Elastic interactions between nano-scale defects in irradiated materials

S. L. Dudarev

CCFE, UK Atomic Energy Authority, Culham Science Centre, Abingdon, Oxfordshire OX14 3DB, United Kingdom

A. P. Sutton

Department of Physics, Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Abstract

Closed form expressions are derived for the energy of elastic interaction between dislocation loops, and between dislocation loops and vacancy clusters, to enable simulations of elastically biased microstructural evolution of irradiated materials. The derivations assume the defects are separated by distances greater than their size. The resulting expressions are well suited for real-space simulations of microstructural evolution involving thousands of elastically interacting defects in 3D. They play a similar role to interatomic potentials in molecular dynamics simulations.

Keywords: Dislocation loops, defects, elastic interaction

1. Introduction

Real-space, real-time simulation of microstructural evolution occurring in materials under irradiation is an outstanding problem in computational materials science. A dislocation-based treatment of mechanical deformation, which is essential for interpreting experimental observations of radiation hardening and embrittlement, requires evaluating the energy of interaction between dislocation

[1]sergei.dudarev@ukaea.uk; s.dudarev@imperial.ac.uk
[2]a.sutton@imperial.ac.uk

loops and other defects, such as vacancies and cavities, in real space, where the loops are treated as three-dimensional objects characterized by their position, size, shape, and spatial orientation.

It is well established that the occurrence of material-dependent temperatures, at which the response to irradiation changes significantly, is related to activation energies of formation and migration of defects. These energies vary from a fraction of an eV to several eV [1, 2]. The energy scales of elastic interactions between defects are similar, depending on the size of defects and the distance between them [3, 4]. Whereas the spectrum of activation energies for reactions between defects is discrete, the energies of elastic interactions are distributed continuously. Thus, although elastic interactions do not give rise to discrete "microstructural transitions" at certain temperatures, their influence on microstructural evolution is just as strong as the thermally activated formation, migration and reaction of defects [5]. These long-range interactions are the subject of this paper.

To what extent are long-range elastic interactions included in current techniques to model microstructural evolution under irradiation? There are two principal approaches. The rate theory approach [6], and its more recent generalizations based either on the Master and Fokker-Planck equations [7], or using the cluster dynamics equations [8, 9], follow the evolution of ensemble-average densities of defect species. Rate theory equations assume that defect densities are spatially homogeneous [8, 9], or that they vary slowly as functions of spatial coordinates [10]. Elastic interactions are included in rate theory through the use of effective parameters, called bias factors [6, 11, 12]. The second approach is to use kinetic Monte Carlo (kMC) simulations where defects are treated as mobile objects undergoing stochastic motion [13, 14]. It is not straightforward to include long-range elastic interactions between defects in such simulations [15, 16, 17]. Wen et al. [18] modelled interactions between small dislocation loops and point defect clusters using kMC simulations that included elastic interactions. These methods were used by Wen et al. [19] to model the evolution of clouds of self-interstitial clusters around edge dislocations, and the subsequent

pinning of these dislocations.

Langevin dynamics simulations of mobile elastically interacting nano-defects[3, 4] show that these interactions strongly influence the evolution of microstructure, leading to trapping of defects, and giving rise to defect clustering and the formation of rafts of defects. Rafts of defects are routinely observed experimentally in materials exposed to irradiation [20, 21, 22, 23, 24, 25, 26].

The computational efficiency of a Langevin dynamics simulation depends primarily on the speed of evaluation of forces acting between defects. In isotropic elasticity the energy of interaction between two dislocation loops is given exactly by Blin's formula. But this involves line integrals around the perimeter of each loop [27, 4], which requires too much computational time when there are very many loops.

To overcome this difficulty we present closed form expressions for the energy of elastic interaction between loops separated by distances larger than their size. The most general case of loops with different Burgers vectors and different loop normals, and with the loops separated by an arbitrary vector, is solved and shown to depend on ten angles. Although the angular dependence is a function of ten independent angles, it is remarkable that it has a closed form. Simpler cases, one of which is well known, involving prismatic loops only are derived as special cases of the general formula.

