Lattice-Statics Green's Function Method for Multiscale Modeling of Point Defects and Extended Defects in Solids*

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Summary

A method is described for multiscale modeling of point defects such as vacancies and interstitials at the atomistic level and extended defects such as free surfaces and interfaces at the macroscopic continuum level in a solid. The method is based upon the use of the lattice-statics Green's functions. It fully accounts for the discrete lattice structure of the solid at the atomistic scale near point defects and reduces asymptotically to the macroscopic continuum model for extended defects. A major advantage of the lattice-statics Green's function is that it can model a large crystallite containing a million atoms without excessive CPU effort. Numerical results are presented for the displacement field on the free surface due to a vacancy in fcc aluminum.

Introduction

We describe a computationally efficient lattice-statics Green's-function method for multiscale modeling of point defects such as vacancies and interstitials and extended defects such as free surfaces and interfaces in solids. The method is especially useful for interpreting and analyzing the elastic response of thin films and semi-infinite solids. Our model treats the point defects at the atomistic scale and extended defects at a macroscopic scale in the same formalism. The lattice-statics Green's function accounts for the discrete lattice structure of the solid and is suitable for atomistic modeling of point defects. It reduces asymptotically to the continuum Green's function that we use to model the extended defects. A major advantage of the Green's-function method is that it is semi-analytic, in contrast to the direct computer simulation methods for lattice statics, which are CPU-intensive. Our method can model a large crystallite containing a million atoms without excessive CPU effort. We use our method to calculate displacement fields in a solid that contains both point and extended defects.

The elastic characteristics of thin films and semi-infinite solids depend upon the strains caused by the point defects near the free surfaces and the interfaces. The point defects need to be modeled at the atomistic scale, whereas free surfaces and interfaces can be adequately modeled at a macroscopic scale. The continuum model is not fully reliable for modeling point defects where the discrete atomistic structure of the crystal lattice is very important (see, for example, [1,2]). Experimentally one measures strain near a free surface. In order to interpret the experimental results, one needs a model to calculate the strains caused by the point defects in the presence of the free surface. It is therefore necessary to use a multiscale model that accounts for the discrete lattice structure of the solid near a point defect and the macroscopic effects near an extended defect. This explains the strong topical interest in multiscale modeling of solids.

Recent papers on multiscale modeling are based upon purely numerical techniques using the finite-element method and/or computer simulation of the lattice structure (for an excellent review

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and other references, see [3]). The purely numerical techniques can be very accurate but they are CPU-intensive and not convenient for parametric design studies. The Green's-function method gives accurate results, is computationally convenient, and can provide quick 'what if' answers, which is useful for design of experiments. For the purpose of illustration, we apply our method to calculate the displacement field at the free surface of a semi-infinite aluminum crystal containing a vacancy. This paper is a preliminary report of our ongoing work on multiscale modeling of point defects in thin films of metals and semiconductors. Details will be published elsewhere.

Theory

We consider a monatomic Bravais lattice with a point defect at the origin. We assume a Cartesian frame of reference. We denote the lattice sites by vector indices **l, l'** etc. A vector index **l** has 3 components, denoted by l_1, l_2, and l_3. The three-dimensional (3D) force-constant matrix between atoms at **l** and **l'** is denoted by $\mathbf{f}^*(\mathbf{l}, \mathbf{l'})$. The force on atom **l** and its displacement from equilibrium position will be denoted, respectively, by **F(l)** and **u(l)**, which are 3D column vectors. The displacement vectors **u(l)** at each lattice site give the relaxation of the lattice or the lattice distortion caused by the defect.

The force-constant matrix for each pair of atoms is 3×3. It is obtained from the interatomic potential as follows:

$$[\mathbf{f}^*(\mathbf{l}, \mathbf{l'})]_{ij} = \partial^2 V(x) / \partial x_i \, \partial x_j, \tag{1}$$

where $V(x)$ is the interatomic potential (assumed central) between the pair of atoms **l** and **l'** separated by vector distance **x.** Similarly, the force at the atom **l** due to the atom at the origin at a distance **x** is given by

$$[\mathbf{F(l)}]_i = - \partial V(x) / \partial x_i. \tag{2}$$

Following the method given in [1,2], we obtain

$$\mathbf{u(l)} \; = \; \Sigma_{\mathbf{l'}} \, \mathbf{G}^*(\mathbf{l}, \mathbf{l'}) \, \mathbf{F(l')}, \tag{3}$$

where **G*** is the defect lattice Green's function defined by

$$\mathbf{G}^* \; = \; [\mathbf{f}^*]^{-1}. \tag{4}$$

The sum in eq. (3) is over all lattice sites and Cartesian coordinates, which have not been shown explicitly for notational brevity.

