Lectures on:

Introduction to and fundamentals of discrete dislocations and dislocation dynamics. Theoretical concepts and computational methods

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Lecture 2: The Theory of Curved Dislocations

The Burgers Displacement Equation
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Volterra Dislocations
• Circular Dislocation Loop
• Rectangular Dislocation Loop
• The stress filed about a straight segment dislocation

The Somigliana Ring Dislocation

References
• Khraishi, T. and Zbib, H.M., The Displacement Field of a Rectangular Volterra Dislocation Loop, Phil Mag,82, 265-277, 2002.
Mixed Dislocation

FIGURE 1-23. (a) Shear of a perfect crystal to form a mixed dislocation. (b) Projection normal to the glide plane in (a). (c) Resolution of (b) into components at point B.
The self-stress

The Peach-Koehler equation for the self-stresses of any curved, closed dislocation loop, is given by the following line integral (see Hirth and Lothe 1982):

\[ \sigma_{\alpha \beta} = -\frac{G}{8\pi} \oint_{C} b_{m} \in_{im\alpha} \frac{\partial}{\partial x'_{i}} \nabla'^{2} R \, dx'_{\beta} - \frac{G}{8\pi} \oint_{C} b_{m} \in_{im\beta} \frac{\partial}{\partial x'_{i}} \nabla'^{2} R \, dx'_{\alpha} \]

\[ -\frac{G}{4\pi(1-\nu)} \oint_{C} b_{m} \in_{imk} \left( \frac{\partial^{3} R}{\partial x'_{i} \partial x'_{\alpha} \partial x'_{\beta}} - \delta_{\alpha \beta} \frac{\partial}{\partial x'_{i}} \nabla'^{2} R \right) \, dx'_{k} \]
The Burgers equation for displacements, for any closed curved dislocation loop, is given in terms of line and area integrals as (see Hirth and Lothe [21]):

\[
u_m(\mathbf{r}) = \frac{-1}{8\pi} \int_A b_m \frac{\partial}{\partial x'_j} \nabla'^2 R dA_j - \frac{1}{8\pi} \oint_C b_i \in_{mik} \nabla'^2 R dx'_k - \frac{1}{8\pi(1-\nu)} \oint_C b_i \in_{ijk} \frac{\partial^2 R}{\partial x'_m \partial x'_j} dx'_k\]
Alternatively, Burgers equation has the following vector form:

\[
\mathbf{u}(\mathbf{r}) = -\frac{\mathbf{b}}{4\pi} \Omega - \frac{1}{4\pi} \oint_{C} \mathbf{b} \times d\mathbf{l}' + \frac{1}{8\pi(1-\nu)} \operatorname{grad} \oint_{C} (\mathbf{b} \times \mathbf{R}) \cdot d\mathbf{l}'
\]

\(\Omega\) is the solid angle through which the positive side of \(A\) is seen from \(r\), and is defined as

\[
\Omega = -\int_{A} \frac{\mathbf{R} \cdot d\mathbf{A}}{R^3}
\]

The displacement field is important in interaction problems between dislocations and embedded particles in a softer metallic matrix, e.g. in metal-matrix composites (MMCs), the boundary condition in the problem is that of zero displacement at a set of collocation points on the interface. The condition is enforced by annulling the undesired displacements caused by the crystal or matrix dislocations with the displacements coming from the distribution of rectangular dislocation loops. In order for this to happen, a quantification of the displacement field of each of the rectangular dislocation loops is necessary and is therefore developed in this paper.

The integration of the Burgers equation to obtain the displacements turns out to be rather involved. It is carried out with respect to the global \(xyz\) system. To perform the integration, the indices in (1) are first expanded. This gives three independent equations, one for each displacement component \((u, v, \text{ and } w)\), corresponding to subscript or index \(m\) values of 1, 2 and 3, respectively. Note that \(u\) is the displacement in the \(x\)-direction, \(v\) in the \(y\)-directions and \(w\) in the \(z\)-direction.