Electron microscope observations of microstructures due to irradiation [20, 21, 22, 23, 24, 25, 26] show that at any moment most loops are separated by distances greater than their size. Reactions between loops, resulting in their annihilation or coalescence, and occurring only when the distance between them is virtually zero, typically involve a small faction of all the defects present in the material.

Our study provides further support for the importance of elastic interactions in the evolution of microstructures of these defects. At separations larger than their sizes the energy of interaction between two dislocation loops separates into purely radial and purely angular dependencies. As a result the angular dependence persists as the distance between the defects increases.

In the next section an approximate formula is derived for the interaction energy between two loops in an infinite anisotropic elastic medium. This formula is directly analogous to the interaction energy between two point defects, involving their elastic dipole tensors. Exploiting this analogy an expression is obtained for the dipole tensor of a small dislocation loop. When the isotropic elastic approximation is made, an approximate closed form expression is derived for the stress field of an arbitrary small loop, and the interaction energy between two arbitrary loops separated by more than their sizes. Using the dipole tensors for a small loop and an isotropic point defect cluster the interaction energy between them is derived. The assumptions underlying the closed form expressions are tested by comparing the approximate interaction energies between prismatic loops with exact numerical results obtained from Blin's formula, where the simplifying approximations in this paper are not made. It is shown that the approximations are remarkably robust and an explanation for their robustness is offered.

2. Interaction energy between small loops

Consider two planar dislocation loops with Burgers vectors $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$, loop normals $\hat{n}^{(1)}$ and $\hat{n}^{(2)}$, loop areas $A^{(1)}$ and $A^{(2)}$, and loop centres at $\mathbf{r}^{(1)}$ and $\mathbf{r}^{(2)}$. Let $\mathbf{r} = \mathbf{r}^{(1)} - \mathbf{r}^{(2)}$. Throughout the paper it is assumed the elastic continuum is infinite with no free surfaces. The elastic interaction energy between the loops is given exactly by the following equivalent surface integrals taken over the areas of the loops:

$$E_{int} = \int_{A^{(2)}} b_i^{(2)} \sigma_{ij}^{(1)} \hat{n}_j^{(2)} \mathrm{d}S = \int_{A^{(1)}} b_i^{(1)} \sigma_{ij}^{(2)} \hat{n}_j^{(1)} \mathrm{d}S. \tag{1}$$

Throughout the paper summation is implied on repeated subscripts. In Eq. (1) the interaction energy is the negative of the work done by the stress field of one loop when the other loop is created in its presence (see Ref. [27], p.106). In the following it is assumed the separation between the loops is much larger than the sizes of the loops. This approximation enables each loop to be treated as

a point-like defect in which the stress field of the other defect is approximately constant. With this approximation Eq. (1) becomes:

$$E_{int} = A^{(2)} b_i^{(2)} \sigma_{ij}^{(1)}(\mathbf{r}^{(2)}) \hat{n}_j^{(2)} = A^{(1)} b_i^{(1)} \sigma_{ij}^{(2)}(\mathbf{r}^{(1)}) \hat{n}_j^{(1)}. \tag{2}$$

Volterra's formula [28] for the displacement field at $\mathbf{r}^{(1)}$ due to the small loop centred at $\mathbf{r}^{(2)}$ becomes:

$$u_j^{(2)}(\mathbf{r}^{(1)}) = C_{kpim} b_k^{(2)} A^{(2)} G_{ij,m}(\mathbf{r}^{(1)} - \mathbf{r}^{(2)}) \hat{n}_p^{(2)}, \tag{3}$$

where $G_{ij}(\mathbf{r}^{(1)} - \mathbf{r}^{(2)})$ is the elastic Green's function relating the displacement $u_i(\mathbf{r}^{(1)})$ to a point force $f_j(\mathbf{r}^{(2)}) : u_i(\mathbf{r}^{(1)}) = G_{ij}(\mathbf{r}^{(1)} - \mathbf{r}^{(2)}) f_j(\mathbf{r}^{(2)})$. Commas denote differentiation, thus $G_{ij,m}(\mathbf{r}) = \partial G_{ij}(\mathbf{r}) / \partial r_m$. The elastic constant tensor is C_{ijkl}.

