Elastic Green's function method for multiscale modeling of point defects and extended defects in solids

Multi-scale model – discrete lattice structure near a point defect and continuum model near a free surface or interface in the same formalism.

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Motivation

Properties of thin films and semi-infinite solids sensitive to concentration of vacancies near a free surface or interface between film and substrate

Examples

- Solid-state lighting devices using III-V semiconductors
- Diffusion near grain boundaries in Copper interconnects

Measurable quantity- strain at or near a free surface

Strains are caused by point defects

Strain – a macroscopic quantity defined in the continuum model.

Continuum model applicable to extended defects such as free surfaces and interfaces

Lattice model very difficult near an extended defect- too much disorder; probably not really needed.

Lattice distortion due to point defects sensitive to discrete lattice structure near the defect- continuum model not valid

Need for a multi-scale model – discrete lattice structure near a point defect and continuum model near a free surface or interface in the same formalism.

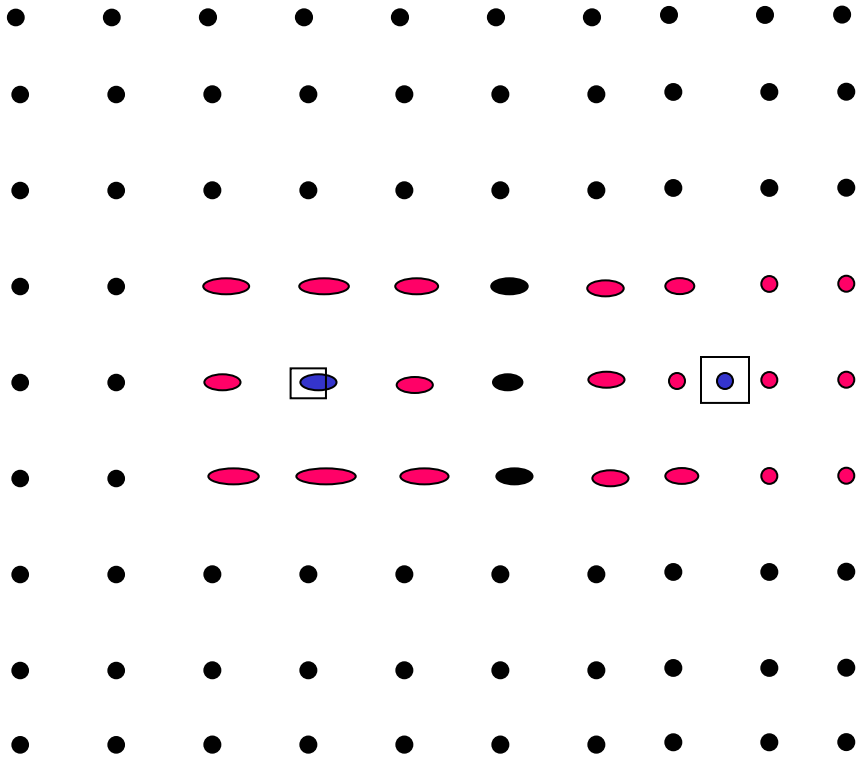
Lattice statics Green's function for point defects.

Lattice statics GF reduces to continuum model GF asymptotically

Continuum GF for extended defects

Objective: To calculate lattice distortion, strains, relaxation energy, change in phonon spectra due to defects, and elastic interaction between the defects

Point defects in a Crystal Lattice



l, l’ - lattice sites (monatomic Bravais)

ϕ (**l, l’**)– 3d matrix – force constants

Obtained by the first and second derivatives of the interatomic potential

F(l) – Force on atom at l

Obtained by the first derivative of the interatomic potential

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

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

- Born- von Karman model
- Pair potential
- Cyclic boundary conditions
- Supercell

u(l) - displacement of the atom at **l**

$$W = - \Sigma \, \mathbf{F(l)} \, \mathbf{u(l)} + (1/2) \, \Sigma \, \phi^{*}(\mathbf{l}, \mathbf{l'}) \, \mathbf{u(l)} \, \mathbf{u(l')}$$

Static displacement

$$\partial W / \partial \, \mathbf{u(l)} = 0$$

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

$$\mathbf{u = G^{*} F}$$

Lattice-statics Green's function

$\mathbf{G}^* = [\phi^*]^{-1}$ 3N x 3N matrices

Relaxation energy: $W = -(1/2)\,\mathbf{F}\mathbf{G}^*\mathbf{F}$

Static interaction energy
between "a" and "b"

$W_{a,b} = W_{a+b} - W_a - W_b$

Thermodynamic interaction energy- Free energy.

