Theory Behind the Stroh Class

The atomman.defect.Stroh class solves the anisotropic elasticity theory for a continuum defect that is infinitely long and periodic along the z-axis such that the stress, strain and displacements are invariant in that direction. The solution was first developed by Eshelby, et al. [1]. Shortly after, Stroh [2, 3] explored the solution in-depth and showed how the problem can be rewritten in an easier to solve form.

1. Theory

Starting with the fundamental equations of elasticity

Compatibility:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \tag{1.1}$$

Strain definition:

$$\varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) \tag{1.2}$$

Force equilibrium:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{1.3}$$

Combining these equations and using the symmetries of Cijkl reveals the partial differential equation (PDE)

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} = 0. \tag{1.4}$$

The infinite periodicity of the defect along the z-axis makes the stress, strain, and displacements invariant along the z direction. Accordingly, $\partial/\partial x_3 = 0$. With this, a solution for Eq. 1.4 is obtained

$$u_k = A_k f(\eta) \qquad \eta = x_1 + p x_2. \tag{1.5}$$

Substituting the solution back into 1.4 gives

$$\left[C_{i1k1} + \left(C_{i1k2} + C_{i2k1}\right)p + C_{i2k2}p^2\right]A_k \frac{\partial^2 f}{\partial \eta^2} = 0, \tag{1.6}$$

or more simply

$$\left[C_{i1k1} + \left(C_{i1k2} + C_{i2k1}\right)p + C_{i2k2}p^2\right]A_k = 0, \tag{1.7}$$

or

$$a_{ik}A_k = 0. \tag{1.8}$$

In order for A_k to be non-zero, the determinate of a_{ik} must be zero. The determinate expression is a sixth-order polynomial expression, giving it six complex roots, p_n with n = 1,2,3,4,5,6. Since the coefficients of the determinate polynomial are real, the roots p_n come in complex conjugate pairs.

With this knowledge, the expression for u_k can be written in one of two forms:

Eshelby: For $p_4 = p_1^* \quad p_5 = p_2^* \quad p_6 = p_3^*$, then

$$u_k = \mathrm{Re}\left[\sum_{n=1}^{3} A_k(n) f_n(\eta_n)\right] \qquad 1.9a$$

Stroh: For p_1, p_2, p_3 having positive imaginary terms and $p_{-1} = p_1^* \quad p_{-2} = p_2^* \quad p_{-3} = p_3^*$, then

$$u_k = \sum_{\alpha=1}^{3} A_{k\alpha} f_\alpha(\eta_\alpha) + \sum_{\alpha=1}^{3} A_{k,-\alpha} f_{-\alpha}(\eta_{-\alpha}) \qquad 1.9b$$

Stroh also defines a stress function vector, ϕ, such that

$$\sigma_{i1} = -\frac{\partial \phi_i}{\partial x_2} \qquad \sigma_{i2} = \frac{\partial \phi_i}{\partial x_1} \qquad 1.10$$

Now, we can find

$$\phi_i = \sum_{\alpha=1}^{3} L_{i\alpha} f_\alpha(\eta_\alpha) + \sum_{\alpha=1}^{3} L_{i,-\alpha} f_{-\alpha}(\eta_{-\alpha}) \qquad 1.11$$

where

$$L_{i\alpha} = (C_{i2k1} + p_\alpha C_{i2k2}) A_{k\alpha} = -(p_\alpha{}^{-1} C_{i1k1} + C_{i1k2}) A_{k\alpha}. \qquad 1.12$$

Additionally,

$$L_{1\alpha} + p_\alpha L_{2\alpha} = 0. \qquad 1.13$$

Going back to the displacement expression,

$$u_k = \sum_{\alpha=1}^{3} A_{k\alpha} f_\alpha(\eta_\alpha) + \sum_{\alpha=1}^{3} A_{k,-\alpha} f_{-\alpha}(\eta_{-\alpha}) \qquad 1.14$$

consider the functions f_α. The requirements for f_α are that it allow for u_k to be multivalued such that a complete circuit around the defect results in a $\Delta u_k = b_k$, while the stresses remain single valued and continuous except at the origin. The most general solution for this is

$$f(\eta) = -\frac{D}{2\pi i} \ln \eta + \sum_{n=-\infty}^{\infty} a_n \eta_n \qquad 1.15$$