Before continuing along with the integration, few steps are in order. First, note that the elevation of the dislocation loop is fixed with respect to the global coordinate system \(xyz\). This means that the dislocation loop lies in a plane parallel to the \(xy\) planes such that \(z'\) is a constant. Second, note that the following holds: \(\nabla' \cdot \mathbf{R} = 2/R\). Third, along segment 1, \(x' = +a\) and \(dx' = 0\), along segment 3, \(x' = -a\) and \(dx' = 0\), along segment 2, \(y' = +b\) and \(dy' = 0\), and along segment 4, \(y' = -b\) and \(dy' = 0\).
A rectangular dislocation loop is composed of four linear dislocation segments (see figure 1). For this work, the Burgers vector $b$ is assumed to be constant, in magnitude and direction, from one point to another along the loop.

The displacement field of a rectangular dislocation loop

\[
\begin{bmatrix}
  u \\
  v \\
  w
\end{bmatrix}
= \begin{bmatrix}
  K_{11} & K_{12} & K_{13} \\
  K_{21} & K_{22} & K_{23} \\
  K_{31} & K_{32} & K_{33}
\end{bmatrix}
\begin{bmatrix}
  b_x \\
  b_y \\
  b_z
\end{bmatrix}
\]

\[K_{11} = -\frac{\Omega(x, y, z)}{4\pi}\]

\[-\frac{(z-z')}{8\pi(1-\nu)} \begin{bmatrix}
  (a-x)\left(\frac{b-y}{\sqrt{(a-x)^2+(b-y)^2+(z'-z)^2}} + \frac{b+y}{\sqrt{(a-x)^2+(b+y)^2+(z'-z)^2}}\right) \\
  (a+x)\left(\frac{b-y}{\sqrt{(a+x)^2+(b-y)^2+(z'-z)^2}} + \frac{b+y}{\sqrt{(a+x)^2+(b+y)^2+(z'-z)^2}}\right)
\end{bmatrix}\]

\[K_{12} = \]

\[-\frac{(z-z')}{8\pi(1-\nu)} \begin{bmatrix}
  1 \frac{1}{\sqrt{(a-x)^2+(b+y)^2+(z'-z)^2}} + \frac{1}{\sqrt{(a+x)^2+(b+y)^2+(z'-z)^2}} \\
  1 \frac{1}{\sqrt{(a-x)^2+(b-y)^2+(z'-z)^2}} - \frac{1}{\sqrt{(a+x)^2+(b-y)^2+(z'-z)^2}}
\end{bmatrix}\]
Figure 3. Three-dimensional carpet plot of $u(x,y,z)$ normalized by the Burgers vector magnitude $|\mathbf{b}|$, where $\mathbf{b}=(bx=0, by=0, bz\neq 0)$. Here, $v=1/3$, $a=b=100bz$, $z'=0$, and $z=20bz$. 
Circular Dislocation loop

\[ r \]

\[ \rho \]

\[ z, z' \]

\[ \theta \]

\[ \phi \]

\[ x \]

\[ y \]

\[ z \]

\[ x' \]

\[ y' \]

\[ z' \]

\[ O \]

\[ C \]

\[ dA \]

\[ R \]

\[ b_z, b_{z'} \]

\[ b_{x'}, b_{y'} \]
Prismatic Dislocation Loops

• Prismatic dislocation loops with a Burgers vector normal to the plane of the loop can form in a material subject to irradiation or quenching by the precipitation of vacancies or interstitial atoms.

![Prismatic dislocation loop diagram](image)

• Glide or shear loops can form readily, e.g., in the glide plane of a Frank-Read source as it continues to emit propagating dislocations. Hence, it is important to quantify the stress field of these loops in order to account for their interaction with other dislocation curves or defects in the crystal.

