ISBN 963 481 623 I
Acta Phys. et. Chem Szeged 33 3-10 (1987)

CHANGE CAUSED IN CHARGE DENSITY OF Si BY A HEXAGONAL SITE SELF-INTERSTITIAL

By

G. PAPP[1], P. BOGUSLAWSKI[2] and A. BALDERESCHI[3]

[1] Department of Theoretical Physics, József Attila University Szeged, Aradi vértanuk tere 1., Hungary

[2] Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

[3] Institut de Physique Appliquée, Ecole Polytechnique Federale, Lausanne, Switzerland

Istituto di Fisica Teoretica, Università di Trieste, Italy

(Received 26 April 1987)

The electronic charge density of a self-interstitial at a hexagonal site in Si is investigated. From the results it can be established that the charge density around the self-interstitial atom is metallic-like and the nearest-neighbour bonds are weakened.

Silicon self-interstitials are poorly understood in comparison with other defects (substitutionals or vacancies, for example). Though vacancies and interstitials should be created in equal numbers by irradiation, only vacancies are observed. There is no experimental evidence for the existence of self-interstitials. However, to understand other interstitial impurities, it is instructive to study self-interstitials.

In this paper we present results on the change caused in the charge density of silicon by a self-interstitial at a hexagonal site.

We calculated the electronic structure by using the self--consistent pseudopotential electron-energy approach [1], with the Appelbaum-Hamann soft-core pseudopotential [2]. In this momentum-space formulation, supercells are used to modell the interstitial [3]. The supercell contains sixteen host atoms and a nearest-neighbour - interstitial distance of 7.6 Å. In our calculations a plane wave basis set (about 700 plane wa es) was treated. When this approach is used for pure silicon test calculations, the results are in good agreement with those obtained by more sophisticated methods.

Let us now proceed to the results. In order to examine the nature of the self-interstitial - lattice bonding, in Fig. 1 we show contour plots of the total valence charge density obtained from our calculations.

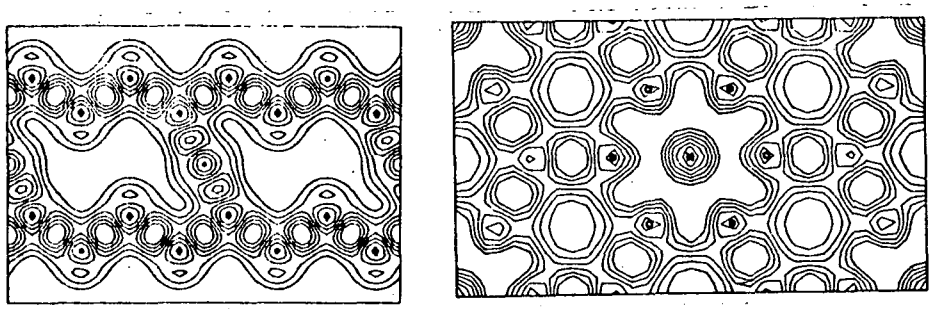

Figure 1: Self-consistent valence charge density contour plot in two different planes: (110) plane (left panel), (111) plane (right panel).

The planes shown are the (110) plane, containing a zigzag chain of atoms (the dark circles) and the self-intersitial (star), and the (111) plane, showing the hexagonal environment. Bonding between the interstitial and the nearest-neighbour atoms is evident, but the charge density accumulation around

the impurity is rather metallic-like. There is a remarkably constant-density region (no contour in the (111) plane) near the Si self-interstitial atom.

Figure 2 shows the $\Delta\rho(\vec{r})$, contour plot for the (110) plane. $\Delta\rho(\vec{r})$ is defined by

$$\Delta\rho(\vec{r})=\rho^{D}(\vec{r})-\rho^{P}(\vec{r}),$$

where $\rho^{D}(\vec{r})$ is the charge density of silicon containing an extra atom, and $\rho^{P}(\vec{r})$ is the pure silicon charge density.