Hooke's law then yields the stress field at $\mathbf{r}^{(1)}$ caused by the second loop at $\mathbf{r}^{(2)}$:

$$\begin{aligned} \sigma_{ab}^{(2)}(\mathbf{r}^{(1)}) &= C_{abjq} u_{j,q}^{(2)}(\mathbf{r}^{(1)}) \\ &= C_{abjq} C_{kpim} b_k^{(2)} A^{(2)} G_{ij,mq}(\mathbf{r}^{(1)} - \mathbf{r}^{(2)}) \hat{n}_p^{(2)}. \end{aligned} \tag{4}$$

Inserting this equation into the second expression on the right of Eq. (2), the following equality is obtained:

$$E_{int} = P_{qj}^{(1)} G_{ij,mq}(\mathbf{r}^{(1)} - \mathbf{r}^{(2)}) P_{mi}^{(2)}, \tag{5}$$

which is also the equation for the interaction energy between two point defects with dipole tensors $P^{(1)}$ and $P^{(2)}$ (see equation (4.100) of Ref. [29]). For the dislocation loops the dipole tensors are:

$$P_{fg}^{(i)} = \frac{1}{2} C_{fgks} A^{(i)} \left(\hat{n}_s^{(i)} b_k^{(i)} + b_s^{(i)} \hat{n}_k^{(i)} \right). \tag{6}$$

Within the approximation of loops separated by distances much greater than their size Eq. (5) is exact, including full elastic anisotropy. Eq. (5) is also the long range interaction energy between point defect clusters, provided their

separation is much greater than their size. It follows that Eq. (5) may also be used to evaluate the interaction energy between dislocation loops and vacancy or interstitial clusters, provided the defects are smaller than their separation.

2.1. The isotropic elastic approximation

Making the approximation of elastic isotropy, the elastic constant tensor becomes:

$$C_{ijkl} = \lambda\ \delta_{ij}\ \delta_{kl} + \mu(\delta_{ik}\ \delta_{jl} + \delta_{il}\ \delta_{jk}), \tag{7}$$

where μ is the shear modulus, $\lambda = 2\mu\nu/(1-2\nu)$ and ν is Poisson's ratio. The elastic dipole tensor for a small loop, as given by Eq. (6), is now

$$P_{ij} = \mu b A \left[(\hat{b}_i \hat{n}_j + \hat{n}_i \hat{b}_j) + \frac{2\nu}{1-2\nu} \hat{b}_k \hat{n}_k \delta_{ij} \right], \tag{8}$$

where $b = |\mathbf{b}|$, $\hat{b} = \mathbf{b}/b$ and $\hat{b}_j = b_j/b$.

The isotropic elastic Green's function $G_{ik}(\mathbf{r})$ is given by [28]:

$$G_{ik}(\mathbf{r}) = \frac{1}{16\pi\mu(1-\nu)r} \left[(3-4\nu)\delta_{ik} + \hat{r}_i \hat{r}_k \right], \tag{9}$$

where $\hat{r}_i$ are the components of the unit vector $\hat{r} = \mathbf{r}/r$ and $r = |\mathbf{r}|$. Differentiating, the following equation is obtained:

$$\begin{aligned} G_{ik,jl}(\mathbf{r}) &= \frac{1}{16\pi\mu(1-\nu)r^3} \times \\ &\{(3-4\nu)\delta_{ik}\,(3\hat{r}_l\hat{r}_j - \delta_{lj}) \\ + \quad & 15\hat{r}_i\hat{r}_j\hat{r}_k\hat{r}_l - 3(\delta_{ij}\hat{r}_k\hat{r}_l + \delta_{il}\hat{r}_j\hat{r}_k + \delta_{jl}\hat{r}_i\hat{r}_k \\ + \quad & \delta_{kj}\hat{r}_i\hat{r}_l + \delta_{kl}\hat{r}_i\hat{r}_j) + (\delta_{il}\delta_{kj} + \delta_{kl}\delta_{ij})\}. \end{aligned} \tag{10}$$

