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Calculation of atomic and electronic structures of dislocations in Si: Nonorthogonal TBMD method

K. Masuda-Jindo [a], M. Menon [b] and K. R. Subbaswamy [b]

[a] Department of Materials Science and Engineering, Tokyo Institute of Technology Nagatsuta, Midori-ku, Yokohama, 227, Japan
[b] Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, U.S.A.

The atomic configurations and electronic states of dislocations in covalent semiconductor Si are calculated by using the improved nonorthogonal tight-binding molecular-dynamics (TBMD) method. This nonorthogonal TB theory, with only two adjustable parameters, gives values of the energies and bonding distances which are in excellent agreement with the ab initio results for Si clusters of size up to N=10. We apply this scheme for the calculations of core structures of dislocations in bulk Si as well as those in the Si clusters. Using the atomic configurations and electronic states of the dislocations, we discuss the size dependence of the dislocation core structure and related mechanical properties of Si clusters.

1. INTRODUCTION

It has been well established that the dislocation mobility in semiconductors is affected quite significantly by doping of electrically active impurities [1]. On the other hand, dislocation motion in covalent semiconductors (e.g., Si, SiC, GaAs, InP, etc) is strongly enhanced by irradiation by electron beam or laser light [2]. The observed exitation enhancement of the dislocation motion can be interpreted in terms of the reduction in activation energy of non-radiative recombination of injected carriers at the dislocation core. In the present study, we focus our attention to the electronic states associated with dislocations in covalent semi-conductors. We calculate the atomic configurations and local electronic states of dislocations in C and Si using the TB molecular dynamics method [3-6]. Using the calculated electronic states of the dislocations, we also discuss the effects of impurity doping and non-radiative recombination of the injected carriers on the dislocation motion in the semiconductors.

2. PRINCIPLE OF CALCULATIONS

The total energy of the system is given by the sum [3-6]

$$U = U_{el} + U_{rep}, \qquad (1)$$

where U_{el} is the sum of the one-electron energies ε_k for the occupied states,

$$U_{el} = \Sigma_{\mathbf{k}} \varepsilon_{\mathbf{k}}, \qquad (2)$$

and U_{rep} is given by a repulsive pair potential

$$U_{rep} = (1/2) \Sigma_i \Sigma_j \phi(r_{ij}), \qquad (3)$$

Here R_{ij} is the separation of atoms i and j. The repulsive potential $\phi(r)$ is taken to be short ranged and varies exponentially with the interatomic distance. To fix absolute energies either a constant or a coordination dependent energy term is added to eq.(1).

In the nonorthogonal TB scheme the characteristic equation is written, in matrix form, as

$$(\mathbf{H} - E_n \mathbf{S})\, \mathbf{C}_n = 0, \qquad (4)$$

where $\mathbf{C}_n$ is a column vector of LCAO coefficients. **H** is the Hamiltonian matrix and **S** the overlap matrix, of the LCAO basis set.

The Hellmann-Feynman theorem for obtaining the electronic part of the force can be obtained from

$$\partial E_n/\partial x = C_n[\partial H/\partial x - E_n \partial S/\partial x]C^n/C^{n*}SC^n, \qquad (5)$$

The $\mathbf{C}_n$ are normalized so that

$$\mathbf{C}^{n*}\mathbf{S}\mathbf{C}^n = 1. \qquad (6)$$

In the conventional TB (orthogonal) approach, the basis set is presumed to be an orthogonal set, $S_{ij} = \delta_{ij}$. In the Slater-Koster scheme the Hamiltonian matrix elements are given in the two-center forms, which are assumed to decrease exponentially with the interatomic distance r. The scaling of the two-body repulsive term is also taken to be exponential.

The eigenvalues of a system with nonorthogonal basis set can then be obtained from

$$\det | H_{ij} - ES_{ij} | = 0. \qquad (7)$$

Evaluation of (7) is expedited by the use of the well known Cholesky factorization in which **S** is factored into

$$\mathbf{S} = \mathbf{B}\mathbf{B}^{+}. \qquad (8)$$

This factorization is always possible provided **S** is positive definite.