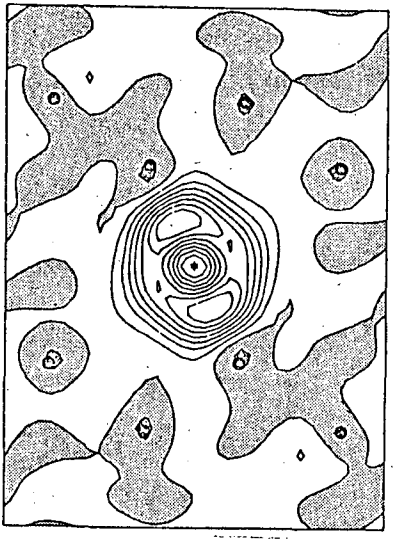

Figure 2: Contour plot of valence charge density difference in (110) plane.

The grey part of Fig. 2 is negative and the remainder is positive. Indifferently, the nearest-neighbour bonds are weakened.

As we have shown earlier [4,5], a hexagnal site self-interstitial produces three main impurity-related states up to the bottom of the conduction band: a hyperdeep state below the valence band, an s-like resonance in the valence band, and a p_z-like bound state in the gap near the top of the valence band. The charge density contour plots in the (110) plane are shown for these states in Fig. 3: the hyperdeep state (panel C), the s-like resonance (panel A) and the p_z-like state (panel B). It can be seen from Fig. 3 that the hyperdeep state and the p_z-like state are well localized around the impurity while the resonance state involves charge

on the nearest neighbours too.

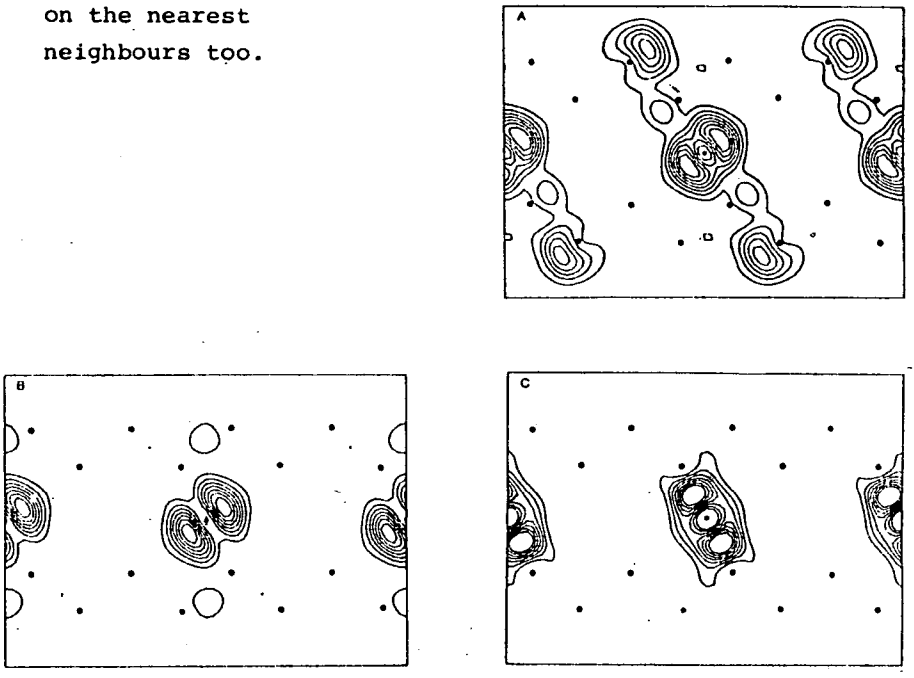

Figure 3: Contour plots of impurity-related states in (110) plane: resonance state (panel A); p_z-like state (panel B); hyperdeep state (panel C).

For the analysis, we decomposed the impurity-related wavefunctions:

$$\psi = P_V \psi + P_C \psi = \psi_V + \psi_C$$

where P_V and P_C are the projectors onto the valence and conduction subspaces, respectively, of perfect Si. In all cases we found that ψ_V consists essentially of host crystal bonding orbitals, and ψ_C corresponds to atomic orbitals of the

self-interstitial orthogonalized to the whole valence states. These results are shown by Figs. 4 and 5 for the hyperdeep state and resonance state in the (211) plane. For the hyperdeep state, contributions from the valence bands dominate, while for the resonance state the effect of the

