Edge-dislocation displacements in an elastic strip

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A Fourier-transform method is used to obtain the displacement field for an edge dislocation. The method reproduces known results and produces new solutions that can be compared with those from atomistic models of edge dislocations.

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I. INTRODUCTION

Because plastic flow occurs through the motion of dislocations, a detailed knowledge of dislocation structure and propagation is desirable.[1] Recent work in molecular dynamics, i.e., solving the equations of motion for crystals containing a few thousand particles, makes it possible to observe dislocations in motion.[2] In comparing these numerical calculations with the predictions of macroscopic elasticity theory, it is necessary to use identical boundary conditions. Thus, both the molecular dynamics and the elasticity theory may be considered in the finite-width strip geometry shown in Fig. 1. Boundary conditions are significant in the dislocation problems, because the displacment field diverges at large R in the absence of boundary constraints.[1]

In this paper, we outline a method for solving the equilibrium-elasticity equations that can be applied to edge dislocations located in a strip having parallel boundaries. The boundaries can be either fixed or stress-free. To illustrate the method, we consider an edge dislocation with Burgers vector parallel to the strip edge and centered in the strip, but these restrictions are not essential. A detailed comparison of dynamical solutions with the results of molecular dynamics is in progress.[3]

II. METHOD

We make use of two fundamental equations from isotropic elasticity theory,

$$\eta\nabla^2\mathbf{U}+(\lambda+\eta)\nabla(\nabla\cdot\mathbf{U})=0, \qquad (1)$$

$$\nabla^4\mathbf{U}=0 \qquad (2)$$

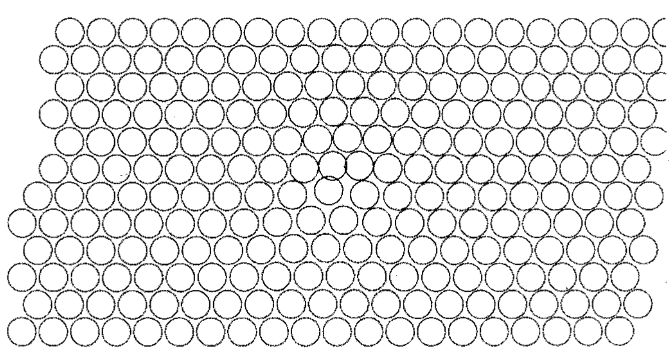

FIG. 1. Geometry for studying the structure of edge dislocations using molecular dynamics and elasticity theory. The particles along the upper and lower edges of the strip are clamped so that the stress well ahead (right) of the dislocation is pure shear and that far behind (left) the dislocation is zero.

where

$$\mathbf{U}=U\hat{\imath}+V\hat{\jmath}+W\hat{k},$$

and U, V, and W are the x, y, and z displacement-vector components, respectively, and λ and η are the Lamé constants. Equation (1) says that the net force on a volume element of material is zero and Eq. (2) is a direct mathematical consequence of Eq. (1). A separable solution of Eq. (2) that satisfies Eq. (1) is

$$U=(b/2\pi)\int_0^\infty (A+By)\ \exp(-ky)\sin kx\,dk,$$

$$V=(b/2\pi)\int_0^\infty [A\ \mathrm{sgn}(y)+\gamma B/k+By\ \mathrm{sgn}(y)]\times\exp(-k|y|)\cos kx\,dk.$$

$$W=0,$$

$\gamma=3-4\nu$ (ν is Poisson's ratio), and b is Burgers vector. The Fourier coefficients A and B appear in both equations, so if $U[V]$ is known, then $V[U]$ is completely determined. Consider an edge dislocation in the infinite xy plane (see Fig. 2) with the pictured boundary conditions,

$$U(x<0,\pm 0)=\pm\tfrac{1}{2}b,\ U(x>0,0)=0.$$

The solution to this problem can be obtained by using the Airy-function method,[1]

$$U=\frac{b}{2\pi}\left(-\tan^{-1}\frac{x}{y}+\frac{xy}{2(1-\nu)(x^2+y^2)}+\frac{\pi}{2}\,\mathrm{sgn}(y)\right),$$

$$V=\frac{b}{2\pi}\left(-\frac{1-2\nu}{4(1-\nu)}\ \ln(x^2+y^2)+\frac{y^2}{2(1-\nu)(x^2+y^2)}\right).$$

