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Finite Element Analysis of Discrete Circular Dislocations

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Abstract: The present work gives a systematic and rigorous implementation of (edge type) circular Volterra dislocation loops in ordinary axisymmetric finite elements using the thermal analogue and the integral representation of dislocations through stresses. The accuracy of the proposed method is studied in problems where analytical solutions exist. The full fields are given for loop dislocations in isotropic and anisotropic crystals and the Peach-Koehler forces are calculated for loops approaching free surfaces and bimaterial interfaces. The results are expected to be very important in the analysis of plastic yield strength, giving quantitative results regarding the influence of grain boundaries, interstitial particles, microvoids, thin film constraints and nano-indentation phenomena. The interaction of few dislocations with various inhomogeneities gives rise to size effects in the yield strength which are of great importance in nano-mechanics.

Keywords: Dislocations, Finite elements, Anisotropic elasticity, Nano-mechanics

1 Introduction

Volterra dislocation loops have Burgers vector normal to the plane of the loop and can form in a solid due to irradiation or quenching by the precipitation of vacancies or interstitial atoms [Khraishi et al. (2000)]. Steketee (1958) indicated that apart from major importance in solid state physics, dislocation theory is of great use in geophysics, since the mechanics involved in earthquakes imply displacement discontinuities across the fractured zones. The mechanics of dislocations is a prominent and difficult subject of Linear Elasticity [Hirth and Lothe (1982)], and closed form solutions exist for relatively simple problems [Mastrojannis et al. (1977); Wang (1996); Khraishi et al. (2000); Kroupa (1960); Vagera (1970); Dundurs and

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Salamon (1972); Ohr (1978)]. The analysis of the interactions of a dislocation loop with other dislocations, with free surfaces, with grain interfaces, with voids and interstitials are important for the physical properties of plasticity, friction, micro and nano-indentation, strength of nano-composites and micro-electro-mechanical devices, see for example Philips (2001), Cotrell (1961), Petch (1953), Hall (1951), Rice (1992).

At the atomic level, a prismatic loop dislocation can be viewed as a stacking fault in an fcc crystal system. An extrinsic stacking fault can be formed, if clusters of interstitials are condensed to form an extra plane of atoms to give a stacking sequence: ABCABCBABCABC... On the other hand, an intrinsic stacking fault can be formed by a collapse of vacancy clusters to form a missing plane of atoms to give a stacking sequence: ABCABCACABCABC... Another appearance of a prismatic loop dislocation is during the growth of a coherent precipitate. In such case, stresses are generated because the lattice dimensions of the precipitate differ from those of the matrix [Baker et al. (1959)]. When the strain energy is large enough, it will be relieved by the precipitate becoming non-coherent (losing continuity with the matrix) and this is done by the formation of dislocation loops at the interface.

Extended prismatic loops have been identified as one possible mechanism of quench hardening in copper [Kimura and Hasiguti (1962)]. In such case, these loops should require an activation energy of about 5eV to disappear. Clarebrough et al. (1964) used electrical resistance measurements and transmission electron microscopy (TEM) to show that dislocation loops predominate as the clustered vacancy defects in gold if, after quenching from high temperature to 0˚C, the gold is rapidly up-quenchened to 100˚C. The oxidation of small amounts of impurities present in the copper give rise to prismatic punching of dislocation loops.

Humphreys (1968) examined single crystals of copper containing coherent precipitates of cobalt. The crystals were deformed in tension and the dislocation distributions were determined by TEM. Coherent particles with a radius of 120Å remained coherent after deformation and were sheared together with the matrix. Particles with a radius of 170Å and above lost coherency spontaneously upon deformation, resulting in rows of prismatic loops of primary Burgers vector.

Weatherly (1968) indicated that a growing precipitate can lose coherency by punching of prismatic dislocation loops, depending on the shape of the precipitate and the dilatation transformation strain. In this way it was explained why Ni-Cr-Ti-Al alloys and Cu-Al_2O_3 alloys showed no evidence of punching, whereas Cu-MgO alloys did. Weatherly and Nicholson (1968) investigated the mechanism of coherency loss of four semi-coherent precipitates (Al-Cu, Al-Cu-Mg, Al-Mg-Si and Ni-Cr-Ti-Al) using TEM. In the last three cases, loss of coherency was due to the attraction of matrix dislocation to the particle/matrix interface. In the first case, loss of coherency was by nucleation of dislocation loops within the plate-shaped precipitate (as the thickness of the precipitate increases).

Humphreys and Stewart (1972) examined single crystals of Cu-20 wt % Zn, containing spherical silica particles, which had been deformed in tension at room temperature. Around the smallest particles (diameter less than 0.11μm), primary prismatic loops are formed. Dislocation debris accumulates at the particles with increasing strain and is responsible for the high rate of work hardening.

