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:

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

Strain definition:

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

Force equilibrium:

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

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

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

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

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

Substituting the solution back into 1.4 gives

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

or more simply

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

or

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

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

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

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

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

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

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

Now, we can find

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

where

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

Additionally,

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

Going back to the displacement expression,

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

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

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

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,

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

and

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

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

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

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

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

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

Defining

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

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

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

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

And equation 1.12 becomes

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

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. Additional Useful Expressions

Stress:

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

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

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

Where E is the pre-ln energy factor

$$E = -\frac{b_i G_{ij} b_j}{4\pi i}$$

and G_{ij} is the energy coefficient tensor

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

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

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

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

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

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

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

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

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

[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.