Self force on dislocation segments in anisotropic crystals

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Abstract. A dislocation segment in a crystal experiences a “self force,” by virtue of the orientation-dependence of its elastic energy. If the crystal is elastically isotropic, this force is manifested as a couple acting to rotate the segment toward the lower energy of the pure screw orientation (i.e. acting to align the dislocation line with its Burgers vector). If the crystal is anisotropic, there are additional contributions to the couple, arising from the more complex energy landscape of the lattice itself. These effects can strongly influence the dynamic evolution of dislocation networks, and via their governing role in dislocation multiplication phenomena, control plastic flow in metals. In this paper we develop a model for dislocation self forces in a general anisotropic medium, and briefly consider the technologically-important example of α-iron, which becomes increasingly anisotropic as the temperature approaches that of the α−γ phase transition at 912°C.
1. Introduction

In addition to interactions with other dislocations, external stresses, image forces and interactions with other parts of the same dislocation, a dislocation segment experiences a force due to the orientation-dependence of its elastic energy, which we call the self force. This force would still be present for a (hypothetical) isolated finite segment, and acts to rotate the segment toward the orientation of lowest energy in the lattice, since symmetry precludes any net linear self force.

In the next section we estimate the elastic contribution to the self force for a straight dislocation in a general anisotropic crystal. This is multiplied by a term depending on the various lengthscales involved, and in the following section we use the isotropic limit to match this to the existing non-singular theory of dislocations [1], using which a well-behaved self force can be calculated for isotropic crystals.

Next we use a simple model to estimate dislocation core effects, which are in principle beyond the scope of continuum elasticity due to the singularity appearing in the elastic fields at a dislocation core. Again we make use of the non-singular isotropic theory to ensure our model has a consistent isotropic limit.

Finally we apply the results derived to the case of α-Fe at high temperatures. Near to the α − γ phase transition occurring at 912°C, α-Fe becomes highly anisotropic, and the self forces depart significantly from their isotropic elasticity approximations. Snapshots of discrete dislocation dynamics (DDD) simulations which implement our prescription for the self force are shown, and they capture the sharp corners characteristic of extreme elastic anisotropy [2, 3, 4].

2. The self force couple

The elastic energy per unit length of a long straight dislocation in an elastic medium is given by [5]

\[
E = K(c_{ijkl}, b, t)F(R, \epsilon),
\]

where the first factor \(K\) depends only on the elastic constant tensor \(c_{ijkl}\) and the dislocation’s Burgers vector and line direction \((b, t)\) respectively, and the second factor \(F\) is independent of the elastic constants and dislocation orientation, depending only on some dislocation lengthscale \(R\) and an inner cutoff \(\epsilon\). This separation stems from the fact that the elastic Green’s tensor is a homogenous function of the source-field separation [5]. The self force arises from the angular variation of the quantity

\[
K = b \cdot B \cdot b = b_i B_{ij} b_j,
\]

where the matrix \(B\) is calculated from \(c_{ijkl}\) and \(t\) (Appendix A). Strictly, this only applies to an infinitely long dislocation, and we make the approximation that the factor \(K\) will still apply to a finite segment, whereas \(F\) will be different (including a possible weak dependence on the elastic moduli).
The work done during an infinitesimal rotation \( t \to t + \delta t \), or \( \phi \to \phi + \delta \phi \), \( \theta \to \theta + \delta \theta \) is

\[
\delta W = L \frac{\partial E}{\partial \phi} \delta \phi + L \frac{\partial E}{\partial \theta} \delta \theta \equiv -Q_\phi \delta \phi - Q_\theta \delta \theta,
\]

