ELECTRONIC ENERGY OF HEXAGONAL SITE SELF-INTERSTITIAL IMPURITY IN SI

by

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(Received 12th October,1986)

A point defect electronic structure calculation with the superlattice model in conjunction with the pseudopotential electronic structure calculation is described. The electronic energy variation of Si caused by self-interstitial impurity at the hexagonal site is investigated. Up to the bottom of the conduction band there are three main point defect-related states: a hyperdeep state at the bottom of the valence band, an s-like resonance near the middle of the valence band and a p_z-like bound state in the gap near the top of the valence band.

Introduction

Self-interstitial impurities in silicon have been studied extensively at different high-symmetry sites in the unit cell [1-5]. In this work we set out to describe the particular features of the electronic energy scheme of the hexagonal site (H) self-interstitial impurity.

Figure 1 shows a cube from the diamond structure. The points denoted by stars are those which have high symmetry and can be occupied by impurities. The letter A shows the host atom position; its point group is T_d. This point is an appropriate site for a substitutional impurity.The letter B denotes the bond centred atom position. If an impurity is situated at this point, it causes considerable distortion. Its point group is D_{3d}.

ISBN 963 481 610 X

Acta Phys. et Chem. Szeged 32 9-15 (1986)

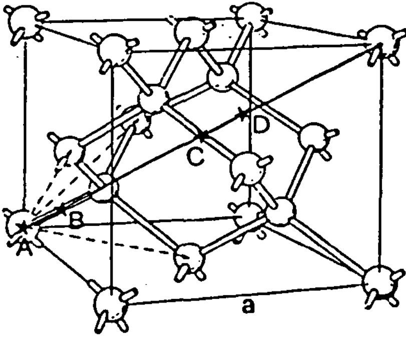

Figure 1: A cube from the diamond structure with highly symmetric points along the diagonal.

The letter C denotes the tetrahedral or antibonding site; its point group is also T_d. The letter D denotes the hexagonal site; its point group is D_{3d}. We examined the electronic structure of Si when the self-interstitial impurity is at the H site.

Model

Superlattice model: the host lattice is superimposed by another lattice which contains the impurities, and a cell is chosen in this lattice (host+impurity). If the impurity lattice constant is larger then the original one, then the impurities are distant from each other and the interactions between them are relatively small.

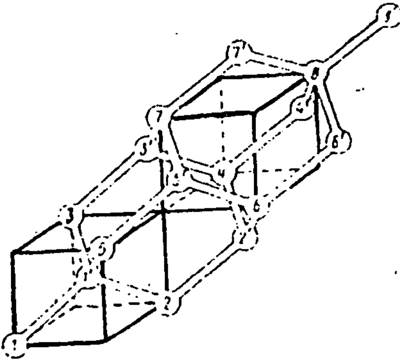
Figure 2: The atomic positions in the chosen cell.

The chosen cell is shown in Figure 2. We selected a FCC impurity lattice with doubled unit vectors (Si_{II}): in this case the cell contains sixteen host atoms and one impurity in the middle.This system retains translational symmetry, as the impurities are repeated periodically. Accordingly any method can be used which is appropriate for periodic systems. To calculate the electronic structure we used the self-consistent pseudopotential method.

Method

It is well known from elementary solid-state physics that there are numerous cases when it is not necessary to know the detailed description of the core electrons [6]: in these cases a pseudopotential can be used to simplify the calculations. The pseudopotential is determined for ions and it can be used as a starting potential for valence electronic structure calculations relating to the solid state.

Figure 3 shows the flow-chart of the procedure [7] leading to a self-consistent screening potential in response to a given structural model.

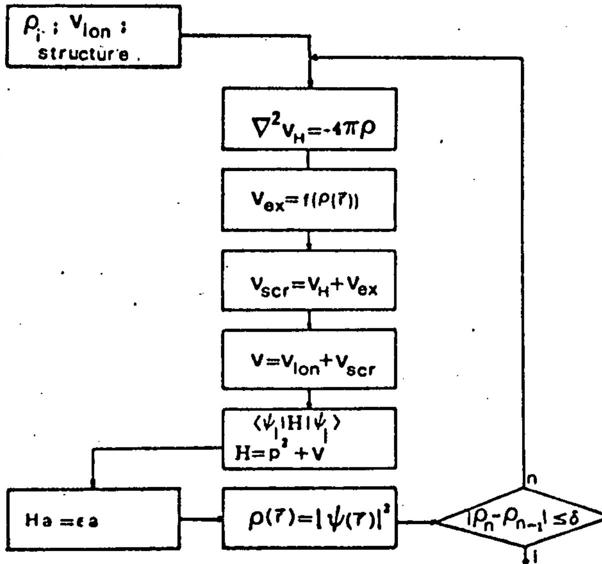

Figure 3: Flow-chart of the calculation

The following input system is required for a calculation:
The structure: the atomic positions in the coordinate system (as mentioned above, we used the FCC lattice).
V_{ion}: we used the soft-core Appelbaum-Hamann pseudopotential for Si^{4+} [8]. The Fourier transform of this potential is:

$$V(q)=2/\Omega_{at}U(q)\exp(-q^2/(4\alpha)) \quad (1)$$

$$U(q)=-4\pi Z/q^2+(\pi/\alpha)^{3/2}(v_1+(3/(2\alpha)-q^2/(4\alpha^2))v_2) \quad (2)$$

where v_1=3.042, v_2=-1.372 and α=0.61. If this potential is applied to the atomic sites, then the ionic potential can be written in the form:

$$V_{ion}(\bar{G}) = \sum_{\bar{G}} S(\bar{G}) V_{ion}^{at}(\bar{G}) \qquad (3)$$

where

$$S(\bar{G}) = 1/M \sum_{\bar{R}} \exp(-i\bar{G}\bar{R}) \qquad (4)$$

is the structure factor, which demands a knowledge of the atomic positions in the cell.

ρ_i: this is the initial value of the charge density. For pure Si, we chose the first component of the charge density to be equal to the number of valence electrons in the cell; the others were taken as 0. For the doped Si, the initial value of the charge was the self-consistent charge density of pure Si.

In the second step, we solved the Poisson equation to obtain the Hartree part of the potential.

For the exchange part of the potential, we used the Xα approximation with α=0.76. Summing up these two potentials, we obtained the screened electronic part of the potential.

Adding to this the ionic part, we found the pseudo-crystal-potential.

The pseudo-wavefunction was expanded on a plane wave basis:

$$\Psi^n(\bar{k},\bar{r}) = \sum_{\bar{G}} a_{\bar{k}}^n(\bar{G}) \exp(i(\bar{k}+\bar{G})\bar{r}) \qquad (5)$$

To obtain convergence results, the kinetic energy cutoff was about 100.68 eV (7.4 Ry) for pure Si, and this cutoff was used for Si_{II} also. About 700 plane waves were used for Si_{II}.

To calculate the charge density, an average is required over the Brillouin zone. We used the mean-value or representative-point technique [9] with $\bar{k}=2\pi a^{-1}(2/3,0,0)$.

Results

We first made test calculations on pure Si. Figures 4a and b show the electronic structure together with degenerations of Si_I and Si_{II}, respectively. The Si_{II} $E(\bar{k})$ curves contain 32 valence bands filled by two electrons. The shaded part of the Figure is the band gap.

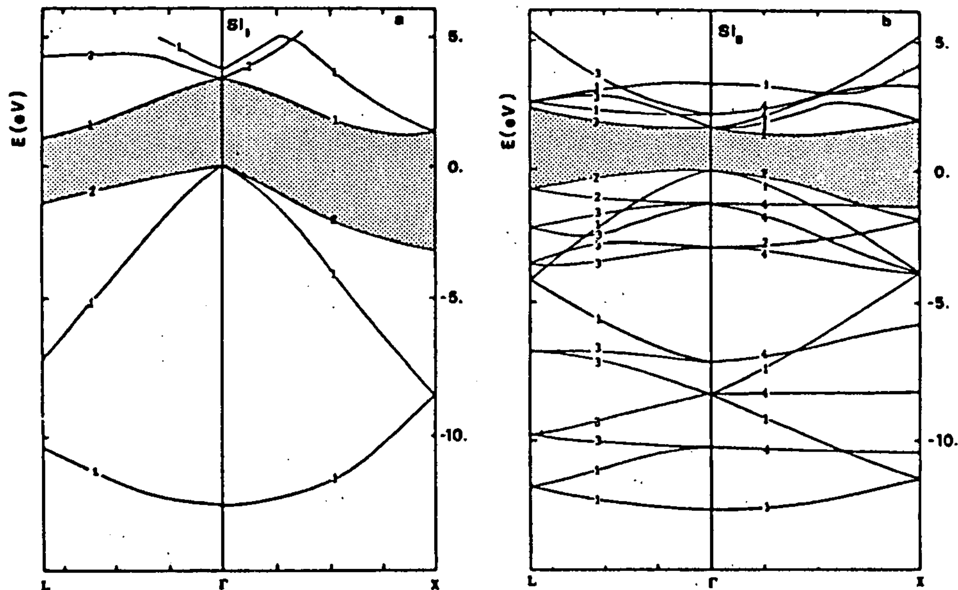

Figure 4: The E(k) curves for Si with a two atomic unit cell (a) and with a sixteen atomic unit cell (b).