The paper is structured as follows. Firstly, we present a thermal analogue of an edge-type loop dislocation. We focus on axisymmetric cases, with the dislocation axis being the axis of axisymmetry. The remaining of the paper presents various applications, comparing with known analytic results, when possible, and presenting new results in cases of material anisotropy. Finally, we investigate the loop dislocations in the context of nano-indentation.

2 The thermal analogue and its implementation in finite elements

2.1 The thermal analogue for discrete circular dislocations

In the present work, we are inspired by the work of Biot (1935) who presented a thermal analogue for the two-dimensional edge dislocation and used it with optical methods to study dislocations. The analysis of a Volterra circular dislocation of radius r_d with a Burgers' vector b_z normal to the plane of the loop requires an axial polar coordinate system (r, θ, z) with the z-axis being in the direction normal to the centre of the dislocation loop, r being the radial direction and θ the circumferential coordinate (Fig. 1).

For any closed circuit embracing the dislocation line we must have (in a Cartesian system (x_1, x_2, x_3) shown in Fig. 1

$$b_3 = b_z = \oint u_{3,j} dx_j \tag{1}$$

where repeated index implies the well known summation from 1 to 3.

In order to make eq. (1) single valued, the displacement field must decay to zero as

$$u_i \to O\left(\frac{1}{\sqrt{x_1^2 + x_2^2 + x_3^2}}\right), \quad i = 1,2,3 \tag{2}$$

The corresponding Peach-Koehler force can be deduced from the corresponding Maxwell tensor according to Eshelby, which in a Cartesian system reads as

$$F_\ell = b_3 \varepsilon_{k\ell j} \oint_L \sigma_{3k} dx_j = \lim_{\delta\xi_\ell \to 0} \frac{\delta U_i}{\delta \xi_\ell}, \quad \ell = 1,2,3 \tag{3}$$

where L is the dislocation line of the loop, $\varepsilon_{k\ell j}$ is the alternating tensor and U is the internal energy. The local coordinates ξ_ℓ describe the radial $(\xi_1 = r)$, the vertical $(\xi_3 = z)$ and the circumferential $(\xi_2 = 2\pi r)$ directions. The last are also called line tension of the dislocation loop. The stress field σ_{ij} includes the influence of other dislocations, free surfaces etc.

In the absence of body forces, the equilibrium equations in polar coordinates are

$$\begin{aligned}&\frac{\partial \sigma_{rr}}{\partial r}+\frac{\partial \sigma_{rz}}{\partial z}+\frac{1}{r}\left(\sigma_{rr}-\sigma_{\theta\theta}\right)=0\\&\frac{\partial \sigma_{rz}}{\partial r}+\frac{\partial \sigma_{zz}}{\partial z}+\frac{\sigma_{rz}}{r}=0\end{aligned}\tag{4}$$

The strains are related to the displacements through the geometric relations

$$\begin{aligned}&\varepsilon_{rr}=\frac{\partial u_r}{\partial r},\quad \varepsilon_{zz}=\frac{\partial u_z}{\partial z},\quad \varepsilon_{\theta\theta}=\frac{u_r}{r}\\&2\varepsilon_{rz}=\gamma_{rz}=\frac{\partial u_r}{\partial z}+\frac{\partial u_z}{\partial r}\end{aligned}\tag{5}$$

and the spin

$$2\omega_{rz}=\frac{\partial u_z}{\partial r}-\frac{\partial u_r}{\partial z}\tag{6}$$

The compatibility equations are

$$\begin{aligned}&2\frac{\partial^2 \varepsilon_{rz}}{\partial r\partial z}=\frac{\partial^2 \varepsilon_{rr}}{\partial z^2}+\frac{\partial^2 \varepsilon_{zz}}{\partial r^2}\\&\varepsilon_{rr}=\frac{\partial}{\partial r}\left(r\varepsilon_{\theta\theta}\right)\end{aligned}\tag{7}$$

Using the axisymmetric coordinates (r,z) we enclose the dislocation by a circuit C, as shown in Fig. 2. Then, from eq. (1) we have

$$b_z=\oint_C du_z=\oint_C\left(\frac{\partial u_z}{\partial r}dr+\frac{\partial u_z}{\partial z}dz\right)\tag{8}$$

If $\mathbf{n}$ is the unit vector normal to the circuit C, then we have the auxiliary relations for the infinitesimal segment ds along C:

$$\begin{aligned}&\frac{\partial}{\partial r}dz-\frac{\partial}{\partial z}dr=\frac{\partial}{\partial n}ds\\&\frac{\partial}{\partial r}dr+\frac{\partial}{\partial z}dz=\frac{\partial}{\partial s}ds\end{aligned}\tag{9}$$