(3)

where the component \( Q_\phi \) acts about the \( z \) axis and \( Q_\theta \) acts about the direction \((-y, x, 0) \propto (-\sin \phi, \cos \phi, 0)\). The total couple can hence be represented by an equal and opposite vector force \( f \) acting at each endpoint:

\[
f = \frac{Q_\phi}{L} e_\phi + \frac{Q_\theta}{L} e_\theta
\]

\[
= -\mathcal{F} \left\{ b_i \frac{1}{s_\theta} \frac{\partial B_{ij}}{\partial \phi} b_j \right\} (-s_\phi, c_\phi, 0) + \left\{ b_i \frac{\partial B_{ij}}{\partial \theta} b_j \right\} (c_\theta c_\phi, c_\theta s_\phi, -s_\theta)
\]

(4)

where \( s_\phi = \sin \phi \) etc. The \( s_\theta^{-1} \) factor arises as we go from couples and rotations to forces and translations, and the factor of \( L \) has cancelled since \( E \) is defined as the energy per unit length. Once \( \mathcal{F} \) is determined, the self-force is completely specified in terms of the derivatives of the matrix \( B \), given in Eq.(A.1).

3. Isotropic elasticity and the non-singular theory

The elastic solutions for the displacement, strain and stress fields generated by a dislocation become singular at the dislocation’s core. This precludes one possible approach to the calculation of the self-force, i.e. evaluating the dislocation’s stress field along its own line and applying the Peach-Koehler formula for the force [6]. However, a non-singular continuum theory of dislocations was developed in Ref.[1], where precisely this procedure was carried out. The variational approach adopted here agrees exactly with that of [1] in the isotropic limit, provided the part of the self-force independent of the variation of the \( B \)-matrix is chosen appropriately, as we now demonstrate. The matrix \( B \) may be calculated analytically for an isotropic crystal, with the result

\[
B_{ij} = \frac{\mu}{4\pi} \left( \delta_{ij} + (M_i M_j + N_i N_j) \frac{\nu}{1 - \nu} \right),
\]

(5)

where \( M, N \) are any fixed pair of mutually orthogonal vectors lying in the plane orthogonal to \( t \), and \( \mu, \nu \) are the shear modulus and Poisson’s ratio respectively. Taking the dislocation to lie along the \( x \)-axis, \( t = (1, 0, 0) \) (with no loss of generality in the isotropic case), for \( b = (b_1, b_2, b_3) \) this gives

\[
b \cdot \frac{\partial B}{\partial \phi} \cdot b = -\frac{\mu \nu}{1 - \nu} \frac{b_1 b_2}{2\pi};
\]

\[
b \cdot \frac{\partial B}{\partial \theta} \cdot b = \frac{\mu \nu}{1 - \nu} \frac{b_1 b_3}{2\pi}.
\]

(6)

The following formula was derived in [1]:

\[
f_{\text{self}} = \frac{\mu}{4\pi} |b_b| \left( \frac{2\nu}{1 - \nu} \mathcal{F}_1(L, a) + \mathcal{F}_2(L, a) \right) b_e,
\]

(7)
where $b_s, b_e$ are the screw and edge components of the Burgers vector respectively. The coefficient of $F_1$ in the above is reproduced in Eqs.6,4. The term involving $F_2$ is due to the finiteness of the segment. The $F_s$ are given by [1]

$$2F_1 = \ln \left( \frac{L_a + L}{a} \right) - 2 \frac{L_a - a}{L} \ln \left( \frac{2L}{a} \right) - 2$$

$$F_2 = -\frac{(L_a - a)^2}{2LL_a} \rightarrow -\frac{1}{2}$$  

(8)

where $a$ is the core scale, and $L_a^2 = L^2 + a^2$ for segment length $L$. Also shown is the limiting behaviour as $a/L \rightarrow 0$. The choice of the parameter $a$ replaces the cutoff $\epsilon$, required in the conventional treatment in order to make the energy integrals convergent [5]. It remains in the final expression for the self force, and affects the calculated values. Arising from the long-range ($\sim 1/r$) nature of the dislocation strain field, it is an unavoidable consequence of using a continuum theory to model a fundamentally discrete object such as a dislocation. Fortunately the dependence is weak, and its effect relatively small. The functions $F_{1,2}$ can be used to estimate the form taken by the elastic-constant-independent part of the self-force in the anisotropic case (see later section).