In the representation of lattice sites, $\mathbf{G}^*$ and $\mathbf{f}^*$ are $3N \times 3N$ matrices, where N is the total number of lattice sites in the Born-von Karman supercell. For an infinite perfect lattice in equilibrium without defects, **F(l)** is 0 for all **l** and the force constant and the Green's function

matrices have translation symmetry. We denote these matrices by $\mathbf{f}$ and $\mathbf{G}$ respectively. When a defect is introduced in the lattice, $\mathbf{F(l)}$ becomes, in general, non-zero and the force constant matrix changes. So

$$\mathbf{f}^* = \mathbf{f} - \mathbf{Df},\tag{5}$$

where $\mathbf{Df}$ denotes the local change in the force constant matrix $\mathbf{f}$. From eqs. (4) and (5), we obtain the following Dyson equation

$$\mathbf{G}^* = \mathbf{G} + \mathbf{G}\,\mathbf{Df}\,\mathbf{G}^*,\tag{6}$$

where

$$\mathbf{G} = [\mathbf{f}]^{-1}\tag{7}$$

is the perfect lattice Green's function. In the same representation, we can write eq. (3) in the following matrix notation:

$$\mathbf{u} = \mathbf{G}^*\,\mathbf{F}.\tag{8}$$

Using eq. (6), we rewrite eq. (8) as

$$\mathbf{u} = \mathbf{G}\,\mathbf{F}^*,\tag{9}$$

where

$$\mathbf{F}^* = \mathbf{F} + \mathbf{Df}\,\mathbf{u}.\tag{10}$$

Equation (9) gives the displacement in terms of the perfect-lattice Green's function and an effective force denoted by $\mathbf{F}^*$, the so called Kanzaki force [1]. From eq. (10), we can identify it as the force due to the defect on relaxed lattice sites, in contrast to $\mathbf{F}$, which denotes the force at the unrelaxed original lattice site. Equation (9) is applicable to any point defect such as a vacancy, an interstitial, or a substitutional impurity.

For the perfect lattice, $\mathbf{G(l,l')}$ has translation symmetry and therefore can be labeled by a single index $\mathbf{l\text{-}l'}$. It is calculated by use of the Fourier representation

$$\mathbf{G(l)} = (1/N)\ \Sigma_{\mathbf{q}}\ \mathbf{G(q)}\ \exp[\ \acute{e}\mathbf{q.l}],\tag{11}$$

where $\acute{e} = \sqrt{-1}$, N is the total number of atoms,

$$\mathbf{G(q)} = [\mathbf{f(q)}]^{-1},\tag{12}$$

$\mathbf{f(q)}$ is the Fourier transform of the force-constant matrix, and $\mathbf{q}$ is a vector in the reciprocal space of the lattice. For brevity of notation, we shall use the same symbol for a function and its Fourier transform, the distinguishing feature being the argument of the function. Since $\mathbf{G(q)}$ and $\mathbf{f(q)}$ are 3 × 3 matrices, eqs. (11) and (12) can be used to calculate the perfect-lattice Green's function $\mathbf{G(l,l')}$.

We define the defect space as the vector space generated by l, l' for which $\mathbf{Df}$ is non-vanishing. We solve the Dyson equation for the defect Green's function by using the matrix partitioning technique [1]. The reduced Dyson equation in defect space is given by

$$\mathbf{g}^* = \mathbf{g} + \mathbf{g} \, \mathbf{Df} \, \mathbf{g}^*, \tag{13}$$

where $\mathbf{g}$, $\mathbf{g}^*$ are components of $\mathbf{G}$ and $\mathbf{G}^*$ in defect space. The matrices in eq. (13) are 3n × 3n matrices, where n is the number of atoms in the defect space. For point defects, n is small so eq. (13) can be solved by direct matrix inversion as given below:

$$\mathbf{g}^* = (\mathbf{I} - \mathbf{g} \, \mathbf{Df})^{-1} \mathbf{g}. \tag{14}$$

For example, for an fcc lattice in which the defect interacts up to its second-neighbor atoms, the matrices in eq. (14) are 57 × 57. Since a point defect such as a vacancy retains the local point-group symmetry of the lattice, we can use group theory to simplify eq. (14) considerably. In the above case of a vacancy in an fcc lattice, eq. (14) can be reduced to a 2 × 2 matrix equation. By definition, the force matrix defined by eq. (2) is nonvanishing only in the defect space. Using eqs. (8) and (13), we obtain for all atoms in the defect space

$$\mathbf{u} = \mathbf{g}^* \, \mathbf{F}. \tag{15}$$

After calculating $\mathbf{u}$ for all atoms in the defect space, we calculate the Kanzaki force in the defect space by using eq. (10). Then the displacement of all atoms in the solid is given in terms of the perfect-lattice Green's function by use of eq. (9). The Kanzaki force contains the full contribution of the discrete lattice structure in the defect space.