![Glide or shear loop diagram](image)
The stress field of a circular Volterra dislocation loop

\[
\sigma_{xx} = \frac{x^2}{\rho} \sigma_{x'x'} - \frac{2xy}{\rho^2} \sigma_{x'y'} + \frac{y^2}{\rho^2} \sigma_{y'y'}
\]

\[
\sigma_{yy} = \frac{y^2}{\rho} \sigma_{x'x'} + \frac{2xy}{\rho^2} \sigma_{x'y'} + \frac{x^2}{\rho^2} \sigma_{y'y'}
\]

\[
\sigma_{zz} = \sigma_{z'z'}
\]

\[
\sigma_{xy} = \frac{xy}{\rho^2} \left( \sigma_{x'x'} - \sigma_{y'y'} \right) + \frac{x^2 - y^2}{\rho^2} \sigma_{x'y'}
\]

\[
\sigma_{xz} = \frac{x}{\rho} \sigma_{x'z'} - \frac{y}{\rho} \sigma_{y'z'}
\]

\[
\sigma_{yz} = \frac{y}{\rho} \sigma_{x'z'} + \frac{x}{\rho} \sigma_{y'z'}
\]
\[
\sigma_{x'x'} = -\frac{Gb_{z'}}{\pi} (C_1 E(k) + C_2 K(k)) - \frac{Gb_{x'}}{2\pi (1-\nu)} (C_3 E(k) + C_4 K(k)) - \frac{Gb_{z'}}{2\pi (1-\nu)} (C_5 E(k) + C_6 K(k)) \\
\sigma_{y'y'} = -\frac{Gb_{x'}}{\pi} (C_7 E(k) + C_8 K(k)) - \frac{Gb_{z'}}{\pi} (C_9 E(k) + C_{10} K(k)) \\
- \frac{Gb_{x'}}{2\pi (1-\nu)} (C_{11} E(k) + C_{12} K(k)) - \frac{Gb_{z'}}{2\pi (1-\nu)} (C_{13} E(k) + C_{14} K(k)) \\
\sigma_{z'z'} = -\frac{Gb_{x'}}{2\pi (1-\nu)} (C_{15} E(k) + C_{16} K(k)) - \frac{Gb_{z'}}{2\pi (1-\nu)} (C_{17} E(k) + C_{18} K(k)) \\
\sigma_{y'z'} = -\frac{Gb_{y'}}{2\pi} (C_{19} E(k) + C_{20} K(k)) - \frac{Gb_{y'}}{2\pi (1-\nu)} (C_{21} E(k) + C_{22} K(k)) \\
\sigma_{x'z'} = -\frac{Gb_{x'}}{2\pi} (C_{23} E(k) + C_{24} K(k)) - \frac{Gb_{x'}}{4\pi (1-\nu)} (C_{25} E(k) + C_{26} K(k)) - \frac{Gb_{z'}}{2\pi (1-\nu)} (C_{27} E(k) + C_{28} K(k)) \\
\sigma_{x'y'} = -\frac{Gb_{y'}}{2\pi} (C_{29} E(k) + C_{30} K(k)) - \frac{Gb_{y'}}{2\pi (1-\nu)} (C_{31} E(k) + C_{32} K(k))
\]
The stress field of a circular loop, and straight segments approximations:

\[
\frac{\sigma_{yy}}{(Gb/z/2\pi)(1-\nu)}
\]

\(\sigma_{zz}/(Gbz/2\pi(1-\nu))\) for varying N:
- N=6
- N=12
- N=18
- N=24

szz, analy.

\(1/r^3\)
Interaction between a defect (Frank sessile loop; defect clusters in irradiated materials) and a glide edge dislocation

Interaction is weak

\[ 1/r^3 \]

Fig. 5. (a) A TEM picture showing dislocation pinning by the dispersed hardening mechanism. (b) A DD picture showing the same mechanism at work as captured in the simulations. The dots in the figure represent defect clusters.
Somigliana Dislocation

Many internal defect, such as broken fiber, debonding etc., can be modeled as a set of discontinuities in the continuum resulting in perturbations (of small or large magnitudes) in an otherwise simple elastic field. The Somigliana dislocation can be considered as one of the most general kinds of such discontinuities and, thus, can be used to model many imperfections.