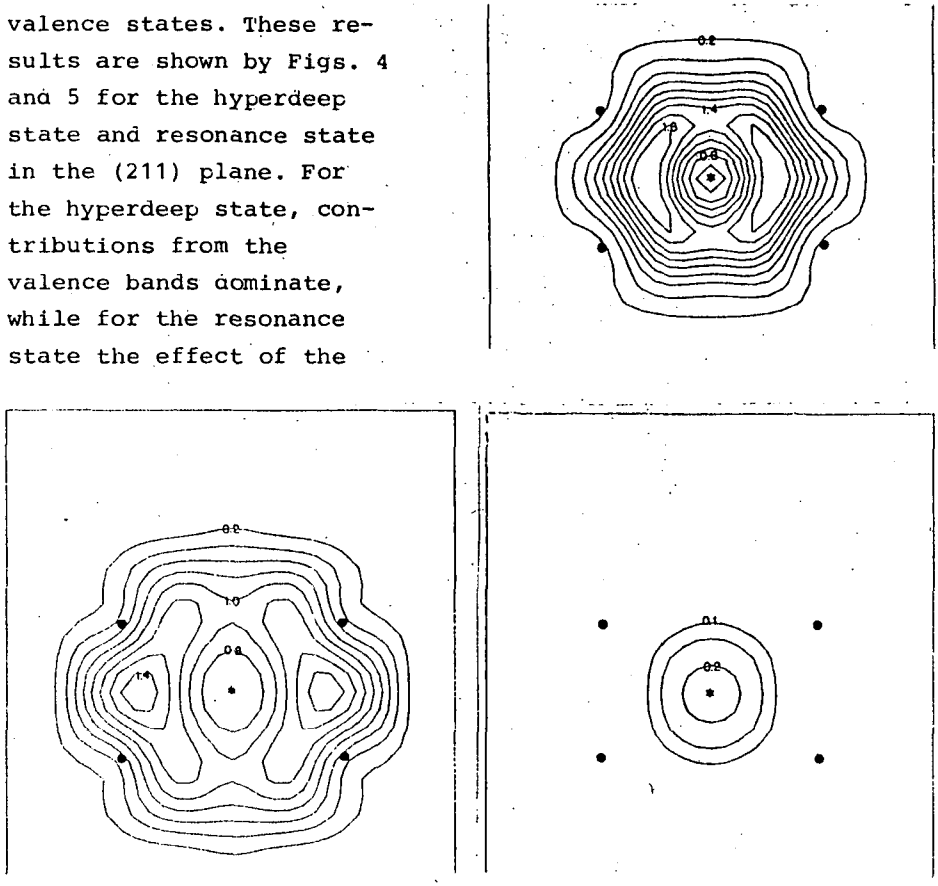

Figure 4: Electron density contour in the (211) plane of the hyperdeep state (top panel), and its projection onto the valence (left panel) and the conduction (right panel) states of perfect Si. Contour values are given in units of one electron/Si unit cell. The self-interstitial and host atoms are indicated by an asterisk and dots, respectively.