We now assume a homogeneous linear thermo-elastic material with cubic elastic symmetry and stress-strain relations taken as

$$\begin{aligned}
\varepsilon_{rr} &= \frac{1}{E}\left(\sigma_{rr} - \nu\left(\sigma_{\theta\theta} + \sigma_{zz}\right)\right) \\
\varepsilon_{\theta\theta} &= \frac{1}{E}\left(\sigma_{\theta\theta} - \nu\left(\sigma_{rr} + \sigma_{zz}\right)\right) \\
\varepsilon_{zz} &= \frac{1}{E}\left(\sigma_{zz} - \nu\left(\sigma_{\theta\theta} + \sigma_{rr}\right)\right) + \alpha_z T(z) \\
\varepsilon_{rz} &= \frac{1}{G}\sigma_{rz}
\end{aligned} \tag{10}$$

Note that in this case we have three independent elastic constants: the elastic modulus E, the Poisson ratio ν and the shear modulus G. Isotropic material implies that

$$G = \frac{E}{2(1+\nu)} \tag{11}$$

It should be also noted that the thermal strain $\alpha_z T(z)$ is added to help establish the thermal analogue and it is not a physical thermal strain (α_z is a “thermal” expansion coefficient and $T(z)$ is a “temperature” distribution).

Misra and Sen (1975) have shown that two stress functions are necessary to describe the stresses in this case, $\Phi(r,z)$ and $R(r,z)$. These functions are continuous with continuous derivatives up to 4^{th} order.

$$\begin{aligned}
\sigma_{rz} &= -\frac{\partial^2\Phi}{\partial r\partial z} \\
\sigma_{rr} &= \frac{\partial^2\Phi}{\partial z^2} + R \\
\sigma_{zz} &= \frac{\partial^2\Phi}{\partial r^2} + \frac{1}{r}\frac{\partial\Phi}{\partial r} \\
\sigma_{\theta\theta} &= \nu\nabla^2\Phi - R
\end{aligned} \tag{12}$$

Integrating with respect to r the compatibility eq. (7), we obtain

$$\frac{\partial}{\partial z}\varepsilon_{rz} = \frac{\partial^2}{\partial z^2}\left(r^2\varepsilon_{\theta\theta}\right) + \frac{\partial}{\partial r}\varepsilon_{zz} \tag{13}$$

Substituting eq. (10) into equation (13), we obtain a relation between Φ and R

$$\frac{\partial^2}{\partial z^2}(rR) = (1-\nu)\frac{\partial}{\partial r}\nabla^2\Phi + \frac{E}{(1+\nu)}\left[\frac{1}{G} - \frac{1+\nu}{E}\right]\frac{\partial^3\Phi}{\partial r\partial z^2} \tag{14}$$

Substituting eq. (10) into equation (7b), we obtain another relation between Φ and R:

$$r\frac{\partial R}{\partial r}+2R=\nu\nabla^2\Phi-\frac{\partial^2\Phi}{\partial z^2} \tag{15}$$

Obviously, eq. (14) and (15) are the driving equations of the problem.

We now turn our attention to the kinematics of the Burgers vector and use Cesaro's integrals, Cesaro (1906). Let C be the amplitude of the disclination. Then

$$C=\oint_C d\omega_{rz}=\oint_C\left(\frac{\partial\varepsilon_{rz}}{\partial r}-\frac{\partial\varepsilon_{rr}}{\partial z}\right)dr+\oint_C\left(\frac{\partial\varepsilon_{zz}}{\partial r}-\frac{\partial\varepsilon_{rz}}{\partial z}\right)dz \tag{16}$$

Continuity of σ_{rz} and the constitutive eq. (10d) implies that

$$C=\oint_C\left(-\frac{\partial\varepsilon_{rr}}{\partial z}dr+\frac{\partial\varepsilon_{zz}}{\partial r}dz\right) \tag{17}$$

Using eq. (12) and the continuity of Φ and R we can conclude that

$$C=0 \tag{18}$$

which assures us that there will be no disclination, precluding a Somigliana type of dislocation. Then Cesaro's integral for b_z becomes

$$b_z=\oint_C\left[\varepsilon_{rz}-r\left(\frac{\partial\varepsilon_{rz}}{\partial r}-\frac{\partial\varepsilon_{rr}}{\partial z}\right)\right]dr+\oint_C\left[\varepsilon_{rz}-r\left(\frac{\partial\varepsilon_{zz}}{\partial z}-\frac{\partial\varepsilon_{rz}}{\partial z}\right)\right]dz \tag{19}$$

Due to continuity of $z\varepsilon_{zz}$ and $r\varepsilon_{rz}$, eq. (19) reduces to

$$b_z=-\oint_C\left(z\frac{\partial\varepsilon_{zz}}{\partial z}+r\frac{\partial\varepsilon_{zz}}{\partial r}\right)dz+\oint_C r\left(\frac{\partial\varepsilon_{rr}}{\partial z}-2\frac{\partial\varepsilon_{rz}}{\partial r}\right)dr-\oint_C r\frac{\partial\varepsilon_{zz}}{\partial r}dz \tag{20}$$

Using eq. (13) and continuity of Φ and R, we obtain

$$b_z=\oint_C z\frac{\partial\left(\alpha_z T(z)\right)}{\partial z}ds \tag{21}$$

