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Elastic interactions between nano-scale defects in irradiated materials

S.L. Dudarev [a, *], A.P. Sutton [b]

[a] CCFE, UK Atomic Energy Authority, Culham Science Centre, Abingdon, Oxfordshire, OX14 3DB, United Kingdom
[b] Department of Physics, Blackett Laboratory, Imperial College London, London, SW7 2AZ, United Kingdom

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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.

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 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 characteristic 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, or migration of 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 [15–17]. Wen et al. [18] modelled interactions between small dislocation loops and point defect clusters using kMC simulations that included elastic interactions. These methods were also 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 [20–26].

* Corresponding author.
E-mail addresses: sergei.dudarev@ukaea.uk, s.dudarev@imperial.ac.uk (S.L. Dudarev), a.sutton@imperial.ac.uk (A.P. Sutton).

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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 computing 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 energy of elastic interaction 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 [20–26] 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 distances 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 given in an explicit analytical form. 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 adopted 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 $\widehat{n}^{(1)}$ and $\widehat{n}^{(2)}$, 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:

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

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:

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

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

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

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 $\mathbf{r}^{(2)}$:

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

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

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

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:

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

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:

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

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

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

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

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

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