planes, and in an isotropic solid together with comparisons of displacements for triangular and hexagonal prismatic loops on Cu $\{111\}$. (b) Similar plots for bcc Fe.
- Figure 5 Displacement contour plots for circular prismatic dislocation loops lying on the $x_2 = 0$ plane: (a) isotropic elasticity and u_1/b_p , (b) isotropic elasticity and u_3/b_p , (c) Fe $\{100\}$ plane and u_1/b_p , (d) Fe $\{100\}$ plane and u_3/b_p , (e) Fe $\{111\}$ plane and u_1/b_p , and (f) Fe $\{111\}$ plane and u_3/b_p . Poisson's ratio is $\nu = 0.3$ for isotropic elasticity. Coordinates are given in Fig. 1 with $b_3 = b_p$.
- Figure 6 Displacement contour plots for circular shear dislocation loops lying on the $x_2 = 0$ plane: (a) isotropic elasticity and u_1/b_p , (b) isotropic elasticity and u_3/b_p , (c) Fe $\{100\}$ plane and u_1/b_p , (d) Fe $\{100\}$ plane and u_3/b_p , (e) Fe $\{111\}$ plane and u_1/b_p , and (f) Fe $\{111\}$ plane and u_3/b_p . Poisson's ratio is $\nu = 0.3$ for isotropic elasticity. Coordinates are given in Fig. 1 with $b_1 = b_s$.
- Figure 7 Contours of strain component ε_{33} for Fe $\{100\}$ and Fe $\{111\}$ interstitial loops (geometry given in Fig. 1) in (a) and (b) respectively. Due to the singularity at the loop core, a cutoff radius of $0.2a$ is introduced. The geometric features of these

distributions are governed primarily by the crystallographic plane of the loop and the elastic anisotropy.

Figure 8 (a) Schematic illustration of a triangular dislocation in its local coordinates. (b) Dislocation loops with different shapes but equal areas on $\{111\}$ planes are plotted. The triangular shape is included for comparison, since actual dislocation loops are not likely to possess such a shape.

Figure 9 Displacements caused by a triangular-shaped prismatic dislocation loop lying on Cu $\{111\}$ plane at $x_3 = 0$: (a) contours of u_3/b_p on (x_1, x_3) plane, (b) mesh plot that corresponds to (a), (c) u_3/b_p mesh plot on the plane of $x_3 = 2a$, and (d) u_3/b_p mesh plot on the plane of $x_3 = 0.2a$. These calculations adopt a quadrature tolerance of 10^{-4} .

Figure 10 Displacements caused by (a) a circular prismatic dislocation loop and (b) a hexagon-shaped prismatic dislocation loop lying on Cu $\{111\}$ plane at $x_3 = 0$. Mesh plots of u_3/b_p are given on the plane of $x_3 = 0.2a$. Insets provide the corresponding contour plots. Calculations for the hexagonal loop adopt a quadrature tolerance of 10^{-5} .

Figure 11 Comparisons between normalized self-energy of circular dislocation loop and normalized indentation modulus. (a) Self-energy pre-factor of a prismatic loop and normal indentation effective modulus are identical. (b) Self-energy pre-factor of a shear dislocation loop and shear effective modulus, if both are normalized by the corresponding values at $\chi = 0$, differ by only a few percent.

Figure 12 Contour plot of the self-energy pre-factor for a prismatic dislocation loop of α -Fe, as in Eq. (67), which replaces the isotropic elastic formulation in Eq. (2) in the standard triangle of inverse pole figures.

Figure 1

Figure 2

(a)

(b)

(c)

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9

Figure 10

(a)

(b)

Figure 11

Figure 12