**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:

 1.1

Strain definition:

 1.2

Force equilibrium:

 1.3

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

. 1.4

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

. 1.5

Substituting the solution back into 1.4 gives

, 1.6

or more simply

, 1.7

or

. 1.8

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

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

Eshelby: For, then

 1.9a

Stroh: For having positive imaginary terms and, then

 1.9b

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

 1.10

Now, we can find

 1.11

where

. 1.12

Additionally,

 1.13

Going back to the displacement expression,

 1.14

consider the functions *fα*. The requirements for *fα* are that it allow for *uk* to be multivalued such that a complete circuit around the defect results in a Δ*uk* = *bk*, while the stresses remain single valued and continuous except at the origin. The most general solution for this is

 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,

 1.16

and

. 1.17

 1.18

The *Dα* 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

. 1.19

Considering only a stationary dislocation, *Fi* = 0, so

 1.20

Defining

 1.21

. 1.22

With this, the displacements can be calculated by knowing *pα*, *Akα*, and *Lkα*.

1. **Finding solutions**

Obtaining values for *pα*, *Akα*, and *Lkα* 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 . In general, these three vectors can be any orientation, but our analysis need only consider , , and . This definition also makes direct comparisons with the previous section possible.

Given two arbitrary vectors  and , use the notation  to indicate a matrix given by:

 2.1

Now, combining this with the previous analysis

 2.2

Equation 1.7 becomes

 2.3

And equation 1.12 becomes

 2.4

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

 for *r*, *s* = 1,2,3,4,5,6 2.5

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

 2.6

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

 2.7a

 2.7b

 2.7c

 2.7d

The eigenvalues and eigenvectors of 2.6 directly give values for *pα*, *Akα*, and *Lkα*.

1. **Derived properties**

Stress:



Energy coefficient tensor:



Energy coefficient:



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

*  for screw dislocations
* for edge dislocations

Elastic energy per unit length in circular ring with inner and outer radii *r*0 and *R*:

,

where is the pre-ln energy factor given by



1. **Consistency checks**

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















1. **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.