The Fourier transform of this solution is

$$U=\frac{b}{2\pi}\left[\int_0^\infty\left(-\frac{1}{k}\mathrm{sgn}(y)+\frac{y}{2(1-\nu)}\right)\times\exp(-k|y|)\ \sin kx\,dk+\ \mathrm{sgn}(y)\frac{\pi}{2}\right],$$

FIG. 2. Displacement boundary conditions for U. The edge dislocation is located at the origin of our coordinate axes.

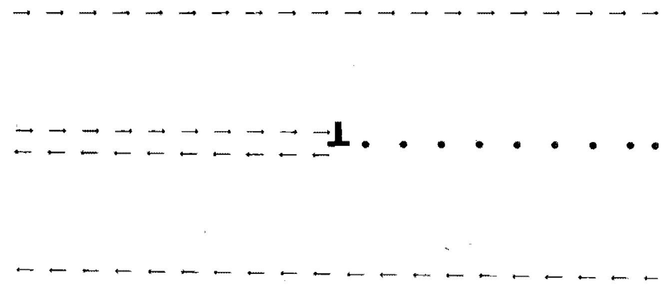

FIG. 3. Boundary conditions for an edge dislocation located in the center of a clamped strip. The stress is pure shear to the far right of the dislocation and is zero to the far left of it.

$$V=\frac{b}{2\pi}\int_0^\infty\left(-\frac{1}{k}+\frac{\gamma}{2(1-\nu)k}+\frac{y\,\mathrm{sgn}(y)}{2(1-\nu)}\right)\times\exp(-k|y|)\cos kx\,dk.$$

We may now obtain the solution to the problem shown in Fig. 3. The boundary conditions are $U(x<0,\pm 0)=\pm\frac{1}{2}b$, $U(x>0,0)=0, U(x,\pm A)=\pm\frac{1}{2}b$, and $V(x,\pm A)=0$, where $\pm A$ is the strip half-width. Figure 3 shows the interaction of an imposed shear displacement b with an edge dislocation that has moved through the strip along the x axis and stopped at $(x,y)=(0,0)$; the arrows display the boundary conditions for U. We construct the displacement field throughout the strip by using an "image" method. The images lie at $(0,\pm 2nA)$, where n is an integer. They are not dislocations, but are instead functional forms that satisfy Eqs. (1) and (2).

$$\begin{aligned}U=\frac{b}{2\pi}\int_0^\infty &\sin kx\,dk\\ &\times\Bigg[\left(-\frac{1}{k}\,\mathrm{sgn}(y)+\frac{y}{2(1-\nu)}\right)\exp(-k|y|)\\ &+\sum_{n=1}^{\infty}(\alpha_n+\beta_n y)\exp[k(y-2nA)]\\ &+\sum_{n=1}^{\infty}(a_n+b_n y)\exp[-k(y+2nA)]\Bigg]\\ &+\frac{b}{4}\,\mathrm{sgn}(y)+\frac{by}{4A},\end{aligned}$$

$$\begin{aligned}V=\frac{b}{2\pi}\int_0^\infty &\cos kx\,dk\\ &\times\Bigg[\left(\frac{1-2\nu}{2(1-\nu)k}+\frac{y}{2(1-\nu)}\,\mathrm{sgn}(y)\right)\exp(-k|y|)\\ &+\sum_{n=1}^{\infty}\left(-\alpha_n+\frac{\gamma\beta_n}{k}-\beta_n y\right)\exp[k(y-2nA)]\\ &+\sum_{n=1}^{\infty}\left(a_n+\frac{\gamma b_n}{k}+b_n y\right)\exp[-k(y+2nA)]\Bigg].\end{aligned}$$