Using Eqns. (4), (7) and (10), the following expression for the stress $\sigma^{(2)}_{ij}(\mathbf{r})$

is obtained:

$$\sigma_{ij}^{(2)}(\mathbf{x}) = -\frac{\mu A^{(2)} b^{(2)}}{4\pi(1-\nu)r^3} \times$$
$$\Big\{ \Big[3(1-2\nu)(\hat{b}^{(2)}\cdot\hat{r})(\hat{n}^{(2)}\cdot\hat{r}) + (4\nu-1)(\hat{b}^{(2)}\cdot\hat{n}^{(2)}) \Big] \delta_{ij}$$
$$+ (1-2\nu)(\hat{b}_i^{(2)}\hat{n}_j^{(2)} + \hat{n}_i^{(2)}\hat{b}_j^{(2)})$$
$$+ 3\nu \Big[(\hat{b}^{(2)}\cdot\hat{r})(\hat{n}_i^{(2)}\hat{r}_j + \hat{r}_i\hat{n}_j^{(2)}) + (\hat{n}^{(2)}\cdot\hat{r})(\hat{b}_i^{(2)}\hat{r}_j + \hat{r}_i\hat{b}_j^{(2)}) \Big]$$
$$+ 3(1-2\nu)(\hat{b}^{(2)}\cdot\hat{n}^{(2)})\hat{r}_i\hat{r}_j - 15(\hat{b}^{(2)}\cdot\hat{r})(\hat{n}^{(2)}\cdot\hat{r})\hat{r}_i\hat{r}_j \Big\}. \qquad (11)$$

Kroupa obtained the same expression in Eqn. (2.11) of Ref. [30] by regarding the dislocation loop as a region that has undergone a transformation strain, and applying Eshelby's procedure to calculate the stress field[31].

To obtain the interaction energy between two small loops, Eq. (11) may be inserted for the stress tensor into the second expression on the right of Eq. (2). Alternatively, Eq. (8) for the dipole tensors and Eq. (10) for the second derivative of the Green's function may be inserted into Eq. (5). Both routes lead to the following general formula for the interaction energy between two small loops separated by the relative position vector $\mathbf{r}$:

$$\begin{aligned}
E_{int}^{(12)} &= \frac{\mu b^{(1)} b^{(2)} A^{(1)} A^{(2)}}{4\pi(1-\nu)r^3} \Big[15(\hat{b}^{(1)}.\hat{r})(\hat{b}^{(2)}.\hat{r})(\hat{n}^{(1)}.\hat{r})(\hat{n}^{(2)}.\hat{r}) \\
&- 3\nu \Big\{ (\hat{b}^{(1)}.\hat{b}^{(2)})(\hat{n}^{(1)}.\hat{r})(\hat{n}^{(2)}.\hat{r}) + (\hat{b}^{(1)}.\hat{n}^{(2)})(\hat{n}^{(1)}.\hat{r})(\hat{b}^{(2)}.\hat{r}) \\
&+ (\hat{n}^{(1)}.\hat{b}^{(2)})(\hat{n}^{(2)}.\hat{r})(\hat{b}^{(1)}.\hat{r}) + (\hat{n}^{(1)}.\hat{n}^{(2)})(\hat{b}^{(1)}.\hat{r})(\hat{b}^{(2)}.\hat{r}) \Big\} \\
&- 3(1-2\nu)(\hat{b}^{(1)}.\hat{n}^{(1)})(\hat{b}^{(2)}.\hat{r})(\hat{n}^{(2)}.\hat{r}) \\
&- 3(1-2\nu)(\hat{b}^{(2)}.\hat{n}^{(2)})(\hat{b}^{(1)}.\hat{r})(\hat{n}^{(1)}.\hat{r}) \\
&- (1-2\nu) \Big\{ (\hat{b}^{(1)}.\hat{b}^{(2)})(\hat{n}^{(1)}.\hat{n}^{(2)}) + (\hat{b}^{(1)}.\hat{n}^{(2)})(\hat{n}^{(1)}.\hat{b}^{(2)}) \Big\} \\
&- (4\nu-1)(\hat{b}^{(1)}.\hat{n}^{(1)})(\hat{b}^{(2)}.\hat{n}^{(2)}) \Big].
\end{aligned} \qquad (12)$$

