

LATTICE STATICS GREEN'S FUNCTION FOR MODELING OF DISLOCATIONS IN CRYSTALS

V.K. Tewary

Materials Reliability Division, National Institute of Standards and Technology, Boulder, CO 80303, vinod.tewary@nist.gov

INTRODUCTION

We describe a lattice statics Green's function (LSGF) method for modeling of dislocation in crystal lattices. The LSGF method was originally developed for point defects [1]. It has been applied [2,3] to small cracks consisting of 10-50 atoms but, so far, it has not been possible to use this method for large defects such as dislocations or cracks involving several hundred or more atoms [4]. In this paper, we describe a defect space Fourier transform method that enables us to apply the LSGF method to extended defects. This paper essentially describes our work in progress. Only the methodology and some preliminary results are reported here. Details will be published elsewhere.

The LSGF method is based upon the Kanzaki method and uses the Fourier representation of the perfect Green's function. Consequently it is possible to model a large crystallite containing several million atoms within a small CPU effort. Alternative methods for modeling dislocations use direct computer simulation based upon molecular dynamics [5, 6] or quasicontinuum [7]. Both these methods are very powerful and have important advantages. The advantage of the LSGF method is that it gives semi-analytical results for large crystallites and is useful for a quick determination of the basic physical characteristics of the defects. It is also useful for providing starting estimates for a detail calculation using massive computer simulation of complicated defect structures.

BASIC FORMULATION

We consider a monatomic Bravais lattice. We assume a Cartesian frame of reference with an atomic site as origin. We denote the lattice sites by vector indices \mathbf{l}, \mathbf{l}' etc. The 3d force constant matrix between atoms at \mathbf{l} and \mathbf{l}' is denoted by $\phi^*(\mathbf{l}, \mathbf{l}')$. The force on atom \mathbf{l} and its displacement from equilibrium position will be denoted, respectively, by $\mathbf{F}(\mathbf{l})$ and $\mathbf{u}(\mathbf{l})$, which are 3d column vectors.

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

$$\mathbf{u}(\mathbf{l}) = \sum \mathbf{G}^*(\mathbf{l}, \mathbf{l}') \mathbf{F}(\mathbf{l}'), \quad (1)$$

where, the defect Green's function,

$$\mathbf{G}^* = [\phi^*]^{-1}. \quad (2)$$

The sum in eq. (1) is over all lattice sites and Cartesian coordinates which has not been explicitly shown for brevity.

In the representation of the lattice sites, \mathbf{G}^* and ϕ^* are $3N \times 3N$ matrices where N is the total number of lattice sites in the Born von Karman supercell. For a perfect lattice in equilibrium without defects, $F(\mathbf{l})$ is 0 for all \mathbf{l} and the force constant and the Green's function matrices have translation symmetry. We denote these matrices by ϕ and \mathbf{G} respectively. When a defect is introduced in the lattice, $\mathbf{F}(\mathbf{l})$ becomes, in general, non-zero and the force constant matrix changes. So,

$$\phi^* = \phi - \Delta \phi, \quad (3)$$

where $\Delta \phi$ denotes the change in the ϕ . From eq. (3), we obtain the following Dyson equation

$$\mathbf{G}^* = \mathbf{G} + \mathbf{G} \Delta \phi \mathbf{G}^*, \quad (4)$$

where

$$\mathbf{G} = [\phi]^{-1}, \quad (5)$$

is the perfect lattice Green's function.

For the perfect lattice, \mathbf{G} is calculated by using the Fourier representation

$$\mathbf{G}(\mathbf{l}, \mathbf{l}') = (1/N) \sum_{\mathbf{q}} \mathbf{G}(\mathbf{q}) \exp[i\mathbf{q} \cdot (\mathbf{l} - \mathbf{l}')], \quad (6)$$

where

$$\mathbf{G}(\mathbf{q}) = [\phi(\mathbf{q})]^{-1}, \quad (7)$$

$\phi(\mathbf{q})$ 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 notations, we shall use the same symbol for a function and its Fourier transform, the distinguishing feature being the argument of the function. Since $\mathbf{G}(\mathbf{q})$ and $\phi(\mathbf{q})$ are 3×3 matrices, eqs. (9) and (10) can be used to calculate the $\mathbf{G}(\mathbf{l}, \mathbf{l}')$.