The coefficients are most conveniently represented as power series in "Ak",

$$a_n=\sum_{m=1}^{n+2}a(m,n)A\,(Ak)^{m-2},$$

$$b_n=\sum_{m=1}^{n+2}b(m,n)(Ak)^{m-2}.$$

For this centered configuration with either fixed or stress-free boundaries, $\alpha_n=-a_n$ and $\beta_n=b_n$. Only four integrals are required to evaluate the Fourier integrals:

$$\int_0^\infty(1/k)\exp(-ky)\,\sin kx\,dk=\tan^{-1}(x/y),$$

$$\int_0^\infty(1/k)\exp(-ky)\,\cos kx\,dk=-\tfrac{1}{2}\ln(x^2+y^2),$$

since

$$-\ln(iz)=-\tfrac{1}{2}\ln(x^2+y^2)+i\tan^{-1}x/y,$$

$$\int_0^\infty k^{p-1}\exp(-ky)\begin{Bmatrix}\sin px\\ \cos px\end{Bmatrix}dk=\frac{\Gamma(p)\begin{Bmatrix}\sin p\theta\\ \cos p\theta\end{Bmatrix}}{(x^2+y^2)^{p/2}}\quad(p\geqslant 1),$$

$$\theta=\sin^{-1}[x(x^2+y^2)^{-1/2}].$$

The problem is solved by considering the boundary conditions and solving the resulting recursion formulas:

$$\begin{aligned}&a(1,1)=-1,\\ &a(2,1)=2(3-4\nu)^{-1},\\ &a(3,1)=-[(3-4\nu)(1-\nu)]^{-1},\\ &b(1,n)=0,\\ &b(2,1)=[2(3-4\nu)(1-\nu)]^{-1},\\ &b(3,1)=-[(3-4\nu)(1-\nu)]^{-1},\\ &b(m,n+1)=-2(3-4\nu)^{-1}[a(m-1,n)\\ &\qquad\qquad+b(m-1,n)]-b(m,n)\qquad(m\geqslant 2),\\ &a(m,n+1)=a(m,n)+b(m,n)+b(m,n+1).\end{aligned}$$

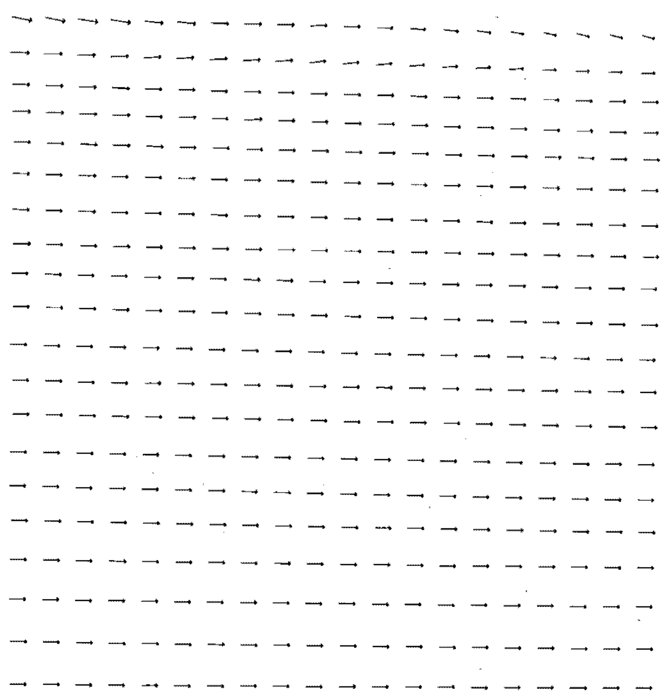

FIG. 4. The convergence of the top-boundary displacements, as 38 additional "images" (19 pairs), are added to the infinite-plane solution, which is shown at the top of the figure.

