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# Elastic modeling of point-defects and their interaction

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ABSTRACT

Different descriptions used to model a point-defect in an elastic continuum are reviewed. The emphasis is put on the elastic dipole approximation, which is shown to be equivalent to the infinitesimal Eshelby inclusion and to the infinitesimal dislocation loop. Knowing this elastic dipole, a second rank tensor fully characterizing the point-defect, one can directly obtain the long-range elastic field induced by the point-defect and its interaction with other elastic fields. The polarizability of the point-defect, resulting from the elastic dipole dependence with the applied strain, is also introduced. Parameterization of such an elastic model, either from experiments or from atomic simulations, is discussed. Different examples, like elastodiffusion and bias calculations, are finally considered to illustrate the usefulness of such an elastic model to describe the evolution of a point-defect in a external elastic field.



## 1. Introduction

Point-defects in crystalline solids, being either intrinsic like vacancies, self-interstitial atoms, and their small clusters, or extrinsic like impurities and dopants, play a major role in materials properties and their kinetic evolution. Some properties of these point-defects, like their formation and migration energies, are mainly determined by the region in the immediate vicinity of the defect where the crystal structure is strongly perturbed. An atomic description appears thus natural to model these properties, and atomic simulations relying either on *ab initio* calculations [1] or empirical potentials have now become a routine tool to study point-defects structures and energies. But point-defects also induce a long-range perturbation of the host lattice, leading to an elastic interaction with other structural defects, impurities or an applied elastic field. An atomic description thus appears unnecessary to capture the interaction arising from this long-range part, and sometimes is also impossible because of the reduced size of the simulation cell in atomic approaches. Elasticity theory becomes then the natural framework. It allows a quantitative description of the point-defect interaction with other defects.

Following the seminal work of Eshelby [2], the simplest elastic model of a point-defect corresponds to a spherical inclusion forced into a spherical hole of slightly different size in an infinite elastic medium. This description accounts for the point-defect relaxation volume and its interaction with a pressure field (size interaction). It can be enriched by considering an ellipsoidal inclusion, thus leading to a interaction with also the deviatoric component of the stress field (shape interaction), and by assigning different elastic constants to the inclusion (inhomogeneity) to describe the variations of the point-defect "size" and "shape" with the strain field where it is immersed. Other elastic descriptions of the point-defect are possible. In particular, it can be modeled by an equivalent distribution of point-forces. The long-range elastic field of the point-defect and its interaction with other stress sources are then fully characterized by the first moment of this force distribution, a second-rank tensor called the elastic dipole. This description is rather natural when modeling point-defects and it can be used to extract elastic dipoles from atomic simulations. These different descriptions are equivalent in the long-range limit, and allow for a quantitative modeling of the elastic field induced by the point-defect, as long as the elastic anisotropy of the matrix is considered.

This article reviews these different elastic models which can be used to describe a point-defect and illustrates their usefulness with chosen examples. After a short reminder of elasticity theory (Section 2), we introduce the different descriptions of a point-defect within elasticity theory (Section 3), favoring the elastic dipole description and showing its equivalence with the infinitesimal Eshelby inclusion as well as with an infinitesimal dislocation loop. The next section (Section 4) describes how the characteristics of the point-defect needed to model it within elasticity theory can be obtained either from atomistic simulations or from experiments. We finally give some applications in Section 5, where results of such an elastic model are compared to direct atomic simulations to assess its validity. The usefulness of this elastic

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description is illustrated in this section for elastodiffusion and for the calculation of bias factors, as well as for the modeling of isolated point-defects in atomistic simulations.

## 2. Elasticity theory

Before describing the modeling of a point-defect within elasticity theory, it is worth recalling the main aspects of the theory [3], in particular the underlying assumptions, some definitions and useful results.

### 2.1. Displacement, distortion and strain

Elasticity theory is based on a continuous description of solid bodies. It relates the forces, either internal or external, exerting on the solid to its deformation. To do so, one first defines the elastic displacement field. If $\vec{R}$ and $\vec{r}$ are the position of a point respectively in the unstrained and the strained body, the displacement at this point is given by

$$\vec{u}(\vec{R}) = \vec{r} - \vec{R}.$$

One can then define the distortion tensor $\partial u_i/\partial R_j$ which expresses how an infinitesimal vector $\overrightarrow{\mathrm{d}R}$ in the unstrained solid is transformed in $\overrightarrow{\mathrm{d}r}$ in the strained body through the relation

$$\mathrm{d}r_i = \left(\delta_{ij} + \frac{\partial u_i}{\partial R_j}\right)\mathrm{d}R_j,$$

where summation over repeated indices is implicit (Einstein convention) and $\delta_{ij}$ is the Kronecker symbol.