We decided to use a simple temperature distribution as in Fig. 3a or Fig. 3b.

$$\begin{aligned}
&\alpha_z T(z)=\Delta\mathrm{T}\quad z=z_d\quad 0\le r\le r_d\\
&\alpha_z T(z)=\Delta\mathrm{T}\frac{(z-z_d+h)}{h}\quad z_d-h\le z\quad 0\le r\le r_d\\
&\alpha_z T(z)=\Delta\mathrm{T}\frac{-(z-z_d-h)}{h}\quad z\le z_d+h\quad 0\le r\le r_d\\
&\alpha_z T(z)=0\quad \text{everywhere else}
\end{aligned} \tag{22}$$

where h is the element size and

$$\alpha_z T(z) = \frac{b_z}{h} \tag{23}$$

Note that eq. (21) is the key theoretical result that needs to be implemented in the finite element codes and then, after selecting an appropriate temperature field as in eq. (22), solve the thermoelastic problem.

2.2 Finite element implementation

Turning to the finite element method, we can discretize the space around the loop dislocation by a uniform fine element distribution of element size h. Assuming linear thermoelastic response, we can assign a temperature distribution as in eq. (22) on the nodes of the mesh as shown in Fig. 3. It should be emphasized that the thermal expansion coefficient α_z is not the physical one, but takes apparent values that are suitable for computations, keeping in mind that there is no actual temperature field in the problem. This procedure forces ordinary finite elements to produce dislocation stress field in a straightforward way.

The ABAQUS general purpose finite element code was used and a uniform mesh of 25,000 axisymmetric, four-noded elements was picked for all applications. The outer boundary was 100 times the Burgers vector in all directions. Note that no special attention was taken for mesh optimization. Mesh optimisation can be achieved by utilising various remeshing techniques and error norms e.g. Zienkiewicz and Zhu (1987).

3 Numerical examples

3.1 The dislocation loop in an infinite medium

In order to test the accuracy of the proposed method, we selected to check the existing analytical solutions for several cases. The simplest case is to consider a circular dislocation loop in an infinite isotropic medium (the geometry of the problem is shown again on Fig. 1).

This problem was studied by Kroupa (1960) and Bullough and Newman (1960). Based on Kroupa's work, Gavazza and Barnett (1976) presented the equation for the self-force per unit dislocation length (tending to shrink the dislocation loop), which is

$$f_r = f_{cut} + f_{tube} = -\frac{\mu b^2}{4\pi(1-\nu)R}\left(\ln\left(\frac{8R}{\varepsilon}\right) - 1\right) - \frac{\mu b^2(3-2\nu)}{16\pi(1-\nu)^2 R} \tag{24}$$

In eq. (24), $R \equiv r_d$ is the dislocation loop radius and $\varepsilon$is the radius of the dislocation core which, from a physical point of view, has magnitude $\varepsilon \approx b_z$. Strictly speaking, the energy density cannot be described inside the core by classic elasticity.

Lubarda and Markenscoff (2007) presented a solution for an edge dislocation which can be used to give an estimation of the core radius. They showed that the width of the dislocation is the region within which the slip discontinuity is less than $b_z/2$, when the maximum discontinuity is b_z. Following their suggestion, we considered $\varepsilon = b_z$ for all our computations, based on the linear distribution of b_z within one element which plays the role of the dislocation width and has size $h = b_z$.

The stress distribution around a Volterra dislocation loop, in the context of isotropic linear elasticity, is given by Khraishi et al. (2000):

$$\begin{aligned}
\sigma_{rr} &= -\frac{Gb_z}{\pi}\left[C_1\mathbf{E}(k)+C_2\mathbf{K}(k)\right]-\frac{Gb_z}{2\pi(1-\nu)}\left[C_5\mathbf{E}(k)+C_6\mathbf{K}(k)\right]\\
\sigma_{\theta\theta} &= -\frac{Gb_z}{\pi}\left[C_9\mathbf{E}(k)+C_{10}\mathbf{K}(k)\right]-\frac{Gb_z}{2\pi(1-\nu)}\left[C_{13}\mathbf{E}(k)+C_{14}\mathbf{K}(k)\right]\\
\sigma_{zz} &= -\frac{Gb_z}{2\pi(1-\nu)}\left[C_{17}\mathbf{E}(k)+C_{18}\mathbf{K}(k)\right]\\
\sigma_{rz} &= -\frac{Gb_z}{2\pi(1-\nu)}\left[C_{27}\mathbf{E}(k)+C_{28}\mathbf{K}(k)\right]
\end{aligned} \tag{25}$$