This is the central result of this paper. It generalises earlier expressions for the interaction energy between infinitesimal prismatic loops derived by Kroupa [30]

and Foreman and Eshelby [32], because in Eq. (12) the loops are of arbitrary character, where the character is prismatic ($\hat{b}\cdot\hat{n}=\pm1$), shear ($\hat{b}\cdot\hat{n}=0$) or a mixture ($0<|\hat{b}\cdot\hat{n}|<1$). The interaction energy separates into an inverse cube dependence on the separation between the loops and a term that depends on ten angles. The ten angles are all the angles, taken in pairs, between the five unit vectors $\hat{r},\hat{b}^{(1)},\hat{b}^{(2)},\hat{n}^{(1)},\hat{n}^{(2)}$. Together with the magnitudes of the Burgers vectors, the loop areas and the distance between the loop centres, the interaction energy is a function of fifteen variables, and it is remarkable that this function has a closed form.

For two pure prismatic loops the interaction energy can be simplified:

$$\begin{aligned} E_{int}^{(12)} = \frac{\mu b^{(1)}b^{(2)}A^{(1)}A^{(2)}}{4\pi(1-\nu)r^3}\{&15(\hat{n}^{(1)}\cdot\hat{r})^2(\hat{n}^{(2)}\cdot\hat{r})^2 \\ -\ &(4\nu-1)-12\nu(\hat{n}^{(1)}\cdot\hat{n}^{(2)})(\hat{n}^{(1)}\cdot\hat{r})(\hat{n}^{(2)}\cdot\hat{r}) \\ -\ &(1-2\nu)[3(\hat{n}^{(2)}\cdot\hat{r})^2+3(\hat{n}^{(1)}\cdot\hat{r})^2+2(\hat{n}^{(1)}\cdot\hat{n}^{(2)})^2]\}. \end{aligned} \tag{13}$$

The angular dependence has been reduced to just three angles between the unit vectors $\hat{r},\hat{n}^{(1)},\hat{n}^{(2)}$ taken in pairs. If the loop normals are parallel to $\hat{n}$ then, as first shown by Foreman and Eshelby [32], the angular dependence is a function of only the angle θ between $\hat{r}$ and $\hat{n}$:

$$E_{int}^{(12)} = \frac{\mu b^{(1)}b^{(2)}A^{(1)}A^{(2)}}{4\pi(1-\nu)r^3}\left(15\cos^4\theta-6\cos^2\theta-1\right). \tag{14}$$

3. Interaction energy between a small loop and a small point defect cluster

The dipole tensor of an isotropic point defect cluster is as follows:

$$P_{ij} = B\Omega_{rel}\delta_{ij}, \tag{15}$$

where Ω_{rel} is the relaxation volume of the defect. In an infinite medium Ω_{rel} is the volume of excess or deficit material in the cluster, Ω_{rel} is positive for

interstitials and negative for vacancies. B is the bulk modulus: $B = 2\mu(1+\nu)/[3(1-2\nu)]$.

Consider the interaction energy between the point defect cluster and another strain field $e_{ij}(\mathbf{r})$. Provided the strain field varies sufficiently slowly that it may be regarded as constant in the cluster then the interaction energy is given by $-P_{ij}e_{ij}$. Inserting Eq. (15) for the dipole tensor, the well known formula is obtained for the interaction energy $E_{int} = p\,\Omega_{rel}$, where $p = -Be_{ii}$ is the hydrostatic pressure acting on the defect [33].