4. Core estimates

A further contribution to the self-force arises from the dislocation core energy, which is beyond the scope of continuum elasticity theory. However, it is reasonable to assume that the core energy $E_c$ follows similar patterns to the elastic energies, for example in temperature-dependence. Refs. [7, 8] describe the elastic energies of certain dislocation configurations falling sharply towards zero with the elastic modulus $C''$; Ref. [8] also utilizes molecular dynamics calculations to verify this, which encompass the effect of the core, and this study supports the notion of the core energy emulating the behaviour of the elastic contribution.

The (isotropic) discrete dislocation dynamics (DDD) simulation program ParaDiS [9] is based on the non-singular theory of dislocations. The following core contributions to the self-force are implemented:

Core torsion $= E_c |b_s| \frac{2\nu}{1-\nu} b_e$

Core longitudinal $= -E_c \left( |b_s|^2 + \frac{|b_e|^2}{1-\nu} \right) t$.  

(9)

Both these expressions can be derived from the elastic energy expression $b \cdot B \cdot b$, by replacing $\mu/4\pi$ with $E_c$ (which is estimated from finer-grained modelling techniques). In this limit

$$b \cdot B \cdot b = \frac{\mu}{4\pi} \left( |b_s|^2 + \frac{|b_e|^2}{1-\nu} \right).$$

(10)

Since the longitudinal self-force is simply the core energy per unit length (the segment’s resistance to elongation, or line tension). Eq.9b follows immediately from this
prescription, with “force = – energy/length.” The core torsional contribution follows from angularly differentiating (10) before making the replacement. In the isotropic approximation, the torsional self-force can only operate in the plane defined by the Burgers vector and line direction.† If \( \alpha \) is the angle made by the Burgers vector with the line direction \( t \), then (c.f. Eq.7)

\[
\mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b} = \frac{\mu |\mathbf{b}|^2}{4\pi} \left( \cos^2 \alpha + \frac{\sin^2 \alpha}{1 - \nu} \right)
\]

\[
\frac{\partial}{\partial \alpha} (\mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b}) = \frac{\mu}{4\pi} \frac{2\nu}{1 - \nu} |\mathbf{b}_s||\mathbf{b}_e|,
\]

and we get Eq.9a. The question now remaining is how to generalize these prescriptions to the anisotropic case.

Various prescriptions exist for the averaging of the anisotropic elastic moduli over orientations, to obtain some “effective” isotropic values for, say, the shear modulus \( \bar{\mu} \) and Poisson’s ratio \( \bar{\nu} \) [10, 11, 12] (see Appendix B). However, it should be emphasized that none of these can capture the anisotropic orientation-dependence of the elastic energy, since in any isotropic approximation there are only two independent parameters, where as a homogenous anisotropic linear elastic medium requires at least three (for high-symmetry examples e.g. cubic crystals) and in principle many more.

5. Anisotropic implementation

In the absence of exhaustive finite-temperature electronic and atomistic studies of dislocation cores in the materials we wish to model, the best that can be offered is a model which captures the prescribed angular energy-dependence and is consistent with the existing benchmarked isotropic implementation.

In the isotropic case, a factor of \( \mu/4\pi \) is extracted and replaced by \( E_c \), or equivalently, the quantity \( \mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b} \) is multiplied by \( 4\pi E_c/\mu \). When the assumption of isotropy is relaxed, \( \mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b} \) can still be calculated exactly, via Eq.A.1, but the prefactor will presumably depend on orientation, \( 4\pi E_c(\theta, \phi)/f(e_{ijkl}, \theta, \phi) \). This is the logarithmic factor mentioned above, though now the cutoff lengthscale must presumably depend on direction. However, if we remain within the remit of our model, the core energy should follow the same angular dependence as the elastic energy, encoded by \( \mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b} \). This requires that the prefactor should not depend strongly on orientation (i.e the core energy and the appropriate function of the elastic moduli should scale in the same way, and the directionality cancels in their ratio). Thus we take an average core energy and divide it by an average shear modulus \( \bar{\mu}/4\pi \) (Appendix B) to get the appropriate prefactor with which to multiply \( \mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b} \). This function captures the orientation-dependence of the dislocation energy, and has the correct isotropic limit, so the core longitudinal self-force