The ln term gives f a change of ±D for every revolution (where the 'cut' is oriented in the +x direction), while the other terms give single valued displacements, which do not apply/matter for an infinitely straight periodic dislocation. So,

$$f_\alpha(\eta_\alpha) = -\frac{D(n)}{2\pi i} \ln \eta_\alpha \qquad 1.16$$

and

$$\sum_{\alpha=1}^{3} A_{k\alpha} D_\alpha - \sum_{\alpha=1}^{3} A_{k,-\alpha} D_{-\alpha} = b_k. \qquad 1.17$$

$$u_k = \frac{1}{2\pi i}\sum_{\alpha=1}^{3} A_{k\alpha} D_\alpha \ln(\eta_\alpha) - \frac{1}{2\pi i}\sum_{\alpha=1}^{3} A_{k,-\alpha} D_{-\alpha} \ln(\eta_{-\alpha}) \quad 1.18$$

The D_α terms are imaginary can be solved by considering the net force on the dislocation.

From Stroh, if the singularity is subsonic, then it can be shown that

$$D_\alpha = \left(L_{i\alpha} b_i + A_{i\alpha} F_i\right) / 2A_{j\alpha} L_{j\alpha} . \quad 1.19$$

Considering only a stationary dislocation, $F_i = 0$, so

$$D_\alpha = \left(L_{i\alpha} b_i\right) / 2A_{j\alpha} L_{j\alpha} \quad 1.20$$

Defining

$$k_\alpha = \frac{1}{2A_{j\alpha} L_{j\alpha}} \quad 1.21$$

$$u_k = \frac{1}{2\pi i}\sum_{\alpha=1}^{3} k_\alpha A_{k\alpha} (L_{k\alpha} b_k) \ln(\eta_\alpha) - \frac{1}{2\pi i}\sum_{\alpha=1}^{3} k_{-\alpha} A_{k,-\alpha} L_{k,-\alpha} b_k \ln(\eta_{-\alpha}) . \quad 1.22$$

With this, the displacements can be calculated by knowing p_α, $A_{k\alpha}$, and $L_{k\alpha}$.

2. Finding solutions

Obtaining values for p_α, $A_{k\alpha}$, and $L_{k\alpha}$ is not a simple task due to the sixth order complex roots. Stroh introduced an idea to create a 6x6 matrix such that the problem can be treated as an eigenvalue expression instead of as a polynomial. Various forms for the eigenvalue expression exist, and atomman.defect.Stroh uses the form listed in Hirth and Lothe [4].

Start by defining three orthogonal vectors $\boldsymbol{\xi} = \mathbf{m} \times \mathbf{n}$. In general, these three vectors can be any orientation, but our analysis need only consider $\mathbf{m} = \mathbf{e}_1$, $\mathbf{n} = \mathbf{e}_2$, and $\boldsymbol{\xi} = \mathbf{e}_3$. This definition also makes direct comparisons with the previous section possible.

Given two arbitrary vectors a_i and b_i, use the notation (ab) to indicate a matrix given by:

$$(ab)_{jk} = a_i C_{ijkl} b_l \qquad 2.1$$

Now, combining this with the previous analysis

$$\eta = m_i x_i + p n_j x_j \qquad 2.2$$

Equation 1.7 becomes

$$\left[(mm) + ((mn) + (nm))p + (nn)p^2\right] A_k = 0 \qquad 2.3$$

And equation 1.12 becomes

$$L_{i\alpha} = -((nm) + p_\alpha (nn)) A_{k\alpha} \qquad 2.4$$

From this, the problem is rewritten as a six dimensional eigenequation:

$$N_{rs}\zeta_r = p\zeta_s \qquad \text{for } r, s = 1,2,3,4,5,6 \qquad 2.5$$

Where N is a 6x6 matrix composed of joining three 3x3 component blocks, NA, NB, NC, and ND, and ζ is a six dimensional vector with components of A and L. Written out:

$$\begin{bmatrix} NA_{11} & NA_{12} & NA_{13} & NB_{11} & NB_{12} & NB_{13} \\ NA_{21} & NA_{22} & NA_{23} & NB_{21} & NB_{22} & NB_{23} \\ NA_{31} & NA_{32} & NA_{33} & NB_{31} & NB_{32} & NB_{33} \\ NC_{11} & NC_{12} & NC_{13} & ND_{11} & ND_{12} & ND_{13} \\ NC_{21} & NC_{22} & NC_{23} & ND_{21} & ND_{22} & ND_{23} \\ NC_{31} & NC_{32} & NC_{33} & ND_{31} & ND_{32} & ND_{33} \end{bmatrix} \bullet \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ L_1 \\ L_2 \\ L_3 \end{bmatrix} = p \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ L_1 \\ L_2 \\ L_3 \end{bmatrix} \qquad 2.6$$

