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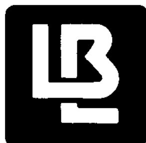

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THEORETICAL STUDY OF STACKING FAULTS IN SILICON

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The *ab initio* pseudopotential method within the local density functional formalism is applied to study stacking faults along the [111] direction in silicon. This is the first case where the stacking fault energy is obtained from first principles and found to be in reasonably good agreement with experimental values. The Hellmann-Feynman theorem is used to study the forces on atoms near the fault. Defect states are found within the energy gap region.

1. Introduction

The electronic and structural properties of defect states in semiconductors have attracted a lot of interest in the recent years. Most studies have concentrated on bond-breaking defects such as vacancies and dislocations. In contrast, there are rather few investigations of the stacking faults in semiconductors because of experimental and theoretical difficulties. The experimental stacking fault energies in silicon along the [111] direction are very small (about 50-60 erg/cm^2)[1,2] since the energy difference comes from the third nearest neighbor arrangement and the systems are only slightly disturbed compared to other bond-breaking defects. There has not been a complete study for the total energy of the silicon stacking faults from first principles[3,4]. A recent charge collection scanning electron microscopy experiment on an extrinsic stacking fault in n-type silicon has suggested the existence of defect states with energies about 0.1 eV below the conduction band minimum[5]. Photoluminescence spectra of plastically deformed silicon suggested a stacking fault state near 0.15 eV above the valence band maximum[6].

In this study, the stacking fault energy is evaluated using the *ab initio* pseudopotential method[7] within the local-density-functional formalism[8]. The tendency of the atoms to relax near the faults is studied by using the Hellmann-Feynman theorem to calculate the forces. The possible existence of defect states in the gap region is also examined.

2. Calculations

The stacking pattern along the [111] direction in a perfect diamond crystal is AA'BB'CC'. Stacking faults correspond to errors in the stacking sequence without any bond-breaking mechanism. For example, the intrinsic stacking fault (ISF) is obtained by removing a pair of atomic planes from the ideal stacking sequence,

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while the extrinsic stacking fault (ESF) is produced by inserting an additional pair of atomic planes (e.g. AA' between BB' and CC'). The atomic positions in the (110) plane are shown in Fig. 1. When passing a fault plane (dashed line in Fig. 1), the orientation of the Si-Si bond is rotated 120 degrees from its normal direction. As a consequence, for the atoms near a fault, e.g., atom *a* in Fig. 1(a) and atoms *a* and *d* in Fig. 1(b), the numbers of first and second nearest neighbors are not changed, but the number of third nearest neighbors is reduced from 12 to 9 with one additional neighboring atom at a distance slightly larger than the second nearest neighbor distance.

We use the geometries of Fig. 1 to calculate the total energies of the ISF and the ESF. The total energy includes the ion-ion, electron-ion, and electron-electron interaction energies. The exchange-correlation functional is approximated by the functional form of Perdew and Zunger[9], which is based on the electron gas calculations of Ceperley and Alder[10]. The one-particle equation is solved self-consistently using a plane wave basis set. The super-cell method is used to maintain the periodicity of the crystal. For the ISF (ESF), 10 (14) atoms are included in the hexagonal super cells with the group symmetry D^3_{3d}. The perfect crystal is also studied in the same symmetry with 6 atoms per cell. The total energies of the perfect crystal and of the crystal with stacking faults are compared to obtain the stacking fault energy. Since the number of atoms per cell is different in each case and an extremely small energy difference is calculated, care is needed in the sampling of k points in the irreducible zone. The grid in the xy plane is chosen to be the same for all cases, while the grid along the z direction is determined according to the relative number of atomic layers in a unit cell. Plane waves with $(k+G)^2$ up to 10 Ryd are included in the calculation. This corresponds to about 70 plane waves per atom. The force at each atom is calculated using the Hellmann-Feynman theorem.

3. Results

The total energies of the perfect crystal with various lattice constants are studied first in this super cell geometry. The minimum energy is found to be at a lattice constant of 5.41 Å, which is very close to the experimental lattice constant 5.43 Å. The following results are all obtained at this calculated lattice constant. The calculated stacking fault energy is 2.3 mRyd per cell for the ISF and 1.5 mRyd for the ESF. These correspond to 40 erg/cm^2 and 26 erg/cm^2 for the ISF and ESF respectively. The error resulting from the finite number of plane waves and k points is estimated to be 20%. The experimental values which are extracted using elasticity models vary from 50 to 60 erg/cm[1,2]. The calculated stacking fault energies are within a factor of two compared to the experimental values. This is the first time that stacking fault energies are obtained from a first-principles calculation.