† Already here the technique of matching core to elastic energies appears questionable. Using the full anisotropic elastic energy to match to is more palatable. It also includes the possibility of contributions to climb forces.
is implemented as
\[-\frac{4\pi E_c}{\mu} (\mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b}) t.\] (12)

As for the core torsion, writing the force as
\[\hat{e}_\alpha \frac{\partial}{\partial \alpha} (\mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b}),\] (13)

with \(\hat{e}_\alpha\) a unit vector in the direction transverse to the segment, is no longer adequate – it cannot account for torsions outside the plane defined by \(\mathbf{b}\) and \(t\). This generalization has been achieved for the elastic energy in the second section – the appropriate directional derivative is
\[\left[ \sum_i \hat{e}_i \frac{\partial}{\partial \alpha_i} \right] (\mathbf{b} \cdot \mathbf{B} \cdot \mathbf{b}),\] (14)

with the sum over the orthogonal angular coordinates. The variational procedure detailed earlier does exactly this, so we arrive at
\[-\frac{4\pi E_c}{\mu} \left[ (\mathbf{b} \cdot \frac{\partial \mathbf{B}}{\partial \phi} \cdot \mathbf{b}) \hat{e}_\phi + (\mathbf{b} \cdot \frac{\partial \mathbf{B}}{\partial \theta} \cdot \mathbf{b}) \hat{e}_\theta \right].\] (15)

Finally we have the elastic torsion. Rewriting the non-singular isotropic limit of this quantity as
\[\frac{\mu}{4\pi |\mathbf{b}| \mathbf{b} \cdot \frac{\nu}{1-\nu} \left( \mathcal{F}_1 + \frac{1-\nu}{\nu} \mathcal{F}_2 \right)},\] (16)

we can immediately read off the appropriate replacement for the first term as half the quantity in square brackets from Eq.15, multiplied by \(\mathcal{F}_1\) of Eq.8. The second term is less clear. Even in an isotropic material, there is a distinction between longitudinal and transverse displacements (hence the need for two independent elastic moduli in three dimensions), and this is manifested by the appearance or two terms, one of which is proportional to \(\mu\), and the other to \(\mu \nu / (1 - \nu)\). In anisotropic materials the clear distinction cannot be made.

\(\mathcal{F}_2\) is much smaller than \(\mathcal{F}_1\) \((L/a \gg 1)\). Rather than neglect it entirely however, we use an averaged Poisson ratio \(\bar{\nu}\) (see Appendix B). Thus the relative contribution of the terms \(\mathcal{F}_{1,2}\) is determined by an isotropically-averaged parameter, but the overall orientation-dependence is retained in the fully anisotropic prefactor. The final expression for the elastic contribution to the torsional self-force is hence
\[\left[ (\mathbf{b} \cdot \frac{\partial \mathbf{B}}{\partial \phi} \cdot \mathbf{b}) \hat{e}_\phi + (\mathbf{b} \cdot \frac{\partial \mathbf{B}}{\partial \theta} \cdot \mathbf{b}) \hat{e}_\theta \right] \left( \mathcal{F}_1 + \frac{1-\bar{\nu}}{\bar{\nu}} \mathcal{F}_2 \right).\] (17)

6. \(\alpha\)-Fe at high temperature: a highly-anisotropic cubic crystal

As the \(\alpha\)–\(\gamma\) bcc-fcc phase transition in Fe is approached, the lattice becomes increasingly elastically-anisotropic \([7, 8, 13]\). The tetragonal shear modulus \(C' = (C_{11} - C_{12})/2\) encodes the crystal’s resistance to deformation in the direction conducive to the martensitic bcc-fcc transformation. As the transition temperature is approached, the
potential barrier between the two lattice structures decreases towards zero, as does $C'$. The trigonal shear modulus $C_{44}$, however, is unrelated to the structural transformation, and falls gradually toward zero at the melting point. The discrepancy between the two independent shear moduli defines the extreme elastic anisotropy of the crystal: the isotropic approximation does not distinguish between the two at all, and hence cannot capture any of the effects reported here and elsewhere e.g. [7, 8, 14].