Burgers vector is NOT conserved along the dislocation line
The Somigliana Ring Dislocation

used to model cylindrical cracks
\[
\begin{bmatrix}
\sigma_r \\
\sigma_\theta \\
\sigma_z \\
\sigma_rz
\end{bmatrix}
= 
\frac{Gb_1}{2\pi(1-\nu)}
\begin{bmatrix}
A_{1,11} & A_{1,12} & A_{1,13} \\
A_{1,21} & A_{1,22} & A_{1,23} \\
A_{1,31} & A_{1,32} & A_{1,33} \\
A_{1,41} & A_{1,42} & A_{1,43}
\end{bmatrix}
\begin{bmatrix}
K(k) \\
E(k) \\
\Pi(k)
\end{bmatrix}
+ 
\frac{Gb_2}{2\pi(1-\nu)}
\begin{bmatrix}
A_{2,11} & A_{2,12} & A_{2,13} \\
A_{2,21} & A_{2,22} & A_{2,23} \\
A_{2,31} & A_{2,32} & A_{2,33} \\
A_{2,41} & A_{2,42} & A_{2,43}
\end{bmatrix}
\begin{bmatrix}
-1 \\
1 \\
0 \\
0
\end{bmatrix}
\begin{bmatrix}
1 \\
1 \\
2\nu \\
0
\end{bmatrix}
\quad \text{for } r < R
+ 
\frac{Gb_1 R}{2(1-\nu)r^2}
\begin{bmatrix}
1 \\
1 \\
0 \\
0
\end{bmatrix}
\quad \text{for } r > R
\]

\[
A_{1,11} = \frac{2b}{r^2 R g^3 p} \left\{ p g \left[ b^2 - \nu (b^2 + r^2 + R^2) \right] - r^2 R^2 b^2 \right\},
\]

\[
A_{1,12} = \frac{-b}{r^2 R p g} \left[ 3b^2 (r^2 + R^2) + (r^2 - R^2)^2 + 2b^4 - 2\nu pg^2 \right] - \frac{2b R}{p^2 g^3} \left[ 4b^2 (r^2 + R^2) + 4(r^2 - R^2)^2 - pg^2 \right].
\]

\[
A_{1,21} = \frac{-b}{g r^2 R} \left[ 2b^2 + 3r^2 - 2\nu (b^2 + R^2 + r^2) \right],
\]

Etc…


A curved dislocation can be approximated as a set of straight dislocation segments.

\[ \sigma(p) = \sum_{j=1}^{N} \sigma_{j,j+1}^p \]
Nodes and collocation points on dislocation loops and curves

\[
\sigma_{\alpha\beta}(\mathbf{p}) = -\frac{G}{8\pi c} \sum_{i=1}^{n} \frac{b_m}{c} \epsilon_{i\alpha\beta} \frac{\partial}{\partial x'_i} \nabla' \cdot \mathbf{R} \; dx'_\beta - \frac{G}{8\pi c} \sum_{i=1}^{n} \frac{b_m}{c} \epsilon_{i\alpha\beta} \frac{\partial}{\partial x'_i} \nabla' \cdot \mathbf{R} \; dx'_\beta \\
- \frac{G}{4\pi(1-v)} \sum_{i=1}^{n} \frac{b_m}{c} \epsilon_{i\alpha\beta} \left( \frac{\partial^3 R}{\partial x'_i \partial x'_\alpha \partial x'_\beta} - \delta_{\alpha\beta} \frac{\partial}{\partial x'_i} \nabla' \cdot \mathbf{R} \right) \; dx'_k
\]
The stress field of a dislocation segment

\[ \sigma(P)_{ij} = \sigma_{ij}(B) - \sigma_{ij}(A) \]