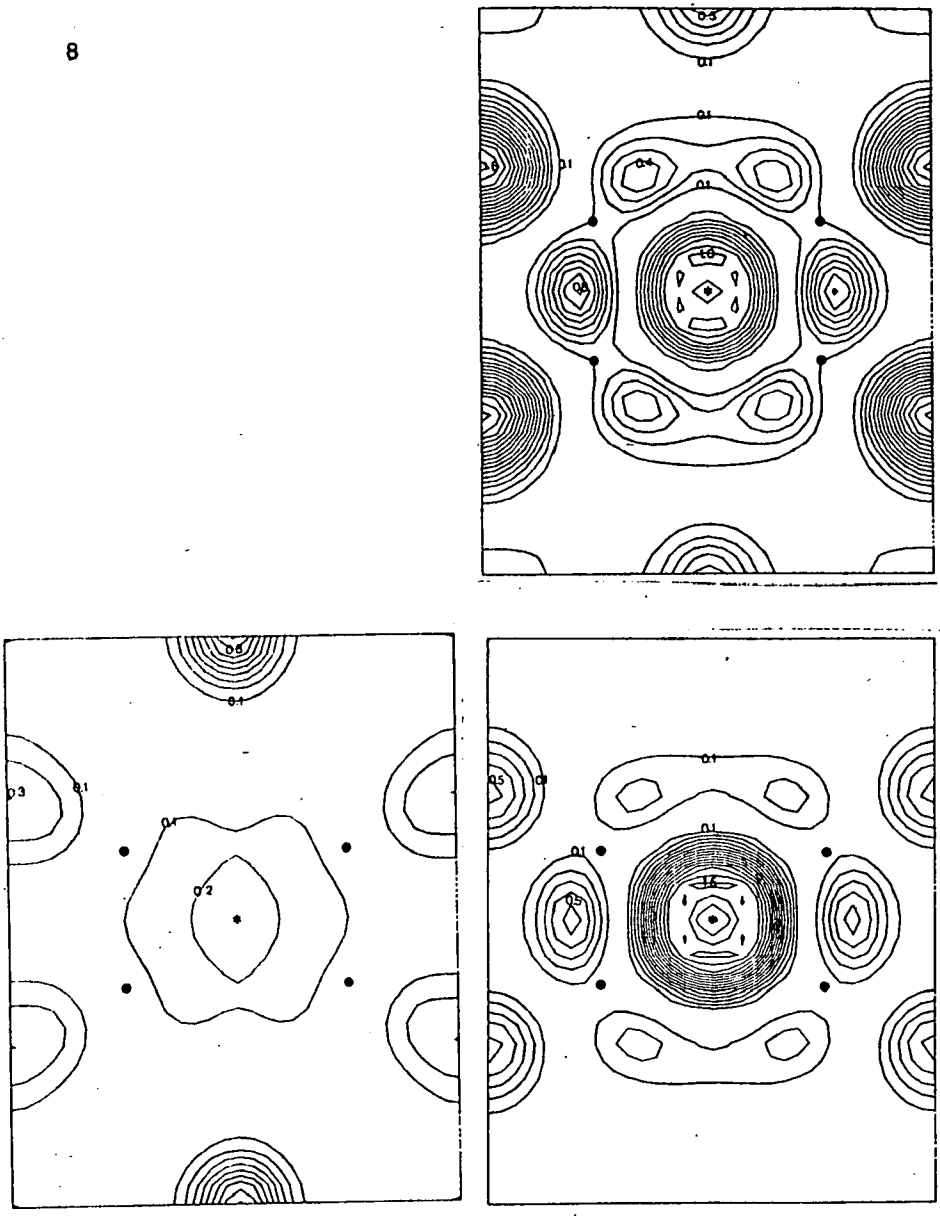

Figure 5: Analysis of the electron density of the s-like resonance state. Same conventions as in Fig. 4.

conduction band is marked. As regards the symmetry properties of the relevant states, we found that the hyperdeep state is a symmetric combination of the nearest-neighbour bonds and the impurity s-orbitals, and the resonance state is an antisymmetric one. Results for the p_z-like state can be found, for example, in [5].

References

[1] *Brust, D.*: Phys. Rev. *A134*, 1337 (1964)

[2] *Appelbaum J.A. and D.R. Hamann*: Phys. Rev. *B8*, 1777 (1973)

[3] Several authors have used the large unit cell approach to study impurity problems. See, for example: *Louie, S.G., M. Schlüter, J.R. Chelikowsky and M.L. Cohen*: Phys. Rev. *B13*, 1654 (1976); *Lindenfelt, U.*: J. Phys. *C11*, 65 and 3651 (1978); *Pickett, W.E., M.L. Cohen and C. Kittel*: Phys. Rev. *B20*, 5050 (1979); *Vanderbilt, D and J.D. Joannopoulos*: Phys. Rev. Lett. *49*, 823 (1982); *Dzwig, P., M.G. Burt, J.C. Inkson and V. Crum*: J. Phys. *C15*, 1187 (1982); *Evarestov, R.A.*: Kvantovokhimicheskie metodi v teorii tverdovo tela, Izdatelstvo Leningradskovo Universiteta (1982)

[4] *Papp, G., P. Boguslawski and A. Baldereschi*: Acta Phys. et Chem. Szeged *32*, 9 (1986)

[5] *Boguslawski, G. Papp and A. Baldereschi*: Solid State Comm. *52*, 155 (1984).

ИЗМЕНЕНИЕ В ПЛОТНОСТИ ЗАРЯДА КРЕМНИЯ ОКАЗЫВАЕМОЙ ГЕКЗАГОНАЛЬНОЙ ТОЧКОЙ САМО-МЕЖДОУЗЛИЯ

Г. Папп, П. Богуславски и А. Балдересски

Исследована плотность электронного заряда само-междоузлия в гекзагональной точке кремния. Из результатов видно, что плотность заряда вокруг атома само-междоузлия и ближайшие связи ослаблены.