The coefficients C_{ij} are functions of spatial coordinates and given by the relations

$$\begin{aligned}
&C_1 = \frac{-(a+b)^{1/2}}{\rho^2},\ C_2 = \frac{a}{\rho^2(a+b)^{1/2}},\\
&C_5 = \frac{(a^2-b^2)\left[ar_d^2+2\rho^2\left(a-3r_d^2\right)\right]+p^2\rho^2\left[8ar_d^2-\left(a^2+3b^2\right)\right]}{\rho^2(a-b)^2(a+b)^{3/2}},\\
&C_6 = \frac{-\left[(a^2-b^2)\left(r_d^2+2\rho^2\right)+p^2\rho^2\left(2r_d^2-a\right)\right]}{\rho^2(a-b)(a+b)^{3/2}},\ C_9 = \frac{(a^2-b^2)+\rho^2\left(2r_d^2-a\right)}{\rho^2(a-b)(a+b)^{1/2}},\\
&C_{10} = \frac{\rho^2-a}{\rho^2(a+b)^{1/2}},\ C_{13} = \frac{a\left(\rho^2-r_d^2\right)}{\rho^2(a-b)(a+b)^{1/2}},\ C_{14} = \frac{-\left(\rho^2-r_d^2\right)}{\rho^2(a+b)^{1/2}},\\
&C_{17} = \frac{(a^2-b^2)\left(a-2r_d^2\right)+p^2\left(a^2+3b^2\right)-8ap^2r_d^2}{(a-b)^2(a+b)^{3/2}}\\
&C_{18} = \frac{-\left[(a^2-b^2)+p^2\left(a-2r_d^2\right)\right]}{(a-b)(a+b)^{3/2}},\ C_{27} = \frac{-p\left[a\left(a^2-b^2\right)-p^2\left(a^2+3b^2\right)\right]}{\rho(a-b)^2(a+b)^{3/2}},
\end{aligned} \tag{26}$$

$$C_{28} = \frac{p\left[\left(a^2-b^2\right)-ap^2\right]}{\rho\,(a-b)^2\,(a+b)^{3/2}}$$

The variables $a,\ b,\ \rho,\ r,\ p$ and k are functions of the Cartesian coordinates (x_1, x_2, x_3) shown in Fig. 1 and given by the relations

$$\rho = \left(x_1^2+x_2^2\right)^{1/2},\ r = \left(\rho^2+z^2\right)^{1/2},\ a = r^2+r_d^2,\ b = 2\rho r_d,\\ p = -z,\ k = \left(\frac{2b}{a+b}\right)^{1/2} \tag{27}$$

The terms $\mathbf{K}(k)$ and $\mathbf{E}(k)$ in eq. (25) are complete elliptic integrals of the first and second kind respectively. Their definition is given in eq. (36).

The analytical solutions are useful only if the infinite medium is isotropic. Anisotropic lattices with cubic crystal symmetry can be studied numerically by implementing the elastic constants in the finite element code.

In Table 1 (Appendix A), the elastic constants c_{ij} of the materials used in this work are given as well as the anisotropy factor $H = 2c_{44}+c_{12}-c_{11}$ and the anisotropy ratio $A = \frac{2c_{44}}{c_{11}-c_{12}}$.

The calculation of the force (F_r, F_z)that acts on the dislocation loop is based on the energy released by a small advancement of the dislocation in the r and z direction respectively. Then

$$F_r = -\frac{\partial U}{\partial r},\ F_z = -\frac{\partial U}{\partial z} \tag{28}$$

where $U$is the total elastic energy of the material with the dislocation.

In the numerical implementation of eq. (28), we move the dislocation (and the associate temperature distribution) by one finite element of length h in the (positive) r and (positive) z direction, separately. Then, we compute the total energy in the initial and in the new positions of the dislocation to find the changes of energy ΔU. The acting forces on the dislocation forces are then

$$F_r = -\frac{\partial U}{\partial r} = -\frac{U_{new}-U_{initial}}{h},\ F_z = -\frac{\partial U}{\partial z} = -\frac{U_{new}-U_{initial}}{h} \tag{29}$$

Note that the resulting from eq. (29) force has to be divided by the loop circumference $2\pi R$ so as it can become self-force per unit length, $f_r = F_r/2\pi R$ and $f_z = F_z/2\pi R$.

In Fig. 4 we present some results for an isotropic material like W. For brevity, only the normalized shear stress component σ_{rz}/G distribution is shown for material W

(Fig. 4a). The normalized self force per unit length f_r/Gb_z (tending to shrink the dislocation loop) calculation is shown in Fig. 4b. The analytical solution is denoted by the continuous line and the FEM results are denoted by the square symbols. As discussed before, we have assumed the dislocation core radius $\varepsilon = b_z$. The force in z direction is zero in this case and indeed our computations based on eq. (29b) verified that.

At the final part of this section, the influence of the anisotropy is investigated. In Fig. 5a, the out of plane normalized stress σ_{zz}/G distribution is shown for materials Cu (upper part) and Cr (lower part). The isocontour spatial and shape difference is obvious. In Fig. 5b, the normalized self force per unit length f_r/Gb_z is given for isotropic W and the anisotropic Cu and Cr.

