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A pseudoinverse for Frank's formula

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In a previous communication, it has been argued that in the Frank–Bilby equation and in the o-lattice equations a pseudoinverse must be used when the reduced displacement-field matrices are not invertible. Here an explicit expression for the pseudoinverse of Frank's formula is derived using a direct vector approach.

1. Introduction

In the geometrical analysis of grain boundaries, the Frank–Bilby equation (see for instance Sutton & Balluffi, 1996) plays a particularly important role in the determination of dislocation content.

Let L^w and L^b be two lattices ('white' and 'black') and let $R(\theta, c)$ be the rotation through an angle θ and around the axis c ($|\mathbf{c}| = 1$) that takes lattice L^w into the lattice L^b. The net dislocation Burger's vector $\mathbf{b}$ traversed when moving from the origin to the point P is given by the Frank–Bilby equation (Sutton & Balluffi, 1996)

$$[I - R^{-1}(\theta, c)]\mathbf{p} = \mathbf{b}, \tag{1}$$

where $T = [I - R^{-1}(\theta, c)]$ is the reduced displacement field, in the terminology of Bollmann (1982). The previous equation assumes a very simple form when one takes as reference lattice the so-called median lattice (see, for instance, Sutton & Balluffi, 1996). The median lattice is the lattice L^m obtained from L^w by a rotation through $\theta/2$ around $\mathbf{c}$ or, alternatively, obtained from L^b by a rotation through $-\theta/2$ around $\mathbf{c}$. In terms of the median lattice, our equation becomes

$$[R(\theta/2, c) - R^{-1}(\theta/2, c)]\mathbf{p} = \mathbf{b}^m, \tag{2}$$

which can be re-cast in the so-called Frank formula (Sutton & Balluffi, 1996):

$$2\sin(\theta/2)(\mathbf{c} \times \mathbf{p}) = \mathbf{b}^m. \tag{3}$$

It can be readily seen that this equation cannot be inverted to yield $\mathbf{p}$ since $\det[I - R^{-1}(\theta, c)] = 0$, however, in a previous communication (Gómez & Romeu, 2000), it has been argued that in such cases one should use the Moore–Penrose pseudoinverse.

Given a matrix T, its (Moore–Penrose) pseudoinverse is the unique matrix T^* that satisfies the four conditions (Noble & Daniel, 1989)

$$\begin{aligned} T\,T^*T &= T \\ T^*T\,T^* &= T^* \\ (T\,T^*)^T &= (T\,T^*) \\ (T^*T)^T &= (T^*T) \end{aligned} \tag{4}$$

If we define

$$T = [R(\theta/2, c) - R^{-1}(\theta/2, c)], \tag{5}$$

then our contention is that the correct inverse formula should read

$$\mathbf{p} = T^*\mathbf{b}^m. \tag{6}$$

An explicit calculation of T^* using matrix methods has been presented by Romeu & Gómez (2001). The purpose of this short communication is to give a succinct vector derivation of T^* and, consequently, of the (pseudo-)inverse of Frank's equation.

2. A pseudoinverse for *T*

Consider the transformation T given by

$$T\mathbf{p} = \mathbf{d} \times \mathbf{p} \tag{7}$$

(where $\mathbf{d}$ is a given vector), then it is straightforward to check that

$$\begin{aligned} T\,T\,T\mathbf{p} &= \mathbf{d} \times [\mathbf{d} \times (\mathbf{d} \times \mathbf{p})] \\ &= \mathbf{d} \times [(\mathbf{d} \cdot \mathbf{p})\mathbf{d} - (\mathbf{d} \cdot \mathbf{d})\mathbf{p}] \\ &= -|\mathbf{d}|^2\mathbf{d} \times \mathbf{p} \\ &= -|\mathbf{d}|^2 T\mathbf{p}. \end{aligned} \tag{8}$$

This in turn means that the pseudoinverse of T is

$$T^* = -[1/|\mathbf{d}|^2]T \tag{9}$$

since it satisfies the pseudoinverse conditions (4) (the fact that $T^T = -T$ has been used).

In terms of cross products,

$$T^*\mathbf{p} = (-1/|\mathbf{d}|^2)(\mathbf{d} \times \mathbf{p}). \tag{10}$$

3. An inverse to Frank's formula

Putting things together,

$$\mathbf{p} = T^*\mathbf{b}^m = \{-1/[2\sin(\theta/2)]\}(\mathbf{c} \times \mathbf{b}^m). \tag{11}$$

This formula gives a (pseudo) inverse to Frank's formula.

4. Discussion

If the transformation T does not have an inverse then it can not be injective. This means that it is possible to have P and P' with $P \neq P'$ and such that $T(P) = T(P')$. Notice that $T(P - P') = 0$ so $P - P'$ lies in the kernel of T. For this reason, the P corresponding to a given $\mathbf{b}^m$ is not unique; if P_0 is given by $T^*\mathbf{b}^m$ then all other possible values for P are of the form $P_0 + k$, where k is any element in the kernel of T. This is well known in o-lattice theory (Bollmann, 1982) where the values of P form lines or planes (depending on the rank of T).

5. Conclusions

An alternative, vector derivation of the pseudoinverse to Frank's formula has been provided.

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