The perfect-lattice Green's function reduces [1] asymptotically to the continuum Green's function. For this purpose, we make $\mathbf{l}$ and $\mathbf{q}$ continuous variables and replace the summation in eq. (11) by integration over the reciprocal space. In conformity with the continuum model notation, we replace $\mathbf{l}$ by $\mathbf{x}$ for large l, which will denote the position vector corresponding to the lattice site $\mathbf{l}$. Thus, in the limit $x \to \infty$,

$$\mathbf{G(x)} = (1/2\pi)^3 \int \mathbf{G_c(q)} \exp(\acute{e}\mathbf{q.x}) \, \mathbf{dq}, \tag{16}$$

where, keeping terms up to q^2 in $\mathbf{f(q)}$,

$$\mathbf{G_c(q)} = \mathrm{Lim}_{q \to 0} \mathbf{G(q)} = \mathrm{Lim}_{q \to 0} [\mathbf{f(q)}]^{-1} = [\mathbf{L(q)}]^{-1}. \tag{17}$$

In eq. (17), **L** is the Christoffel matrix, defined as follows:

$$\Lambda_{ij}(\mathbf{q}) = c_{ikjl}\, q_k\, q_l, \tag{18}$$

where i,j,k,l, etc. are Cartesian indices that assume the values 1-3, and **c** is the elastic constant tensor. Summation over repeated indices is implied.

Equation (9) is our master equation for multscale modeling. At large distances from the point defect, we replace **G** by the continuum Green's function defined by eq. (17) but use the lattice value of **F*** as defined in terms of the lattice Green's function by eqs. (8) and (9). Thus the displacement field in our multiscale model at the position vector **x** is given by

$$\mathbf{u(x)} = \Sigma_{l'}\, \mathbf{G_c(x\text{-}l')}\, \mathbf{F^*(l')}. \tag{19}$$

Since the distance between the lattice sites in the defect space over which **F*** is distributed is much less than x, $\mathbf{G_c(x\text{-}l')}$ can be calculated in terms of the derivatives of the Green's function.

We incorporate the effect of extended defects in $\mathbf{G_c}$ by imposing appropriate boundary conditions using the standard techniques of the continuum model. As an example, we consider a semi-infinite solid with a free surface. We choose a frame of reference in which the origin and the X- and Y- axes are on the free surface and the positive Z-axis points into the solid. The zero-traction boundary condition at the free surface, which is taken to be the plane at $x_3=0$, is given by

$$\tau_{i3}(\mathbf{x}) = c_{i3jk}\, e_{jk}(\mathbf{x}) = 0 \qquad (x_3=0), \tag{20}$$

where

$$e_{jk} = \partial u_j(\mathbf{x})/\partial x_k. \tag{21}$$

Various computationally efficient representations of the continuum Green's function for anisotropic semi-infinite solids are available in the literature [4,5]. In this paper, since our objective is just to illustrate the multiscale modeling technique, we will assume for simplicity that the solid is elastically isotropic. The solution for the isotropic continuum case was obtained by Mindlin [6]. The result for the displacement field at the free surface at a radial distance r from the origin is quoted below:

$$4\pi u_r/f = -rh/R^3 + \mu r/[(\lambda+\mu)(R-h)R], \tag{22}$$

$$4\pi u_z/f = (R^2 + h^2)/R^3 + \mu/[(\lambda+\mu)R], \tag{23}$$

where we have used cylindrical coordinates; u_r and u_z are, respectively, the radial and the Z-components of the displacement field; f is the magnitude of the force in units of $8\pi\mu\,(\lambda+2\mu)/(\lambda+\mu)$ acting at (0,0,h); λ and μ are the Lame constants; and $R^2 = (r^2 + h^2)$.
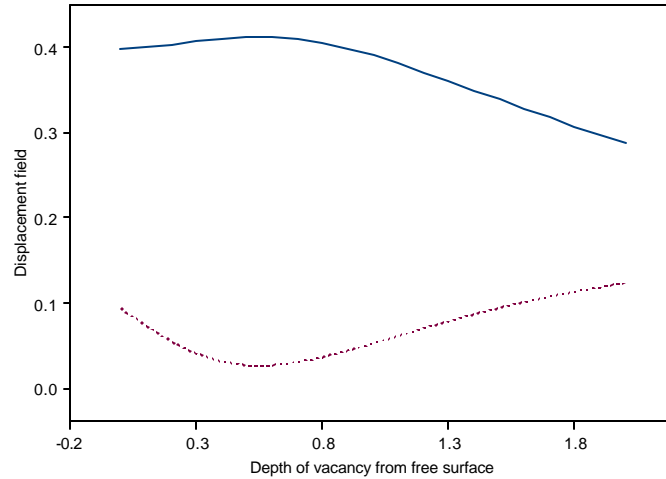
Figure 1 Displacement field at the free surface of fcc aluminum due to a vacancy as a function of h, the depth of the vacancy from the free surface. Solid line- u_z, the Z-component; broken line- u_r, the radial component in cylindrical coordinates.

Results and Conclusions

Figure (1) gives the calculated values of u_r and u_z as a function of h at the free surface (1,0,0) at r=1 due to a vacancy at (0,0,h) in fcc aluminum. We assumed a simple model interatomic potential due to Bullough and Hardy (see [1]) extending up to 2nd neighbors. The lattice-statics Green's function is calculated for a million atom model by use of the method given in [1], which gives **F***. The main conclusion of this paper is that the Green's function method for multiscale modeling can be used to model a large crystallite at the atomistic level without excessive CPU effort and, in the same formalism, include macroscopic defects such as free surfaces.

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