Of central importance to the elasticity theory is the dimensionless strain tensor, defined by

$$\begin{aligned}\varepsilon_{ij}(\vec{R}) &= \frac{1}{2}\left[\left(\delta_{in} + \frac{\partial u_n}{\partial R_i}\right)\left(\delta_{nj} + \frac{\partial u_n}{\partial R_j}\right) - \delta_{ij}\right] \\ &= \frac{1}{2}\left(\frac{\partial u_i}{\partial R_j} + \frac{\partial u_j}{\partial R_i} + \frac{\partial u_n}{\partial R_i}\frac{\partial u_n}{\partial R_j}\right).\end{aligned}$$

This symmetric tensor expresses the change of size and shape of a body as a result of a force acting on it. The length d$L$ of the infinitesimal vector d$\vec{R}$ in the unstrained body is thus transformed into d$l$ in the strained body, through the relation

$$\mathrm{d}l^2 = \mathrm{d}L^2 + 2\varepsilon_{ij}\mathrm{d}R_i\mathrm{d}R_j.$$

Assuming small deformation, a common assumption of linear elasticity, only the leading terms of the distortion are kept. The strain tensor then corresponds to the symmetric part of the distortion tensor, as

$$\varepsilon_{ij}(\vec{R}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial R_j} + \frac{\partial u_j}{\partial R_i}\right). \tag{1}$$

The antisymmetric part of the distortion tensor corresponds to the infinitesimal rigid body rotation. It does not lead to any energetic contribution within linear elasticity in the absence of internal torque.

With this small deformation assumption, there is no distinction between Lagrangian coordinates $\vec{R}$ and Eulerian coordinates $\vec{r}$ when describing elastic fields. One can equally write, for instance, $\vec{u}(\vec{r})$ or $\vec{u}(\vec{R})$ for the displacement field, which are equivalent to the leading order of the distortion.

### 2.2. Stress

The force $\overrightarrow{\delta F}$ acting on a volume element $\delta V$ of a strained body is composed of two contributions, the sum of external body forces $\vec{f}$ and the internal forces arising from atomic interactions. Because of the mutual cancellation of forces between particles inside the volume $\delta V$, only forces corresponding to the interaction with outside particles appear in this last contribution, which is thus proportional to the surface elements $\overrightarrow{\mathrm{d}S}$ defining the volume element $\delta V$. One obtains

$$\delta F_i = \int_{\delta V} f_i \mathrm{d}V + \oint_{\delta S} \sigma_{ij}\mathrm{d}S_j,$$

where $\sigma$ is the stress tensor defining internal forces.

Considering the mechanical equilibrium of the volume element $\delta V$, the absence of resultant force leads to the equation

$$\frac{\partial \sigma_{ij}(\vec{r})}{\partial r_j} + f_i(\vec{r}) = 0, \tag{2}$$

whereas the absence of torque ensures the symmetry of the stress tensor.

At the boundary of the strained body, internal forces are balanced by applied forces. If $\vec{T}^{\mathrm{a}}\mathrm{d}S$ is the force applied on the infinitesimal surface element d$S$, this leads to the boundary condition

$$\sigma_{ij}n_j = T_i^{\mathrm{a}}, \tag{3}$$

where $\vec{n}$ is the outward-pointing normal to the surface element d$S$.

The work $\delta w$, defined per volume unit, of these internal forces is given by

$$\delta w = -\sigma_{ij}\delta\varepsilon_{ij},$$

where $\delta\varepsilon_{ij}$ is the strain change during the deformation increase, and the sign convention is $\delta w > 0$ when the energy flux goes outwards the elastic body. This leads to the following thermodynamic definition of the stress tensor

$$\sigma_{ij} = \left(\frac{\partial e}{\partial \varepsilon_{ij}}\right)_s = \left(\frac{\partial f}{\partial \varepsilon_{ij}}\right)_T,$$

where $e, s$, and $f = e - Ts$ are the internal energy, entropy, and free energy of the elastic body defined per volume unit.

### 2.3. Hooke's law

To go further, one needs a constitutive equation for the energy or the free energy. Taking as a reference the undeformed state corresponding to the elastic body at equilibrium without any external force, either body or applied stress, the energy is at a minimum for $\varepsilon = 0$ and then

$$\sigma_{ij}(\varepsilon = 0) = \left.\frac{\partial e}{\partial \varepsilon_{ij}}\right|_{\varepsilon=0} = 0.$$

The leading order terms of the series expansion of the energy are then

$$e(T,\varepsilon) = e^0(T) + \frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl},$$

where $e^0(T) = e(T, \varepsilon = 0)$ is the energy of the unstrained body at temperature $T$. The elastic constants $C_{ijkl}$ entering this expression are thus defined by

$$C_{ijkl} = \frac{\partial^2 e}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}}.$$

This is a fourth-rank tensor which obeys minor symmetry $C_{ijkl} = C_{jikl} = C_{ijlk}$ because of the strain tensor symmetry and also major symmetry $C_{ijkl} = C_{klij}$ because of allowed permutation of partial derivatives. This leads to at most 21 independent coefficients, which can be further reduced by considering the symmetries of the solid body [4].

This series expansion of the energy leads to a linear relation, the Hooke's law, between the stress and the strain

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \tag{4}$$