The hydrostatic pressure of a small dislocation loop is obtained directly from Eq. (11) and the interaction energy is then:

$$E_{int} = \frac{\mu A b \Omega_{rel}}{6\pi r^3}\frac{(1+\nu)}{(1-\nu)}\left[3(\hat{b}\cdot\hat{r})(\hat{n}\cdot\hat{r}) - (\hat{b}\cdot\hat{n})\right]. \tag{16}$$

If the loop is prismatic, with $\hat{b}\cdot\hat{n} = 1$ Eq. (16) has a particularly simple form:

$$E_{int} = \frac{\mu A b \Omega_{rel}}{3\pi r^3}\frac{1+\nu}{1-\nu}P_2(\cos\theta), \tag{17}$$

where the sign of E_{int} is reversed if $\hat{b}\cdot\hat{n} = -1$, $P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$ is a Legendre polynomial and $\cos\theta = \hat{b}\cdot\hat{r}$.

4. Comparisons with exact results

To assess the accuracy of our formulae for the isotropic elastic interaction energy between small dislocation loops in an infinite medium, the energies calculated using Eq. (13) and (14) are compared with the exact results of Blin's formula for the interaction energy (see Eq. (4-40) of Ref. [27]), which takes into account fully the variation of the stress field of one loop within the other.

In the first calculation two identical circular prismatic loops are considered in tungsten with radius 10 Å, and Burgers vector $a[001]$, where a is the lattice constant. As they are prismatic loops their normals are also [001]. One loop is placed at the origin. The second moves along the straight line $\mathbf{r} = d\hat{i} + \alpha\hat{k}$, where $\hat{i}$ and $\hat{k}$ are unit vectors along the x_1 and x_3 Cartesian axes, and $-400\text{Å} \leq \alpha \leq 500\text{Å}$. Three values of d are compared: $30, 50, 100\text{Å}$. Values computed for

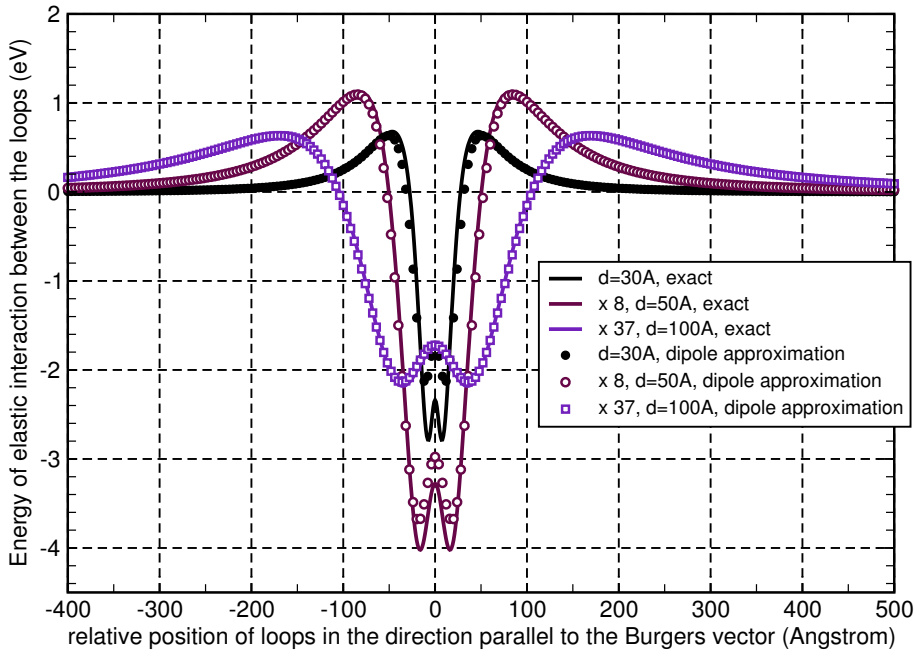


Figure 1: Comparison of the elastic interaction energies between two prismatic loops calculated with Eq. (14) ('dipole approximation') compared with the exact Blin formula [27], see text. For $d = 100$Å the curves computed using the exact and approximate formulae are not distinguishable on the scale of the figure.