3.2 The dislocation loop near a free surface

Consider a circular dislocation loop of radius R lying in an isotropic half space at a distance a from the free surface $z = 0$ as shown in Fig. 6. This problem has been studied by Bastecka (1964). The stress fields in this case become asymmetric in the z direction and a force towards the free surface is exerted to the dislocation loop.

An examination of Bastecka's solution for the attractive force and its corresponding values leads to the conclusion that the printed version of this work contains some misprints.

The force per unit length that exerts on the dislocation loop is given by the equation

$$f_z = \frac{a^2 b_z^2 G}{R^3 (1-\nu)} \int_0^\infty t^3 J_1^2(t)\, e^{-(2a/R)t} dt \tag{30}$$

where J_1 denotes a Bessel function of the first kind and first order.

By introducing $d = a/R$ and doing the integration, we obtain

$$f_z = \frac{b_z^2 G}{8\pi R(1-\nu)} \left\{ \frac{-3d^4 + 7d^2 + 2}{(1+d^2)^3} \mathbf{E}\left(-\frac{1}{d^2}\right) + \frac{3d^4 + 2d^2 - 1}{(1+d^2)^3} \mathbf{K}\left(-\frac{1}{d^2}\right) \right\} \tag{31}$$

where $\mathbf{K}(k)$ and $\mathbf{E}(k)$ are complete elliptic integrals of the first and second kind respectively.

Then, we calculate the theoretical values of f_z for different values of d. Turning to the finite elements, we use the methodology described in the previous section to calculate the resulting force per unit length for the isotropic material W. The results are presented in Fig. 6a. It is obvious that the match is almost exact.

Again, we investigate the variation of the result in anisotropic materials. In Fig. 6b, the results for the material Cu and Cr are shown. We observe that for low values of a/R, anisotropy plays a significant role: the force that attracts the loop to the surface is stronger if $H < 0$ and weaker if $H > 0$ compared to the isotropic case $H = 0$.

3.3 The dislocation loop in a two phase material

3.3.1 The displacement field of the two-phase material

Consider a two-phase material, idealized as two isotropic half spaces with perfect adhesion and a dislocation loop in a plane parallel to the interface. The geometry of the problem is shown in Fig. 8. This problem was solved by Salamon and Dundurs (1971).

For consistency reasons the loop radius is denoted by R and the positive z-axis is placed as shown so that a positive force would mean attraction of the loop to the interface. The distance from the loop to the interface is denoted by z'. The shear modulus and the Poisson ratio of the two materials are G_1, ν_1 and G_2, ν_2 respectively. The influence of the elastic constants can be reduced to two parameters α and β(Dundurs constants)

$$\alpha = \frac{(G_2/G_1)(\kappa_1+1)-(\kappa_2+1)}{(G_2/G_1)(\kappa_1+1)+(\kappa_2+1)},\ \beta = \frac{(G_2/G_1)(\kappa_1-1)-(\kappa_2-1)}{(G_2/G_1)(\kappa_1+1)+(\kappa_2+1)} \tag{32}$$

where $\kappa_1 = 3-4\nu_1$ and $\kappa_2 = 3-4\nu_2$.

The representation of the elastic fields is given through integrals of the Lipschitz-Hankel type. The following special functions of the space coordinates are used

$$\begin{aligned} J^{(1)}(m,n;p) &= \int_0^\infty J_m(t)J_n(\rho t)\,e^{-|\zeta-\zeta'|t}t^p dt \\ J^{(2)}(m,n;p) &= \int_0^\infty J_m(t)J_n(\rho t)\,e^{-|\zeta+\zeta'|t}t^p dt \end{aligned} \tag{33}$$

where J_k denotes a Bessel function of the first kind and order k. Also, the dimensionless variables $\rho = r/R$, $\zeta = z/R$ and $\zeta' = z'/R$ are used.

The displacement field in the regions *I* and *II* is given by the equations

$$u_\gamma^I = \frac{b_z \gamma}{2(\kappa_1+1)r}\Big\{-(\kappa_1-1)J^{(1)}(1,1;0)+2\left|\zeta-\zeta'\right|J^{(1)}(1,1;1)- \\ -\left[\frac{(\alpha-\beta)\kappa_1}{1+\beta}-\frac{\alpha+\beta}{1-\beta}\right]J^{(2)}(1,1;0)+ \\ +\frac{2(\alpha-\beta)}{1+\beta}\left[\left(\zeta-\kappa_1\zeta'\right)J^{(2)}(1,1;1)+2\zeta'\zeta J^{(2)}(1,1;2)\right]\Big\} \tag{34}$$

$$u_\gamma^{II} = -\frac{(1-\alpha)b_z\gamma}{2(\kappa_2+1)r} \\ \left\{\left(\frac{\kappa_2}{1-\beta}-\frac{1}{1+\beta}\right)J^{(1)}(1,1;0)+2\left(\frac{\zeta}{1-\beta}-\frac{\zeta'}{1+\beta}\right)J^{(1)}(1,1;1)\right\}$$

