Theoretical Model

1. Yoffe-Shaibani-Hazzeldine Model for an Inclined Threading dislocation

In the original derivation by Yoffe (1961) [1], two auxiliary coordinate systems are utilized by rotating the right-handed standard Cartesian coordinates around the x axis: x, η, ζ and x, $\eta^{'}$, $\zeta^{'}$. The dislocation terminating at the origin $(0, 0, 0)$ is in the $-z$ half space with an inclination angle of α to the $-z$ axis. Yoffe's original analytical solution for a threading dislocation was later revisited by Shaibani and Hazzeldine (1981) who introduced a number of simplifications in addition to several typographical corrections [2]. The relationships between the different coordinate systems are expressed as:

$$\eta = y \cos\alpha - z \sin\alpha, \tag{1a}$$

$$\zeta = z \cos\alpha + y \sin\alpha, \tag{1b}$$

$$\eta^{'} = -y \cos\alpha - z \sin\alpha, \tag{1c}$$

$$\zeta^{'} = -z \cos\alpha + y \sin\alpha, \tag{1d}$$

$$R^2 = x^2 + y^2 + z^2 = x^2 + \eta^2 + \zeta^2 = x^2 + \eta^{'2} + \zeta^{'2}. \tag{1e}$$

For a Burgers vector $\mathbf{b} = b_x\mathbf{e_x} + b_y\mathbf{e_y} + b_z\mathbf{e_z}$, the YSH model aligns a screw dislocation's Burgers vector along the $-\zeta^{'}$ axis and an edge dislocation's Burgers vector along the $-\eta^{'}$ axis:

$$b_e = b_y \cos\alpha + b_z \sin\alpha, \tag{2a}$$

$$b_s = b_z \cos\alpha - b_y \sin\alpha, \tag{2b}$$

with a special case when the Burgers vector of the edge dislocation is perpendicular to the y-z plane, i.e., along the x direction (b_x). In the case of a mixed dislocation, the Burgers vector $\mathbf{b}$ can be resolved into edge (b_e) and screw (b_s) components using equations 2. The total displacement field of a mixed dislocation also follows the superposition principle.

To reduce the complexity of the analytical forms, a few auxiliary parameters are introduced:

$$\omega = \arctan\frac{y}{x} - \arctan\frac{\eta}{x} + \arctan\frac{xR\sin\alpha}{y\eta + x^2\cos\alpha}, \tag{3a}$$

$$\omega^{'} = \arctan\frac{y}{x} - \arctan\frac{\eta^{'}}{x} + \arctan\frac{xR\sin\alpha}{y\eta^{'} - x^2\cos\alpha}, \tag{3b}$$

and

$$A = (R - z); B = (R - \zeta); B^{'} = (R - \zeta^{'}) \tag{4}$$

Below, the displacement fields of different dislocation types are listed without derivation.

1.1. Dislocation in the y-z plane: screw component b_s

The displacement field $\mathbf{u} = [u_x, u_y, u_z]$ of the screw component of an inclined dislocation with magnitude of Burgers vector b_s in the y-z plane at any point (x, y, z) is shown below. These equations also apply to the case of a pure screw dislocation when the Burgers vector is along the dislocation line, i.e., along the $-\zeta^{'}$ direction.

$$\begin{aligned} u_x = \{&xm_s + \frac{2\eta\cos^2\alpha}{B} + 2(1-2\nu)\cot\alpha[-1 + \cos\alpha + \cos\alpha\log A \\ &- \frac{y\sin\alpha}{A} - \log B] - \sin 2\alpha\}/(2SG), \end{aligned} \tag{5}$$

$$\begin{aligned} u_y = \{&ym_s - \frac{2x\cos\alpha}{B} - \sin\alpha(\omega^{'} - \omega) + 2(1-2\nu)\cot\alpha[x\sin\alpha/A \\ &- \omega\cos\alpha]\}/(2SG), \end{aligned} \tag{6}$$

$$u_z = \{zm_s + \cos\alpha(\omega^{'} - \omega) - 2(1-2\nu)\omega\cos\alpha\}/(2SG), \tag{7}$$

where

$$m_s = \frac{x\sin 2\alpha}{RB}; S = (\frac{Gb_s}{2\pi})^{-1} \tag{8}$$

and G is the shear modulus and ν the Poisson ratio.