$d = 100$Å are scaled up by the factor of 37, and the values computed for $d = 50$Å are scaled by the factor of 8. The results in Fig. 1 show that the small loop approximation of Eq. (14) is remarkably accurate even when $d = 30$Å for which the closest approach of the two loops is 10Å. The reasons for the accuracy of the approximation are discussed in the next section.

In the second example the elastic interaction energy is considered between two circular prismatic loops of radius 10Å. The first loop has Burgers vector $a[001]$ and is located at the origin. The second loop has Burgers vector $a/2[111]$ and moves along the line $\mathbf{r} = d\hat{i} + \frac{\alpha}{\sqrt{3}}[111]$, where $-250\text{Å} \leq \alpha \leq 250\text{Å}$. The approximate energies were calculated using Eq. (13), and the exact energies were obtained using Blin's formula. It is seen in Fig. 2 that the agreement is again remarkably good, even when the separation between the loops is comparable to

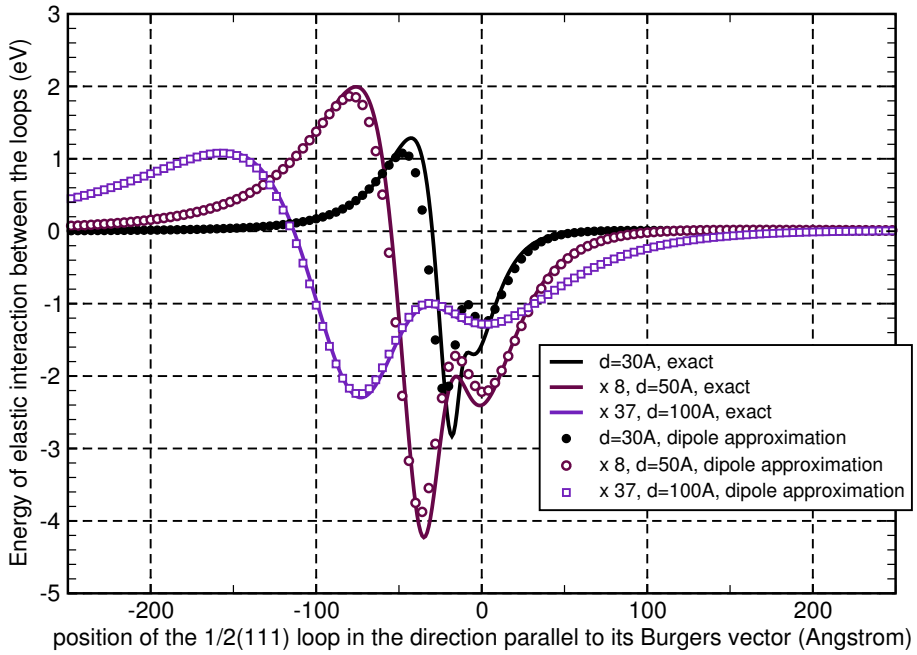


Figure 2: Energy of elastic interaction between two circular prismatic dislocation loops with Burgers vectors $a[001]$ and $a/2[111]$ and loop radius 10Å. The curves labelled 'dipole approximation' were calculated with Eq. (14), while the exact results were obtained with the Blin formula [27], see text. For $d = 100$Å the curves computed using the exact and approximate formulae are not distinguishable on the scale of the figure.

the loop size.

5. Discussion

5.1. Accuracy of the approximations

It is instructive to consider the first order corrections to the approximate energy of interaction between two dislocation loops, to understand why Eqs. (13) and (14), and presumably Eq. (12), are so accurate. Consider Volterra's

formula [28] for the displacement field of a dislocation loop:

$$u_i(\mathbf{r}) = \int_S C_{jklm}\, b_l\, G_{ij,k}(\mathbf{r}-\mathbf{r}')\, \hat{n}_m\, \mathrm{d}S(\mathbf{r}'). \tag{18}$$