Force Const for perfect lattice ϕ

$\phi^* = \phi - \Delta\phi,$

$\mathbf{G^* = G + G\,\Delta\phi\,G^*,}$

where

$\mathbf{G = [\phi]^{-1}}$

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

$\mathbf{u = (G + G\,\Delta\phi\,G^*)\,F}$

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

$\mathbf{F^* = F + \Delta\phi\,u.}$ **Kanzaki Force**

G(l,l') has translation symmetry

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

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

Solution of the Dyson equation

F and $\Delta\phi$ nonvanishing only in defect space- matrices of finite dimensions

$$\Delta\Phi \;=\; \begin{bmatrix} \Delta\phi & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{g}^* = \mathbf{g} + \mathbf{g}\,\Delta\phi\,\mathbf{g}^*$$

$$\mathbf{g}^* = (\mathbf{I} - \mathbf{g}\,\Delta\phi)^{-1}\mathbf{g}$$

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

Calculate **u** in defect space

Calculate Kanzaki force in def space

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

G reduces to cont GF for large l

Replace sum by an integral

Treat **l** and **q** as continuous variables

Write **x** for position vector of site **l**

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

$$\mathbf{G_c(q)} = \mathrm{Lim}_{q\to 0}\, \mathbf{G(q)} = \mathrm{Lim}_{q\to 0}\, [\phi(\mathbf{q})]^{-1}$$

$$= [\Lambda(\mathbf{q})]^{-1}.$$

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

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

$G_c(x-l')$ can be calculated in terms of the derivatives of the continuum Green's function.

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

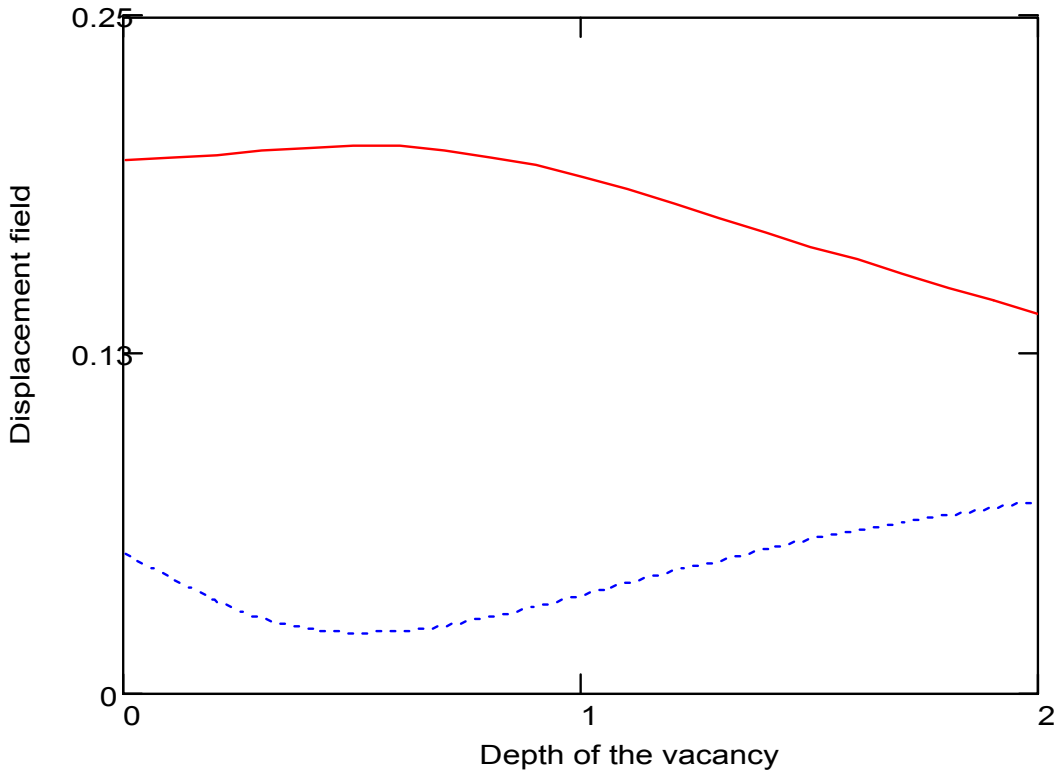
$e_{jk} = \partial u_j(\mathbf{x})/ \partial x_k$

Efficient methods for calculating GF and derivatives for anisotropic solids are available

Mindlin solution for isotropic solids

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

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



- MSGF method can model a large crystallite at the atomistic level without excessive CPU effort
- In the same formalism, include the extended defects using the standard techniques of the continuum model.