We define the defect space as the vector space generated by \mathbf{l}, \mathbf{l}' for which $\Delta \phi$ is non-vanishing. The lattice sites in the defect space will be denoted by λ, λ' . We partition the matrices in eq. (4), and take only their components in the defect space. The Dyson equation in defect space is given by

$$\mathbf{g}^* = \mathbf{g} + \mathbf{g} \Delta \phi \mathbf{g}^*, \quad (8)$$

where \mathbf{g}, \mathbf{g}^* are components of \mathbf{G} and \mathbf{G}^* in defect space. The matrices in eq. (8) are $3n \times 3n$ matrices, where n is the number of atoms in the defect space. For point defects, n is small, so eq. (12) can be solved by direct matrix inversion. For extended defects such as dislocations, cracks, etc., n is quite large. In earlier calculations, eq. (8) is solved numerically by restricting n to less than 50. In the computer simulation work, n is taken to

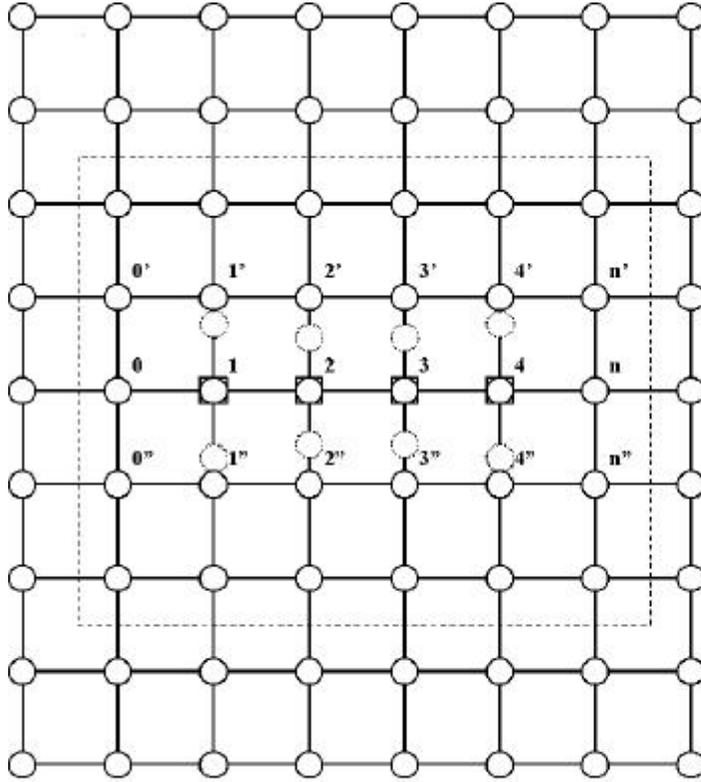


Fig. 1: Defect space for an edge dislocation dipole. Unrelaxed lattice sites are indicated by solid circles. Vacancies are created at sites marked by rectangles covering circles. The defect space consists of all sites inside the dashed rectangle. The end space in this model consists of sites $0, 0', 0''$, and n, n', n'' . The dotted circles show the relaxed positions of the atoms 1-4 calculated using the model given in [3]. The relaxation of other atoms is not shown.

be of the order 10-50, with N to be 50-100, which requires huge CPU effort. In the conventional LSGF method for cracks [3], although N can be 100-1000, n is typically less than 50. These values are unrealistically low. We show that by taking Fourier transform in the defect space, we can solve eq. (8) for $n=1000$ or larger with minimal CPU effort.

Defect space Fourier transform method

We assume that the atoms interact through pair potentials and the interatomic potential is short range. This is a reasonable assumption since even the embedded atom potential that accounts for multibody interactions, can be expressed into an effective dominant short range pair potential. For simple straight dislocations or planar cracks, the defect space has translation symmetry except near the ends. We exploit this translation symmetry in the defect space Fourier transform (DSFT) method for partially diagonalizing the Dyson equation.

Consider an edge dislocation. Although the DSFT method is applicable to 3d, for the sake of illustration in the present paper, we consider an infinite straight dislocation that makes the problem 2d. Following Volterra's construction, we create a half plane of vacancies, pull the atoms across the vacancy plane together by a distance u_c and bond them. Then we allow the lattice to relax to its new equilibrium position.

Figure 1 illustrates the model. Instead of a single edge dislocation, we create a dislocation dipole so that the sum of all forces in the lattice is 0. A single dislocation implies unbalanced forces at the ends which makes the lattice unstable and introduces singularity in the displacement field. Atoms 1 - 4 are the created vacancies. The defect space includes all atoms in the box, 0-n, 0'-n', and 0''-n''. Notice that the defect space has translation symmetry except for the end atoms, 0,1, 4,n, and the corresponding primed and double primed atoms.

The displacement field for atoms in the defect space is given by

$$\mathbf{u}(\lambda) = \mathbf{u}_c + \mathbf{v}(\lambda) \quad (9)$$

where \mathbf{u}_c constant for all λ . We determine \mathbf{u}_c by a minimization procedure and \mathbf{v} by solving the Dyson equation. The determination of \mathbf{u}_c includes nonlinear effects. We assume $\mathbf{v}(\lambda)$ to be small and neglect cubic and higher order terms in v .

