

4. Энергия взаимодействия

Теперь энергию взаимодействия $2D$ -вихря с круговой цилиндрической полостью найдем, подставив в (3) ток (4) и градиент фазы (12) и исключив собственную энергию вихря в совершенном сверхпроводнике. Вычисляя интеграл, получим окончательный результат в виде

$$U(R) = \frac{\phi_0^2}{8\pi^2 \Lambda} \ln \left(1 - \frac{a^2}{R^2} \right).$$

Это взаимодействие является притягивающим и дальнедействующим. Полученное выражение совпадает с ближними асимптотиками для энергии взаимодействия с круговой полостью пирловского и абрикосовского вихрей [2,3].

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MAGNETIC INTERACTION OF TWO-DIMENSIONAL VORTEX WITH COLUMNAR DEFECT IN LAYERED SUPERCONDUCTOR

The energy of interaction between two-dimensional vortex and a circle cavity in a layered superconductor is calculated. It is shown that its dependence on cavity radius a and distance R between the vortex and the cavity obeys the same rule $\ln(1 - a^2/R^2)$ as the short-range asymptotics of the energy of interaction of both Pearl and Abrikosov vortices with the cavity.

Fig. 1. Circle cavity of radius a in an infinite superconducting layer. The $2D$ -vortex center is at point x_0

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THE ELECTRONIC STRUCTURE AND CHARGE DISTRIBUTION IN DOPED AND UNDOPED DIAMOND AND ZIRCONIA

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The electronic structures of impure lithium in diamond and of impure chromium or yttrium in zirconia were calculated by the tight-binding theory (TBT). The results show that lithium in interstitial positions of a diamond forms donor levels (a shallow donor in H-site and a deep level in T-site). Lithium in the substitutional position forms acceptor levels. Chromium and yttrium in the substitutional positions of the zirconium form deep donor and shallow acceptor levels, respectively.

1. Introduction

The problem of describing the electronic states of defects and impurities in diamond and zirconia is one of great importance, both from the fundamental and practical point of view. It is well known that the *p*-type conductivity can easily be obtained. To obtain the *n*-type conductivity is a more difficult problem [1]. Active electronics is in need of *n*-type semiconductor diamond and zirconia. The mechanism of the formation of different defects and their properties in diamond and zirconia have been unknown until now. Both these aspects of the problem of defects in diamond and zirconia are closely related, and the progress in one field enables it to be achieved in the other.

The electronic structure of impure nitrogen in diamond was studied in [2]. Recently, the electronic structure of impure phosphorus in diamond has been studied in some of our papers [3] using the theory of shallow donor states and the tight-binding theory (TBT).

The theoretical calculations and the experimental results on lithium in diamond lattice are contradictory [4]. Some theoretical and experimental papers reported that lithium in a diamond lattice can form shallow donor levels, while in others it is stated that it forms deep levels, or even acceptor levels.

A detailed discussion of calculations of the zirconia electronic structure and their comparison with other approaches as well as with experimental photoemission (PES) and bremsstrahlung isochromat (BIS) spectra can be found in [5–7].

The present work is devoted to the simulation of lithium entering into interstitial or substitutional position of a diamond lattice and chromium or yttrium entering the substitutional position of zirconia, by using the methods of the work [3].

2. The tight-binding cluster model

We use the tight-binding theory [8,9]. In this theory of *SP*-bonded systems the electronic eigenstates are written in terms of a basis set consisting of a single *S*-state and three *P*-states at each atom of diamond. In the theory of *SPD*-bonded systems the electronic eigenstates are written in terms of a basis set consisting of a single *S*-state, five *D*-states of each metal atom and three *P*-states at each oxygen atom of zirconia. The corresponding one-electron eigenvalues and eigenfunctions are then obtained by diagonalizing an $N \times N$ Hamiltonian matrix based upon these *N*-orbitals.

In the given work, the basis system of diamond is limited by *SP*³-hybridized orbitals made of one *S*-orbital and three *P_x*, *P_y*- and *P_z*-orbitals of the valence shell of each diamond atom. These are *2s*- and *2p*-atom wave functions of carbon. We use parameters consisting of values for diagonal terms $\epsilon_s = -19,5$ eV, $\epsilon_p = -10,7$ eV and forms $V_{ss\sigma} = -5,1$ eV, $V_{sp\sigma} = 2,55$ eV, $V_{pp\sigma} = 5,1$ eV, $V_{pp\pi} = -1,7$ eV for interactions between nearest neighbour orbitals from [10]. The first two subscripts indicate the orbital coupled and the last one indicates the component of the angular momentum around the internuclear axis.

The basis system of zirconia is made of one *5S*-orbital and five *4D*-orbitals of zirconium and three *2P_x*, *2P_y*- and *2P_z*-orbitals of the oxygen atom of zirconia. We use parameters consisting of values for diagonal terms $\epsilon_s = -5,68$ eV, $\epsilon_d = -8,46$ eV, $\epsilon_p = -14,13$ eV.

Our consideration is based upon simulation of the diamond crystal by means of a large group of atoms (cluster).

3. Substitutional lithium in diamond

To calculate the energy levels of substitutional lithium in diamond we have used a group of seventeen carbon atoms, inclusive the central unit – (0,0,0) plus all its first – (1,1,1) and second – (2,2,0), nearest neighbours in the diamond lattice. During simulation the lithium

impurity is placed in the cluster's central unit.