3.RESULTS AND DISCUSSIONS

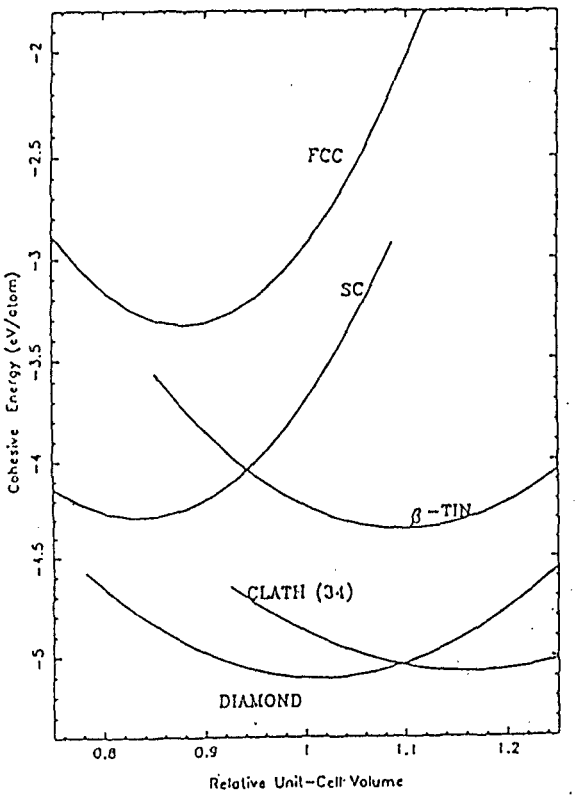

Fig.1 The cohesive energies of various structures of Si using the present scheme.

In Fig.1, we present the zero-temperature phase diagram for silicon obtained by the present method. Compared to the higher coordinated structure, the diamond structure is lower in energy. We have found that inclusion of nonorthogonality is crucial in correctly differentiating the clathrate and diamond structures, which are so close energetically.

We have performed the non-orthogonal basis TB-MD simulations of the atomic configurations for 90° and 30° partial dislocations in covalent semiconductors C, Si and Ge. The similar calculations have also been performed for small clusters composed of ~ 150 atoms. In Fig.2, we present the calculated atomic configurations of a 90° partial dislocation in a Si crystallite composed of 142 Si atoms. It is interesting to note that reconstruction defects "soliton" often appears in the central region of the small Si cluster. This is due to the fact that atomic reconstruction starts from the both ends of the finite dislocation line, and propagate to the central region of the cluster. Therefore, one dangling bond often remains unreconstructed at the central region of the cluster, which has no dangling bonds coupled with.

The electonic structures of the dislocation are calculated by using the sp^3s^* basis recursion method [3,4]. We have found that the atomic configurations calculated by conventional TB-MD method is almost identical to those obtained by the non-orthogonal TB-MD, except for minor changes in the heavily distorted bond region. Both for 90° and 30° partial dislocations in Si, we have found that point like singularities "solitons" in the dislocation core can produce prominent deep levels in the band gap, and they are expected to act as (non-radiative) recombination centers of the injected carriers: Kink sites do not produce prominent deep levels. The latter is a consequence of the fact that there are four nearest-neighbour atoms (around kink site atom) and cancellation of the electronic effects occurs from compressed and stretched bonds.

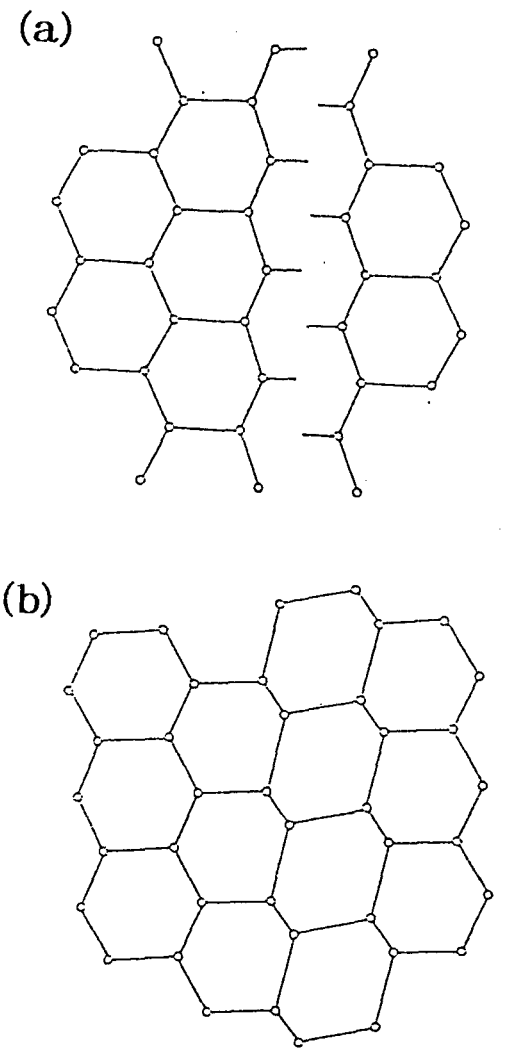

Fig.2 Calculated atomic configuration of dislocation in Si cluster. (a) unreconstructed, (b) reconstructed.

These theoretical findings are in agreement with the experimental results that the observed reduction in the activation energy (0.68-0.82 eV for intrinsic Si) of the enhanced dislocation motion under irradiation of electron beam or laser light corresponds to the deep energy levels associated with the straight dialocation sites (rather than the kink sites) [2].

Furthermore, because of the higher density of "soliton" in the small cluster, it may be concluded that small semiconductor clusters can be deformed more easily, compared to the bulk crystal, via the enhanced dislocation motion.

Fig.3 Atomic displacements u_0 and u_1 at temperature kT/ε_0 =0.4 and 0.6.

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