The four component blocks that satisfy Eqs. 2.3 and 2.4 are:

$$NB_{ij} = -\left((nn)_{ij}\right)^{-1} \qquad 2.7a$$

$$NA_{ik} = NB_{ij}(nm)_{jk} \qquad 2.7b$$

$$NC_{ik} = (mn)_{ij} NA_{jk} + (mm)_{ik} \qquad 2.7c$$

$$ND_{ik} = (mn)_{ij} NB_{jk} \qquad 2.7d$$

The eigenvalues and eigenvectors of 2.6 directly give values for p_α, $A_{k\alpha}$, and $L_{k\alpha}$.

3. Derived properties

Stress:

$$\sigma_{ij} = \frac{1}{2\pi i}\sum_{\alpha=1}^{3} k_\alpha C_{ijkl}\left[m_l + p_\alpha n_l\right]A_{k\alpha}(L_{k\alpha}b_k)\frac{1}{\eta_\alpha} - \frac{1}{2\pi i}\sum_{\alpha=1}^{3} k_{-\alpha} C_{ijkl}\left[m_l + p_{-\alpha} n_l\right]A_{k-\alpha}(L_{k-\alpha}b_k)\frac{1}{\eta_{-\alpha}}$$

Energy coefficient tensor:

$$K_{ij} = i\sum_{\alpha=1}^{3} k_\alpha L_{i\alpha}L_{j\alpha} - i\sum_{\alpha=1}^{3} k_{-\alpha}L_{i-\alpha}L_{j-\alpha}$$

Energy coefficient:

$$K = \frac{b_i K_{ij} b_j}{b_i b_j}$$

The energy coefficient tensor depends only on the elastic constants and the orientation of the system. It can be used to separate out the edge and screw components of the energy coefficient tensor and see if terms are coupled. The energy coefficient is a scalar that depends on the character of a particular dislocation.

Note that in isotropic materials

- $K = \mu$ for screw dislocations
- $K = \dfrac{\mu}{1-\nu}$ for edge dislocations

Elastic energy per unit length in circular ring with inner and outer radii r_0 and R:

$$\frac{W}{L} = \alpha \ln\left(\frac{R}{r_0}\right),$$

where α is the pre-ln energy factor given by

$$\alpha = \frac{b_i K_{ij} b_j}{4\pi} = \frac{Kb^2}{4\pi}$$

4. Consistency checks

A number of consistency checks exist that be used to verify that the eigenvalues and vectors have been properly calculated:

$$\sum_{\alpha=\pm1}^{\pm3} k_\alpha A_{i\alpha} L_{j\alpha} = \sum_{\alpha=\pm1}^{\pm3} k_\alpha L_{i\alpha} A_{j\alpha} = \delta_{ij}$$

$$\sum_{\alpha=\pm1}^{\pm3} k_\alpha A_{i\alpha} A_{j\alpha} = \sum_{\alpha=\pm1}^{\pm3} k_\alpha L_{i\alpha} L_{j\alpha} = 0$$

$$k_\alpha^{1/2} k_\beta^{1/2} \left(A_{i\alpha} L_{i\beta} + A_{i\beta} L_{i\alpha} \right) = \begin{cases} 1 & \alpha = \beta \\ 0 & \alpha \neq \beta \end{cases}$$

$$\sum_{\alpha=\pm1}^{\pm3} p_\alpha k_\alpha A_{i\alpha} L_{j\alpha} = NA_{ij}$$

$$\sum_{\alpha=\pm1}^{\pm3} p_\alpha k_\alpha A_{i\alpha} A_{j\alpha} = NB_{ij}$$

$$\sum_{\alpha=\pm1}^{\pm3} p_\alpha k_\alpha L_{i\alpha} L_{j\alpha} = NC_{ij}$$

$$\sum_{\alpha=\pm1}^{\pm3} p_\alpha k_\alpha L_{i\alpha} A_{j\alpha} = ND_{ij}$$

5. References

[1] J.D. Eshelby, W.T. Read, W. Shockley, Acta Metall Mater, 1 (1953) 251-259.
[2] A.N. Stroh, Philosophical Magazine, 3 (1958) 625-&.
[3] A.N. Stroh, J Math Phys Camb, 41 (1962) 77-&.
[4] J.P. Hirth, J. Lothe, Theory of Dislocations, 2nd ed., Wiley, New York, 1982.