\[
\begin{align*}
\sigma_{xx} &= -b_x \frac{y \lambda}{\rho^2 R} \left(1 + \frac{x^2}{R^2} - \frac{2x^2}{\rho^2} \right) - b_y \frac{x \lambda}{\rho^2 R} \left(1 - \frac{x^2}{R^2} + \frac{2x^2}{\rho^2} \right) \\
\sigma_{yy} &= b_x \frac{y \lambda}{\rho^2 R} \left(1 - \frac{y^2}{R^2} - \frac{2y^2}{\rho^2} \right) + b_y \frac{x \lambda}{\rho^2 R} \left(1 + \frac{y^2}{R^2} + \frac{2y^2}{\rho^2} \right) \\
\sigma_{zz} &= b_x \left(- \frac{2\nu y}{R \rho^2} + \frac{y \lambda}{R \rho^3} \right) + b_y \left(- \frac{2\nu x}{R \rho^2} - \frac{x \lambda}{R \rho^3} \right) \\
\sigma_{xy} &= b_x \frac{x \lambda}{\rho^2 R} \left(1 - \frac{x^2}{R^2} - \frac{2x^2}{\rho^2} \right) - b_y \frac{y \lambda}{\rho^2 R} \left(1 - \frac{x^2}{R^2} + \frac{2x^2}{\rho^2} \right) \\
\sigma_{xz} &= -b_x \frac{x \lambda}{R^3} + b_y \left(- \frac{\nu}{R} + \frac{x^2}{R^3} \right) + b_z \frac{y \lambda (1 - \nu)}{R(R + \lambda)} \\
\sigma_{yz} &= b_x \left(\frac{\nu}{R} - \frac{y^2}{R^3} \right) + b_y \frac{x \lambda}{R^3} - b_z \frac{x \lambda (1 - \nu)}{R(R + \lambda)} \\
\rho^2 &= x^2 + y^2, \quad R^2 = \rho^2 + z^2, \quad \lambda = z' - z
\end{align*}
\]

Other forms are given in Hirth and Lothe (1982, p. 134)
This form is most convenient to use
Discrete Circular Volterra Dislocation Loop
Observed in quenched metals and metals and alloys of low stacking-fault energy. It consists of a tetrahedron of intrinsic stacking faults on \{111\} planes with \(1/6\langle110\rangle\) type stair-rod dislocations along the edges of the tetrahedron. A dislocation loop (of Frank partial dislocation formed by the collapse of vacancies), may dissociate into a low-energy stair-rod dislocation and a Shockly partial on an intersecting slip plane, leading to the formation of a SFT.
Comparison between the Stress Fields of Unit Defects

To contrast the differing stress fields of a FS loop and a SFT, we calculate the Peach-Koehler force that both exert at a point on a straight edge dislocation situated an x-distance from the loop plane (or correspondingly, from the tetrahedron's base plane). An edge view of the loop and its possible SFT offspring (shown in dashed line) is exhibited in this figure along with a nearby edge dislocation. In this figure, the glide force (in the direction of the dislocation's Burgers vector) is plotted versus the y-coordinate of the dislocation at a given x. Note that in the force exerted by the SFT is smaller than that caused by the FS loop. An exception to this is the case when x=9b where the edge dislocation almost cuts the tip of the tetrahedron in question. In such a case, the SFT force is stronger than the loop's. Moreover, if the dislocation line collides with a SFT (a more probable event than a loop collision, considering volume differences), then their inelastic interaction is also expected to be strong. In this figure, the edge length of the triangular FS loop, or correspondingly the SFT, is equal to 10b, which is a typical defect dimension as measured experimentally. Now, if one fixes the y value and varies the x-coordinate instead, it would still be observed that overall, and as long as elastic interactions are concerned, the FS loop causes a stronger glide force on the dislocation. The results demonstrate a higher stress field associated with the FS loop, which should be in-line with physical reasoning. Since the SFT forms from a FS loop (i.e. it's a preferred lower energy state), it is then expected that a more relaxed strain-field accompany such geometry over that of a loop.
Dislocation multiplication
Frank-Read sources