The forces on each atom near the faults in the ideal geometry is shown in

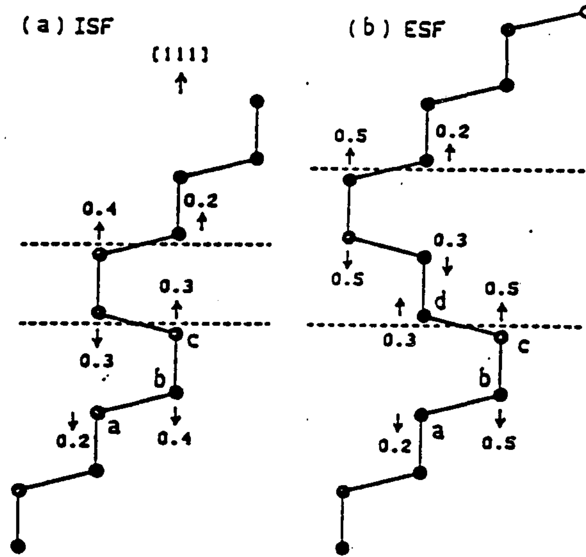

Fig. 1 Atomic positions in the (110) plane of Si for (a) ISF and (b) ESF. The dashed line indicates a stacking fault plane. The net force on each atom in this ideal geometry is marked in units of 10^{-2} Ryd/a.u.

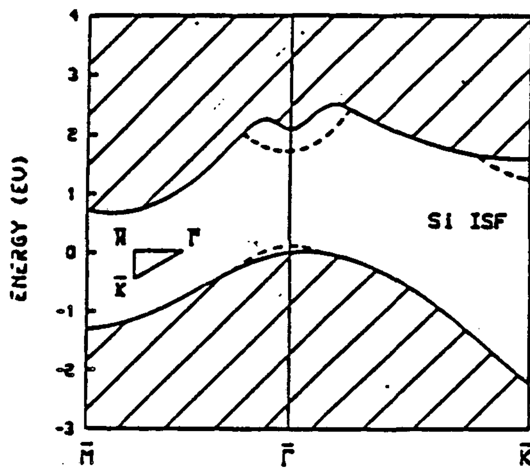

Fig. 2 The energy dispersions of the defect states (dashed lines) for the ISF in the two dimensional Brillouin zone perpendicular to the [111] direction. The shaded region is the projected bands of the perfect crystal. The valence band maximum is set equal to zero.

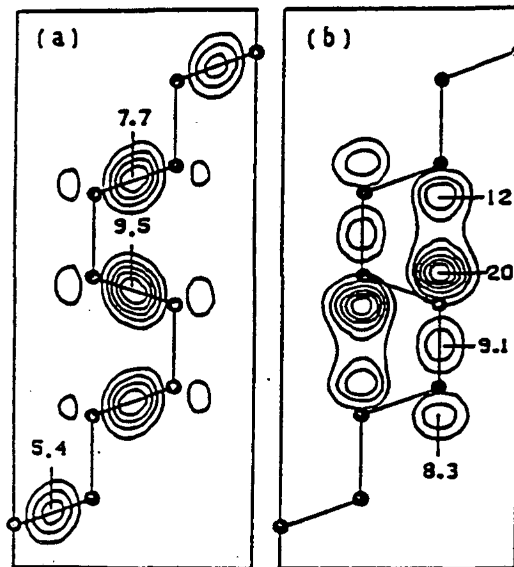

Fig. 3 Charge density of the ISF states at $\bar{\Gamma}$ with energies (a) 0.1 eV above the valence band maximum, and (b) 0.3 eV below the conduction minimum. The charge density is in units of electron per cell volume and is normalized to one electron per cell. The contours are drawn in the interval of (a) 1.5 and (b) 3.0.

Fig. 1. Since the three-fold rotational symmetry around the [111] axis is maintained, the only forces existing are along the [111] direction. The atoms belonging to the same double layer near the fault, e.g., atoms *b* and c in Fig. 1(a) and 1(b), tend to stretch the covalent bond between them. The atoms belonging to different double layers, e.g. atoms *a* and *d* in Fig. 1(b), also tend to repel each other. Therefore the fully relaxed unit cell would have a larger length along the [111] direction.

The calculated band structure in the two dimensional Brillouin zone is plotted in Fig. 2 for the ISF. The projected bands in the [111] plane of the perfect crystal are shaded in the figure. Defect states in the gap region associated with stacking faults are found near $\bar{\Gamma}$ and $\bar{K}$. There are two states in the gap for the ISF at $\bar{\Gamma}$. One is a two-fold degenerate state about 0.1 eV above the valence band maximum; another state is about 0.3 eV below the conduction band minimum. The former level position is consistent with the photoluminescence spectrum finding[6]. The charge density of these states for the ISF is plotted in Fig. 3. The state above the valence band maximum is a bonding state with higher charge density concentrated between fault atoms as is shown in Fig. 3(a). The state below the conduction band minimum is basically an anti-bonding state also with charge accumulated near the fault atoms. However, this state has energy higher than the indirect band gap and may be detected only in momentum dependent experiments. Defect states in the ESF are found at similar positions to those of the ISF.

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