$$u_z^I = \frac{b_z}{2(\kappa_1+1)}\Big\{\pm(\kappa_1+1)J^{(1)}(1,0;0)+2\left(\zeta-\zeta'\right)J^{(1)}(1,0;1)+ \\ +\left[\frac{(\alpha-\beta)\kappa_1}{1+\beta}+\frac{\alpha+\beta}{1-\beta}\right]J^{(2)}(1,0;0)+ \\ +\frac{2(\alpha-\beta)}{1+\beta}\left[\left(\zeta+\kappa_1\zeta'\right)J^{(2)}(1,0;1)+2\zeta'\zeta J^{(2)}(1,0;2)\right]\Big\} \tag{35}$$

$$u_z^{II} = -\frac{(1-\alpha)b_z}{2(\kappa_2+1)} \\ \left\{\left(\frac{\kappa_2}{1-\beta}+\frac{1}{1+\beta}\right)J^{(1)}(1,0;0)-2\left(\frac{\zeta}{1-\beta}-\frac{\zeta'}{1+\beta}\right)J^{(1)}(1,0;1)\right\}$$

In the expression of u_z^I, the upper sign is to be taken for $\zeta-\zeta'>0$ and the lower for $\zeta-\zeta'<0$. In the expressions of u_γ^I and u_γ^{II}, $\gamma = x$ or y.

In order to evaluate numerically the equations above, it is better to use the complete elliptical integrals representation. The special functions $J(m,n;p)$ can be expressed in terms of the complete elliptic integrals of the first, second and third kind

$$\mathbf{K}(k) = \int_0^{\pi/2}\left(1-k^2\sin^2\varphi\right)^{-1/2}d\varphi \\ \mathbf{E}(k) = \int_0^{\pi/2}\left(1-k^2\sin^2\varphi\right)^{1/2}d\varphi \\ \mathbf{\Pi}(h,k) = \int_0^{\pi/2}\left(1-h\sin^2\varphi\right)^{-1}\left(1-k^2\sin^2\varphi\right)^{-1/2}d\varphi \tag{36}$$

where

$$k^2 = \frac{4\rho}{(1+\rho)^2+\xi^2},\; k'^2 = 1-k^2 = \frac{(1-\rho)^2+\xi^2}{(1+\rho)^2+\xi^2},\; h = \frac{4\rho}{(1+\rho)^2} \tag{37}$$

Also, $\xi = |\zeta - \zeta'|$ for $J^{(1)}(m,n;p)$ and $\xi = |\zeta + \zeta'|$ for $J^{(2)}(m,n;p)$.

Below, we quote the necessary special functions for the calculation of the displacement components.

$$2\pi J(1,0;0) = \begin{cases} -k\rho^{-1/2}\xi\left(\mathbf{K}(k) + \frac{1-\rho}{1+\rho}\mathbf{\Pi}(h,k)\right) + 2\pi & (\rho < 1) \\ -k\xi\mathbf{K}(k) + \pi & (\rho = 1) \\ -k\rho^{-1/2}\xi\left(\mathbf{K}(k) - \frac{\rho-1}{\rho+1}\mathbf{\Pi}(h,k)\right) & (\rho > 1) \end{cases}$$

$$2\pi J(1,0;1) = k\rho^{-1/2}\left(\frac{k^2\left(1-\rho^2-\xi^2\right)}{4k'^2\rho}\mathbf{E}(k) + \mathbf{K}(k)\right)$$

$$2\pi J(1,0;2) = \frac{k^3\xi}{4k'^2\rho^{3/2}} \left\{\left[\frac{k^4\left[1-\left(\rho^2+\xi^2\right)^2\right]}{4k'^2\rho^2} + 3\right]\mathbf{E}(k) - \frac{k^2\left(1-\rho^2-\xi^2\right)}{4\rho}\mathbf{K}(k)\right\}$$

$$2\pi J(1,1;0) = \frac{4}{k\rho^{1/2}}\left[\left(1-\frac{1}{2}k^2\right)\mathbf{K}(k) - \mathbf{E}(k)\right] \tag{38}$$

$$2\pi J(1,1;1) = k\rho^{-3/2}\xi\left[\left(1-\frac{1}{2}k^2\right)\left(k'\right)^{-2}\mathbf{E}(k) - \mathbf{K}(k)\right]$$

$$2\pi J(1,1;2) = k\rho^{-3/2} \left\{\frac{k^2}{4k'^2\rho}\left[\frac{k^4\xi^2}{k'^2} - \left(1+\rho^2\right)\right]\mathbf{E}(k) + \left[1 - \frac{k^2\left(2-k^2\right)\xi^2}{8k'^2\rho}\right]\mathbf{K}(k)\right\}$$

The special cases of a dislocation loop in a homogeneous medium and a dislocation loop near a free surface can be studied using eq. (34) and (35). Ohr (1978) used these equations to visualize the displacement fields of a dislocation loop near a free surface ($\alpha = -1.0$, β = - 0.5).