This is an exact result in anisotropic linear elasticity. The surface integral in Eq. (18) may be taken over the area of the plane enclosed by the dislocation loop. Let $\mathbf{R}$ be the centre of the loop and let $\boldsymbol{\rho}$ be a vector from $\mathbf{R}$ to any point inside the loop. Then $\mathbf{r}' = \mathbf{R} + \boldsymbol{\rho}$ and $\mathbf{r} - \mathbf{r}' = (\mathbf{r} - \mathbf{R}) - \boldsymbol{\rho}$. For a plane loop the normal $\hat{n}$ is constant. Thus the only spatial dependence in the integrand is in the Green's function, which may be expanded as follows:

$$\begin{aligned} G_{ij,k}(\mathbf{r}-\mathbf{R}-\boldsymbol{\rho}) &= G_{ij,k}(\mathbf{r}-\mathbf{R}) - \rho_p\, G_{ij,kp}(\mathbf{r}-\mathbf{R}) \\ &+ \frac{1}{2}\,\rho_p\,\rho_q\, G_{ij,kpq}(\mathbf{r}-\mathbf{R}) + \ldots \end{aligned} \tag{19}$$

The approximations made in this paper amount to taking just the first term on the right hand-side of Eq. (19). If this expansion is substituted into the integral in Eq. (18) the surface integral becomes a set of moments of the loop area. If the loop is centrosymmetric, such as a circle, ellipse, rectangle or hexagon, the first moments are zero. In that case there is no contribution from $G_{ij,kp}(\mathbf{r}-\mathbf{R})$ and the lowest order correction arises from the second moment giving terms proportional to $G_{ij,kpp}(\mathbf{r}-\mathbf{R})$. These terms give rise to contributions to the stress field of the loop that decay with distance r as L^2/r^5, where L is a characteristic size of the loop. Thus the first order correction to the interaction energy between centrosymmetric loops decays as L^2/r^5. This explains the remarkable accuracy of the approximation seen in Figs. 1 and 2. It is consistent with the statement on p.140 of Ref. [27] 'For finite loops with shapes similar to circles of radius R, the long-range stress fields at distances from the loop greater than $2R$ converge rapidly to the stress field of the infinitesimal loop, in accord with the expectation from St. Venant's principle.'

5.2. Boundary conditions

Throughout this paper it has been assumed the defects are in an infinite medium. In reality any body is finite with its surface subject to boundary conditions. This is particularly important for point defects where the volume of relaxation can change by about a factor of two between the solution for an infinite body and the solution for a finite body with free surfaces, no matter how far the surfaces are from the defect [34]. Secondly, isotropic point defects, for which the dipole tensor is proportional to δ_{ij}, do not interact in an infinite body in isotropic elasticity. Formally this is because $G_{ij,ij} = 0$ in Eq.5. However, they do interact in a finite body through 'image' interactions. Nabarro [35] presented the corrections to the displacement field of a small shear loop in an infinite medium that result when the loop is at the centre of a sphere with no tractions applied to its surface.

In a finite body with *surfaces free of tractions* the relaxation volume of a small dislocation loop is as follows [29]:

$$\Omega_{rel}^{loop} = P_{jj}/(3B) \tag{20}$$

Inserting the dipole tensor of a loop from Eq. (8) into this equation leads to the result that $\Omega_{rel}^{loop} = A(\mathbf{b} \cdot \hat{n})$. Thus, the relaxation volume in a finite body is zero for a shear loop, and for a prismatic loop it is equal to the number of interstitial atoms or vacancies in the loop multiplied by the atomic volume.

6. Summary

A closed form expression (Eq. (12)) has been derived for the interaction energy in an infinite isotropic elastic medium between two small dislocation loops with arbitrary loop normals and Burgers vectors. The assumption was made that the loops are separated by more than their size. Comparisons were made for the interaction energies calculated for prismatic dislocation loops between the approximate formulae and exact numerical values obtained with Blin's formula. The results agreed well even at small loop separations, and an explanation was

offered. Closed form expressions have also been derived under the same conditions for elastic interactions between dislocation loops and isotropic vacancy clusters. These formulae are useful for simulations of the evolution of radiation damage microstructures including elastic interactions.

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