1.2. Dislocation in the y-z plane: edge component b_e

The displacement field $\mathbf{u} = [u_x, u_y, u_z]$ of the edge component of an inclined dislocation with magnitude of Burgers vector b_e in the y-z plane at any point (x, y, z) is given by:

$$\begin{aligned} u_x = \{ & xm_e + \lambda + 2\frac{\cos\alpha}{B}(z + 2(1-\nu)\eta\sin\alpha) - 4(1-\nu)\sin^2\alpha \\ & + k[1 - \cos\alpha - \cos\alpha\log A + \frac{y\sin\alpha}{A} + \log B]\}/(2D_eG), \end{aligned} \tag{9}$$

$$u_y = \{ym_e + q_e\sin\alpha + \theta\cos\alpha + k[-\frac{x\sin\alpha}{A} + \omega\cos\alpha]\}/(2D_eG), \tag{10}$$

$$\begin{aligned} u_z = [& zm_e + q_e\cos\alpha + \theta\sin\alpha - 2x\cos a(\frac{1}{B'} + \frac{1-2\nu}{B}) \\ & + k\omega\sin\alpha]/(2D_eG), \end{aligned} \tag{11}$$

where:

$$q_e = x[\frac{1}{B'} - \frac{1}{B} + \frac{2z\cos\alpha}{B^2}], \tag{12a}$$

$$m_e = -\frac{q_e}{R} - \frac{4(1-\nu)x\cos^2\alpha}{RB}, \tag{12b}$$

$$D_e = [\frac{Gb_e}{4\pi(1-\nu)}]^{-1}, \tag{12c}$$

$$\lambda = (1-2v)\log(\frac{B'}{B}), \tag{12d}$$

$$\theta = 2(1-\nu)(\omega' - \omega), \tag{12e}$$

$$k = 4(1-\nu)(1-2\nu)\cot^2\alpha, \tag{12f}$$

1.3. Pure Edge dislocation in the x-z plane: $|\mathbf{b}| = b_x$

In this case, the Burgers vector of the edge dislocation is perpendicular to the y-z plane for all angles α, i.e., a pure edge dislocation.

$$u_x = \{xm_x + \theta + k[\frac{x \tan\alpha}{A} - \omega]\}/(2D_xG), \tag{13}$$

$$\begin{aligned} u_y = \{ &ym_x + q_x \sin\alpha - \lambda\cos\alpha - \frac{2\cos\alpha}{B}[z\cos\alpha + (1-2\nu)y\sin\alpha] \\ &+ k[-1 + \cos\alpha - \log A + \frac{y\tan\alpha}{A} + \cos\alpha\log B]\}/(2D_xG), \end{aligned} \tag{14}$$

$$\begin{aligned} u_z = \{ &zm_x + q_x\cos a - \lambda\sin\alpha - \frac{2\eta^{'}\cos\alpha}{B^{'}} + \frac{4\cos\alpha}{B}[(1-\nu)y\cos\alpha \\ &- (1-2\nu)z\sin\alpha] + k\tan\alpha(\cos\alpha - \log A + \cos\alpha\log B) \\ &+ 4(1-\nu)\cos\alpha\cot\alpha\}/(2D_xG) \end{aligned} \tag{15}$$

where:

$$q_x = \frac{\eta^{'}}{B^{'}} - \frac{\eta}{B} - \frac{2z\eta\cos\alpha}{B^2}, \tag{16a}$$

$$m_x = -\frac{q_x}{R} + \frac{2(1-2\nu)y\cos\alpha}{RB}, \tag{16b}$$

$$D_x = (\frac{Gb_x}{4\pi(1-\nu)})^{-1}, \tag{16c}$$

$$\lambda = (1-2v)\log(\frac{B^{'}}{B}), \tag{16d}$$

$$\theta = 2(1-\nu)(\omega^{'} - \omega), \tag{16e}$$

$$k = 4(1-\nu)(1-2\nu)\cot^2\alpha, \tag{16f}$$

References

[1] E. H. Yoffe, A dislocation at a free surface, Philosophical Magazine 6 (1961) 1147–1155.

[2] S. J. Shaibani, P. M. Hazzledine, The displacement and stress fields of a general dislocation close to a free surface of an isotropic solid, Philosophical Magazine A 44 (1981) 657–665.