We consider a material that consists of Cu in region I to study the free surface case. The material properties of Cu will be taken to be isotropic (see Table 1). The distance from the dislocation loop b_z to the interface is selected $z' = 10b_z$. The comparison between the analytical solution and the finite elements prediction of the displacement fields is illustrated in Fig. 9.

3.3.2 *The forces acting on the dislocation loop*

The existence of the bimaterial interface changes the elastic field around the dislocation loop. As a result, a force is exerted on the dislocation. The force can be either attractive towards the interface or repulsive, depending on the elastic constants of the two materials.

Dundurs and Salamon (1972) give the expression for the force components (per unit length). The expression of the component f_r contains the variable ε (the radius of the dislocation core) which does not have an exact value. We will focus on the calculation of the component f_z which is of great practical value in dislocation stacking close to bimaterial interfaces. The following special function of the space coordinates is defined

$$J^*(m,n;p) = \int_0^\infty J_m(t) J_n(t) e^{-2\zeta' t} t^p dt \tag{39}$$

where J_k denotes a Bessel function of the first kind and order k.

Then, the force per unit length of the dislocation loop is given by

$$f_z = \frac{2G_1 b_z^2}{(1+\beta)(\kappa_1+1)R} \left\{ \frac{(1+\alpha)\beta}{1-\beta} J*(1,1;1) + 2(\alpha-\beta)\zeta'^2 J*(1,1;3) \right\} \tag{40}$$

Using this formula, we investigate the force distribution in a variety of material combinations. We solve the same problems using the finite element code and the thermal analogue and calculate the force per unit length as described in previous sections. The results are shown in Fig. 10. The analytical results are presented on the left side and the FEM results on the right. A force with a positive sign means attraction of the loop to the interface (negative sign implies repulsion of the loop from the interface). For certain material combinations, there is either attraction or repulsion depending on the size of the loop or the distance from the interface. To the best of our knowledge, it is the first time that eq. (40) has been checked, independently.

3.3.3 The nano-indentation problem

In the nano-indentation problem, it is often the case that a metallic substrate is probed by a diamond punch. Dislocation loops are often created near the surface (Fig. 11). The stress field created by the punch forces to the substrate influences the dislocation kinematic inside the substrate. Regardless of applied load, the punch-substrate interface creates self-stresses that can repel or attract dislocations to the interface. Fig. 12a indicates that a diamond punch would lead to the repulsion of dislocations from the surface for most cases. On the other hand, a steel punch could lead to attraction of dislocations in some cases, as shown in Fig. 12b. The present methodology can be very useful in cases when several dislocations can be trapped in stable or unstable locations.

4 Conclusions

We have used a thermal analogue to describe an edge-type circular Volterra dislocation loop by ordinary axisymmetric finite elements. We were able to reproduce all available analytic solutions regarding displacement and self-stress field, as well as the Peach-Koehler configuration forces acting on loop dislocations. Moreover, we were able to extend the existing solution for anisotropic crystals. Our approach can be readily implemented in any finite element code as a thermoelasticity problem.

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Appendix A Elastic constants

The elastic constants of the materials used throughout the text are listed in Table 1 (Hirth and Lothe, 1982).

Table 1: Elastic constants of the materials used in this work.

Crystal	c_{11} (10^{10}Pa)	c_{12} (10^{10}Pa)	c_{44} (10^{10}Pa)	H (10^{10}Pa)	A	G (10^{10}Pa)	ν
Al	10.82	6.13	2.85	1.01	1.22	2.65	0.347
Ag	12.40	9.34	4.61	6.16	3.01	3.38	0.354
Au	18.60	15.70	4.20	5.50	2.90	3.10	0.412
Cr	35.00	5.78	10.10	-9.02	0.69	11.90	0.130
Cu	16.84	12.14	7.54	10.38	3.21	5.46	0.324
Fe	24.20	14.65	11.20	12.85	2.35	8.63	0.291
Ge	12.89	4.83	6.71	5.36	1.67	5.64	0.200
K	0.457	0.374	0.263	0.443	6.34	0.17	0.312
Mo	46.00	17.60	11.00	-6.40	0.77	12.28	0.305
Na	0.603	0.459	0.586	1.028	8.14	0.38	0.201
Nb	24.60	13.40	2.87	-5.46	0.51	3.96	0.392
Ni	24.65	14.73	12.47	15.02	2.51	9.47	0.276
Pb	4.66	3.92	1.44	2.14	3.89	1.01	0.387
Ta	26.70	16.10	8.25	5.90	1.56	7.07	0.339
Th	7.53	4.89	4.78	6.92	3.62	3.40	0.254
Si	16.57	6.39	7.96	5.74	1.56	6.81	0.218
V	22.80	11.90	4.26	-2.38	0.78	4.74	0.352
W	52.10	20.10	16.00	0.00	1.00	16.00	0.278
Diamond	107.60	12.50	57.60	20.10	1.21	53.58	0.068