We write

$$\Delta\phi(\lambda, \lambda') = \Delta\phi_0(\lambda, \lambda') - \delta\phi(\lambda, \lambda'), \quad (10)$$

$$\mathbf{F}(\lambda) = \mathbf{F}_0 + \mathbf{f}(\lambda), \quad (11)$$

where \mathbf{F}_0 and $\Delta\phi_0(\lambda, \lambda')$ are have translation symmetry. Hence, \mathbf{F}_0 is independent of λ and $\Delta\phi_0(\lambda, \lambda')$ depends upon λ , and λ' only through their difference. The end correction is given by $\mathbf{f}(\lambda)$ and $\delta\phi(\lambda, \lambda')$ which are non-vanishing only for atoms at the ends of the defect space. The atomic sites at the ends constitute the end space.

We introduce Fourier transforms in the defect space as follows

$$\Delta\phi_0(\lambda, \lambda') = (1/n) \sum_{\mathbf{k}} \Delta\phi_0(\mathbf{k}) \exp[i\mathbf{k} \cdot (\lambda - \lambda')] \quad (12)$$

$$\mathbf{g}(\lambda, \lambda') = (1/n) \sum_{\mathbf{k}} \mathbf{g}(\mathbf{k}) \exp[i\mathbf{k} \cdot (\lambda - \lambda')] \quad (13)$$

where \mathbf{k} takes n values between $-\pi$ and $+\pi$ such that $k \cdot \lambda(n)$ is a multiple of π . The DSFT of the Green's function is given by

$$\mathbf{g}(\mathbf{k}) = \sum_{\lambda} \mathbf{g}(\mathbf{0}, \lambda) \exp(i\mathbf{k} \cdot \lambda), \quad (14)$$

or

$$\mathbf{g}(\mathbf{k}) = (1/N) \sum_{\mathbf{q}} \mathbf{G}(\mathbf{q}) \mathbf{M}(\mathbf{k}, \mathbf{q}), \quad (15)$$

where \mathbf{M} is a projection function that projects the Green's function from the reciprocal space of the lattice to that of the defect space. It is given by

$$\mathbf{M}(\mathbf{k}, \mathbf{q}) = \sum_{\lambda} \exp[i(\mathbf{k} - \mathbf{q}) \cdot \lambda]. \quad (16)$$

In general, the lattice sum in eq. (16) can be obtained analytically. It gives a discrete analogue of the Hilbert transform.

Using eq. (10) in eq. (8), and partitioning the matrix in the end space, we obtain for the Dyson equation in the end space

$$\mathbf{g}^* = \mathbf{g}_d - \mathbf{g}_d \delta\phi \mathbf{g}^* \quad (17)$$

where

$$\mathbf{g}_d = [\mathbf{I} - \mathbf{g} \Delta\phi_0]^{-1} \mathbf{g} \quad (18)$$

We evaluate \mathbf{g}_d using DFST given by eqs. (12) and (13) and then solve eq. (17) in the defect space by using matrix partitioning technique [1].

Results of a preliminary calculation are shown in Fig. 1. For these calculations, we assumed the same force constant model as given in [3]. Only the displacement field for atoms 1-4 in the defect space has been shown in Fig. 1. The displaced positions of these atoms are shown as dotted circles.

CONCLUSIONS

To summarize, the main advantage of the LSGF method using DSFT is that it is semianalytic which allows to model large crystallites and large defects with minimal CPU effort - even for 3d dislocation problems. It can account for nonlinear effects locally in the defect space but assumes the harmonic approximation for atoms outside the defect space. Since the method involves independent sums over \mathbf{q} and \mathbf{k} space, the the computational program can be easily vectorized if needed. The main disadvantage of our method is that it can not give time evolution of the equilibrium and is limited to simple defect structures.

REFERENCES

1. V. K. Tewary, Green's function method for lattice statics, Adv. Phys. **22**, p757 (1973).
2. R. Thomson, S.J. Zhou, A.E. Carlsson, and V.K. Tewary, Lattice imperfections studied by use of lattice Green's functions, Phys. Rev. **B46**, p 10613 (1992).
3. V.K. Tewary and R. Thomson, Lattice statics of interfaces and interfacial cracks in bimaterial solids, J. Mater. Res. **7**, p1018 (1992).
4. A.E. Carlsson and R. Thomson, Fracture toughness of materials: From atomistics to continuum theory, Solid State Physics **51**, p233 (1998).
5. P. Vashishta, A. Nakano, R.K. Kalia, et. al. Crack propagation and fracture in ceramic films- Million atom molecular dynamics simulations on parallel computers, Mat. Sci. Eng.-Solids **B37**, p56 (1996).
6. R. Pasionot, D. Farkas, and E.J. Savino, Dislocation core structure in ordered intermetallic alloys, J. Physique III **1**, p997 (1991).
7. E.B. Tadmor, M. Ortiz, and R. Phillips, Quasicontinuum analysis of defects in solids, Phil. Mag. **A73**, p1529 (1996).