The dramatic effect of anisotropy on the dislocation self force in $\alpha$-Fe is displayed in Fig.1, for $b = [100]$ (top) and $1/2[111]$ (bottom). The vector from the origin to a point on the surface represents the dislocation line direction, and the distance from the origin (centre of the spheroid) to the surface corresponds to the dislocation’s energy per-unit-length, the longitudinal contribution to the self-force. The colour corresponds to the torsional contribution. Firstly consider the right-hand plots, which use a simple isotropic approximation ($C', C_{44} \rightarrow (C' + C_{44})/2$). The ellipsoids which result are circularly-symmetric about the direction of the Burgers’ vector, since all pure edge orientations are equivalent in an isotropic crystal. As more screw component is included, the radius reduces, reaching a minimum at the pure screw orientation. The colour indicates zero
The torsional self force at the energy extrema, the stable minimum of the screw and the degenerate maxima of the equivalent edge orientations.

The situation is markedly different when the full anisotropic calculation is used in the left-hand plots \( \left( C' = 13.3, C_{44} = 99.0 \text{GPa} \right) \), particularly for the \( b = [100] \) case. The most significant feature is the huge relative increase in the energy of the \( b = [100] \) screw, and the powerful self force acting to rotate the line away from this unfavourable orientation. This has important consequences for the evolution of dislocation sources (see below). For the \( b = 1/2[111] \) case, the opposite is true: the energy of the screw falls dramatically and the self-force acts to favour this orientation. It should be noted that no isotropic averaging procedure can reproduce these effects. The only degrees of freedom offered by such an approximation are the overall scale of the spheroid (set by \( \bar{\mu} \)) and its eccentricity (set by \( \bar{\nu} \)). The striking variation of energy with orientation leads to conspicuous effects on the lowest-energy configurations adopted by dislocations, as the lines are driven away from unfavourable orientations by the anisotropic self-force.

Fig. 2 shows a series of snapshots taken from DDD simulations of Frank-Read sources operating in high-temperature \( \alpha \)-Fe in various geometrical configurations (see caption).

When the dislocation density is low, the self-force is the dominant contribution to the force on each segment, exceeding that of the stresses from interaction with other segments. The evolution of a bowing pinned dislocation is governed by the competition between the applied stress and the dislocation’s resistance to elongation (“line tension”, or longitudinal self-force), and, especially in the highly-anisotropic limit, the energy landscape of the lattice itself (torsional self-force). For this reason, we calculate the self-force according to the prescription detailed above, and use isotropic elasticity for the sub-leading interaction stresses, avoiding possible non-uniqueness problems with the anisotropic stress field of an unclosed dislocation loop.

The sharp corners which emerge, especially in the \( b = [100] \) example, are the result of the anisotropic self-force acting to avoid the highest-energy orientations. The loops would always be smooth and elliptical according to the isotropic approximation, where the only variability in shape comes from the edge-screw energy difference. The eccentricity of the ellipse is related to Poisson’s ratio, analogous to the energy surfaces. Since the high-energy orientations avoided, all of the generated loop is essentially low-energy, and hence is more easily generated. In other words, a lower applied stress is required to operate the source than would otherwise be the case. These results are in agreement with those reported elsewhere, see e.g. [2, 3].