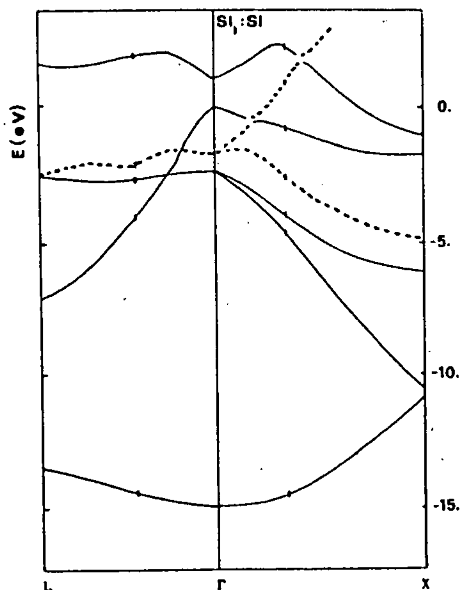

Figure 5: The electronic structure of Si with a self-interstitial impurity at the H site.

We studied the interactions between the impurities. We took a normal Si cell and placed a self-interstitial impurity at the hexagonal site. This gave the electronic structure shown in Fig. 5. The decreasing symmetry along the Γ-X axis caused the degeneration of the bands to decrease and an impurity-related band arose. Due to the interaction of the extra atoms, the dispersion of this band was very great. The band gap disappeared and a metallic like electronic structure resulted. The bottom of the valence band remained almost the same, but the top was changed drastically.

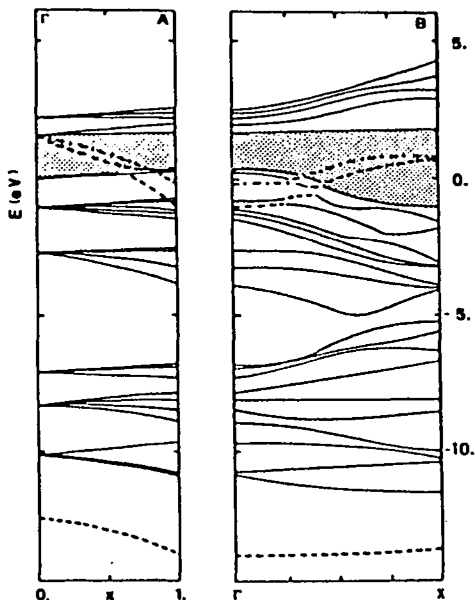

Figure 6: The electronic structure of Si_{II} : Si_H along the Γ-X axis (B); the identification of the impurity-related states (A).

Figure 6B shows the band structure of Si_{II} : Si_H along the Γ-X axis. The impurity-related states are indicated by dashed and dashed-dotted lines. There is an s-like hyperdeep level below the valence band, an s-like resonance in the valence band (dashed lines), and a p_z-like state near the top of the valence band (dashed-dotted line). The dispersion of the impurity-related bands is inherent in our method.

Figure 6A depicts one of the methods we used for the identification of impurity-related states. With the help of a switching parameter, we solved the eigenvalue problem of the following Hamiltonian:

$$H(x,\bar{r})=p^2/(2m)+V^p(\bar{r})+x(V^d(\bar{r})-V^p(\bar{r})) \qquad (5)$$

where $V^p(\bar{r})$ and $V^d(\bar{r})$ are the pure and the doped Si crystal potentials, respectively; $0 \leq x \leq 1$. x=0 gives the pure Si, and x=1 gives the doped Si states. It can bee seen from the left panel that at the hexagonal site two states are depressed from the conduction band and the results are the above-mentioned states.

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ЭЛЕКТРОННАЯ ЭНЕРГИЯ Si МЕЖДОУЗЛИЯ В КРЕМНИИ В ТОЧКЕ ГЕКСАГОНАЛЫ

Г.Папп, П.Богуславски и А.Балдерески

Описываются рассчеты электронной структуры точечного дефекта в модели суперрешетки методом псевдопотенциала. Исследуются изменения электронной структури кремния за счет самомеждоузлия в точке гексагоналы. До дна проводимости существуют три состояния связанные с точечным дефектом: гиперглубокое состояние на дне балентной зоны, s типа резонанс близко к середине валентной зоны и связанное состояние типа p_z в запрещенной зоне, близко к потолку валентной зоны.