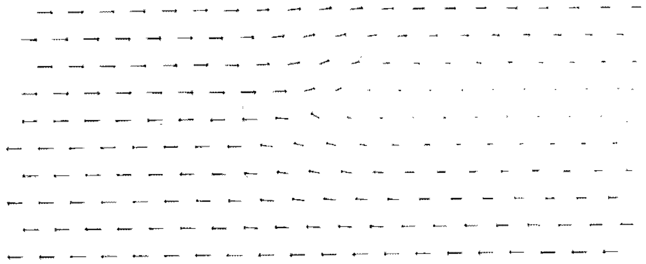

FIG. 5. Displacements obtained in a fixed-boundary strip after summing 38 images. The displacements are shown at the sites of a triangular lattice in order to visualize the effect of a finite lattice on the field. The tails of the arrows represent the atoms in an unstrained lattice; the heads represent present atomic sites.

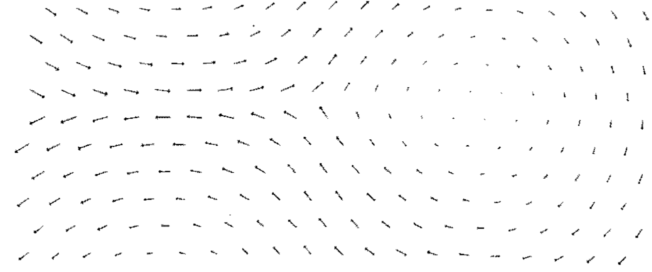

FIG. 6. Displacements obtained in a stress-free boundary strip after summing 40 images. (Same comments apply as in Fig. 5.).

To solve the stress-free strip $\sigma_{yy}(x\pm A) = \sigma_{xy}(x,\pm A) = 0$ one obtains the stresses from the general displacements given above. The constant shear $b/4A$ in U is set equal to zero. These stresses along with the boundary conditions yield the following recursion formulas:

$$a(1,1)=1,$$
$$a(2,1)=-2,$$
$$a(3,1)=(1-\nu)^{-1},$$
$$b(1,n)=0,$$
$$b(2,1)=-4[2(1-\nu)]^{-1},$$
$$b(3,1)=(1-\nu)^{-1},$$
$$b(m,n+1)=2[a(m-1,n)+b(m-1,n)] + b(m,n)(3-4\nu) \quad (m\geqslant 2),$$
$$a(m,n+1)=b(m,n+1)+a(m,n)+b(m,n)+2(1-\nu) \times [b(m+1,n)-b(m+1,n+1)].$$

III. RESULTS

Figure 4 shows the rigid boundary displacement field at $y=A$ as a function of the number of images n included in the solution. The error falls off as $1/n$. In Figs. 4–6, Poisson's ratio is 0.25. This same value is appropriate to the molecular-dynamics calculations.[4] The Burgers vector equals unity. (For this centered configuration, it is possible to analytically sum all the arctans, ln's, and k^0 terms. This decreases the error but does not change the $1/n$ dependence.) Figure 5 shows the displacement field throughout the rigid boundary strip after taking 38 images. To sum V, because the logarithmic terms appear to cause V to diverge, we let $V_{\text{image}}(\pm 2nA)$ represent the image contributions to the y displacement field:

$$V = V_{\text{core}} + \tfrac{1}{2}[V_{\text{image}}(2A) + V_{\text{image}}(-2A)] + \tfrac{1}{2}[V_{\text{image}}(2A) + V_{\text{image}}(-2A) + V_{\text{image}}(4A) + V_{\text{image}}(-4A)] + \cdots,$$

where V_{core} is the infinite-plane solution. This procedure demonstrates the convergence of V. The U terms add directly:

$$U = U_{\text{core}} + U_{\text{image}}(2A) + U_{\text{image}}(-2A) + U_{\text{image}}(4A) + U_{\text{image}}(-4A) + \cdots.$$

Figure 6 shows the displacement field throughout the stress-free strip after summing 40 images. Using Kroupa's calculation[5] of the bend angle of the strip, we find that the error in the displacement field falls off less rapidly than in the fixed-boundary case. Nabarro and Kostlan[6] have used an Airy-function approach to solve this same stress-free problem.

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