MICROSCOPIC NATURE OF LITHIUM INTERACTION WITH ACCEPTOR-TYPE DEFECTS IN SILICON

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Lithium is traditionally used for compensation of electrically activ acceptor-type defects in crystalline sillicon. Very little, however, is known about the nature of such compensation. To establish the microscopic nature of lithium interaction, calculations have been carried out of the electronic structure and geometrical configuration of defects with lithium by the discrete variational X_α-method /1/. The interaction of lithium atoms with vacancies, atoms of the acceptor impurity (B, Al, Ga) and with oxygen representing one of the most abundent impurities in Si has been analyzed. The Li atoms have been found to interact with lattice vacancies by forming various complexes. As follows from the calculations, Li atoms can passivate the vacancy states if they (four Li atoms) form a cubic-tetrahedral complex (fig. 1).

In this complex, the Li atoms lie on the axes connecting the vacancy center with the empty vertices of the cube $Li_4+V+Si_4H_{12}$ (T_d symmetry). The ground state of the $Li_4+V+Si_4H_{12}$ system is degenerate which should lead to a Jahn-Teller lattice distortion near the complex /2,3/.

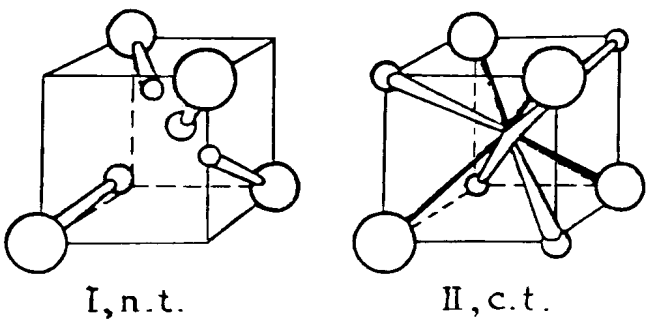

Fig. 1. Models fo possible configurations for systems of T_d symmetry containing four impurity atoms and a core of Si atoms. *I* — normal tetrahedral configuration (n. t.); *II* — cubic tetrahedral configuration (c. t.)

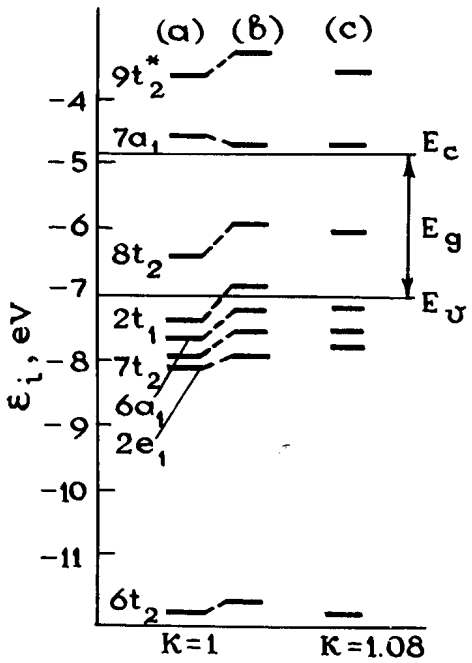

Fig. 2. One-electron energy spectrum for $Li_4+Si_4H_{12}$ cluster at total energy minimum for different Si core expansion coefficients: (*a*) for the first minimum R=2.4 a. u.; (*b*) for the second, R= =3.4 a. u.; (*c*) for the third, R≅2.4 a. u.

Fig. 2 shows the valence level diagram for the unrelaxed (K=1) and relaxed (K=1.08) c.t. geometry of the $V+Li_4$ at the total energy minimum. As seen from fig. 2a,b, the $8t_2$ level is to lie close to midgap or slightly lower and to be filled completely by 6 electrons. Let us see in which case the $8t_2$ level should be a multiple donor, and when the c. t. configuration may be considered as passivated. Clearly enough, the barrier for electron transfer $8t_2$—$7a_1$ is ~1.5 eV. By our calculations, the gap width for Si_5H_{12} cluster (called ideal) is E=2.25 eV. Therefore if the Fermi level (E_F) in a sample lies at midgap, such a system should be electrically inactive. If, however, the Fermi level lies below the midgap, the system should act as a multiple electron donor for the valence band in p—Si. In n—Si there should be no such effect.

An isolated Li atom can also interact with atoms of the acceptor impurity (B, Al, Ga) forming an unstable metastable state. The B—Li—Si_4H_{12} complexes (C_{3v} symmetry) do not have states in the gap. If the oxygen atom interacts with the Li atom, the O—Li+Si_4H_{12} complex (C_{2v}) with be energetically stable, so that to produce compensation, the oxygen concentration in the original Si should be reduced. To confirm the results of the calculations, irradiated fast neutron studies of Si with Li have been carried out.

It is shown that at exceeding by far the concentration of the dopant and of the radiation-induced defects the electrical parameters of irradiated silicon recover to their original levels which agrees with the proposed model of Li atoms bound in a cubic-tetrahedral geometrical configuration. The recovery by lithium should apparently be observed also on other semiconductor materials having vacancylike lattice defects.

Thus our experiments show that Li passivation does indeed occur, and the theory predicts c. t. to be a possible stable configuration.

REFERENCES

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