7. Conclusions

In this paper we have investigated the impact elastic anisotropy has on dislocation self-force. We have developed a procedure for computational implementation which captures the orientation-dependence of a dislocation segment’s elastic energy, and hence self-force, and which leads to an isotropic limit consistent with the computationally-convenient
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Figure 2. Snapshots of DDD simulations of critical Frank-Read sources. Pairs, left to right: ⟨100⟩{001}, ⟨100⟩{011}, 1/2⟨111⟩{011}, 1/2⟨111⟩{112}. Top: initial edge; bottom: initial screw. The snapshots are rotated to align similar crystallographic directions in each case. The anisotropic self-force acts to align the dislocation along the lowest-energy directions. All the above loops would be elliptical in the isotropic approximation.

non-singular theory of dislocations developed in [1, 15]. The rich variation in the dislocation energy landscape of an anisotropic lattice leads to stronger and more variable self-forces, which in turn lead to interesting geometric dislocation configurations. The jagged, sharp-cornered structures we predict also emerge from the analytical variational approaches adopted in [2, 3], and have also been observed in irradiated α-iron in the electron microscope [3, 4].

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Appendix A. Calculation of B matrix

\[ \mathcal{K} = b_i B_{ij} b_j; \quad B_{ij} = \frac{1}{8\pi^2} \int_0^{2\pi} \left\{ (mm)_{ij} - (mn)_{ik} (nn)^{-1}_{kl} (nm)_{lj} \right\} d\omega, \quad (A.1) \]

where

\[ (uv)_{ij} = u_k c_{kj} i j v_l \quad (A.2) \]
for any pair of vectors \( u, v \), and \( n, m, \omega \) are defined relative to \( t \) as in Fig.A1[5]. Note that some authors define \( B \) as \( 4\pi \times B \) as defined above, and compensate the factor in Eq.1.

**Appendix B. Voigt and Reuss averages**

In cubic crystals, the following relations hold, where \( \mu \) is the shear modulus, \( B \) is the bulk modulus, \( \nu \) is Poisson’s ratio and \( E \) is the Young’s modulus.

\[
\begin{align*}
\mu_V &= \frac{1}{5} (2C'' + 3C_{44}) \\
B_V &= \frac{1}{3} (2C'' + 3C_{12}) \\
\nu_V &= \frac{1}{2} \frac{12C'' + 5C_{12} - 2C_{44}}{4C'' + 5C_{12} + C_{44}} \\
E_V &= \frac{4C'' + 6C'' C_{12} + 6C'' C_{44} + 9C_{12}C_{44}}{4C'' + 5C_{12} + C_{44}} \\
\end{align*}
\]

\[
\begin{align*}
\mu_R &= \frac{5C''C_{44}}{2C_{44} + 3C''} \\
B_R &= \frac{1}{3} (2C'' + 3C_{12}) \\
\nu_R &= \frac{1}{2} \frac{12C_{44} C_{12} + 2C''^2 + 3C'' C_{12} - 2C'' C_{44}}{2C_{44} C_{12} + 2C''^2 + 3C'' C_{12} + 3C'' C_{44}} \\
E_R &= \frac{5C'' C_{44} (2C'' + 3C_{12})}{3C' C_{44} + 2C''^2 + 2C_{12} C_{44} + 3C_{12} C''} \\
\end{align*}
\]

Subscripts \( V \) and \( R \) refer to Voigt- and Reuss-averaging respectively. Voigt’s procedure [10] assumes the strain is uniform everywhere (and results in inter-grain forces being out
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of equilibrium), whereas Reuss’ procedure [11] assumes the stress is uniform (leading to deformed grains which do not fit together). Hill [12] demonstrates that:

\[ \mu_R < \mu_V, \quad B_R < B_V, \quad E_R < E_V, \]  

(B.3)

and further reports that taking values for \( \mu, B, E \) between the Voigt and Reuss procedures agree well with experiment. Either the arithmetic or geometric mean will do, and

\[ \nu = \frac{1}{2} \left( 1 - \frac{3\mu}{3B + \mu} \right). \]  

(B.4)

References