The one-electron molecular-orbital energies resulted from the calculation when the central atom of the cluster is replaced by substitutional lithium (ionization potentials of 5,34 eV and 3,42 eV for 2S- and 2P-orbitals, respectively [8]) is shown in Fig. 1 (A, B, C), here (A), (B), (C) are electronic levels of Li, 17C and Li + 16C, accordingly.

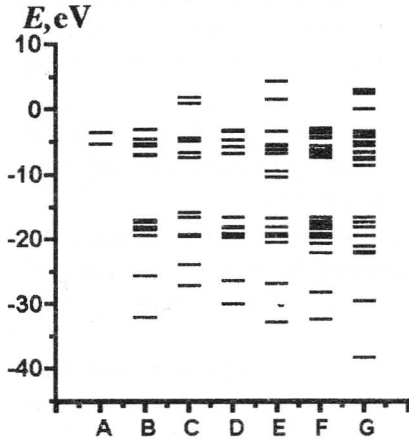


Fig. 1. Energies of one-electron MO's for a diamond cluster as a function of lithium position. It shows that (A) is Li, (B) is 17C, (C) is Li+16C, (D) is 14C, (E) is Li+14C, (F) is 18C and (G) is Li+18C

3.1. Conclusion. The orbitals connected with lithium appear in the conduction band. These orbitals are unoccupied. Triply degenerate orbital appears in the forbidden gap near the valence-band edge. Unpaired electron of the lithium is not localized at the lithium (Fig. 1 (C)).

4. Interstitial lithium in diamond

In the diamond lattice there will be two such sites as illustrated in Fig. 1 (D, E, F, G). One site, which we shall call tetrahedral, is characterized by four nearest neighbours at a distance of $0,433a_0$ from the center, and six next – nearest neighbours at a distance of $0,500a_0$; a_0 is the unit-cell edge length. The center of the hexagonal site is at a distance of $0,415a_0$ from six nearest neighbours, and $0,649a_0$ from eight next-nearest neighbours. It is clear that consideration of nearest neighbours only makes the hexagonal site one of greater repulsive energy for the impurity than the tetrahedral site.

4.1. Energy levels of interstitial lithium at T-site. To calculate the energy levels of interstitial lithium at T-site, we have used a group of fifteen atoms, inclusive the central unit $(-1,-1,-1)$ plus all its first- and second-nearest neighbours in the diamond lattice. During simulation the lithium impurity is placed in the cluster's central unit.

The one-electron molecular-orbital energies resulted from the calculation, when the central atom of the cluster is replaced by interstitial lithium, is shown in Fig. 1 (D, E), here (A), (D), (E) are electronic levels of Li, 14C and Li +14C, accordingly.

4.1.1. Conclusion. The orbitals connected with lithium appear in the forbidden gap. Comparing the calculations for the central atom of lithium at the T-site we may conclude that the lithium unpaired electron is localized at the lithium (Fig. 1(E)).

4.2. Energy levels of interstitial lithium in H-site. To calculate the energy levels of interstitial lithium at H-site, we have used a group of nineteen atoms, inclusive the central unit $(-1,5, -1,5, -1,5)$ plus all its first- and second- nearest neighbours in the diamond lattice. During simulation the lithium impurity is placed in the cluster's central unit.

The one-electron molecular-orbital energies resulted from the calculations, when the central atom of the cluster is replaced by interstitial lithium, is shown in Fig. 1(F, G), here (A), (F), (G) are electronic levels of Li, 18C and Li + 18C, accordingly.

4.2.1. Conclusion. The orbitals connected with lithium appear in the conduction band. These orbitals are unoccupied. The nondegenerate orbital appears in the forbidden gap near the conduction-band edge. Comparing the calculation for central atom of lithium in H-site we may conclude that the lithium unpaired electron is not localized at the lithium (Fig. 1(G)).

5. Substitutional chromium or yttrium in zirconia

To calculate the energy levels of substitutional chromium or yttrium in zirconia, we have used a cell of 12 atoms, inclusive the 8 oxygen atoms and 4 atoms of zirconium. During simulation the chromium or yttrium impurity is placed in the cell's zirconium unit.

The one-electron molecular-orbital energies resulted from the calculations, when the zirconium atom of the cell is replaced by substitutional chromium (ionization potentials of 6,9 eV and 13,4 eV for 4*S*- and 3*D*-orbitals, respectively [8]), is shown in Fig. 2 (C) here (A), (B), (C) are electronic levels of Cr, Zr₄O₈ and Cr + Zr₃O₈, accordingly. The one-electron molecular-orbital energies resulted from the calculations, when the zirconium atom of the cell is replaced by substitutional yttrium (ionization potentials of 5,34 eV and 6,80 eV for 5*S*- and 4*D*-orbitals, respectively [8]), is shown in Fig. 2 (D) here (B), (E), (D) are electronic levels of Zr₄O₈, Y, Y + Zr₃O₈, accordingly.

5.1. Conclusion. Orbitals connected with chromium appear in the forbidden gap. Two doubly degenerate and one non-degenerate levels appear in the forbidden gap. Unbonding electrons of the chromium are localized at the chromium. Thus, the substitutional chromium must be deep double donor (i.e. with two donor electrons at each atom of chromium) (Fig. 2 (C)).

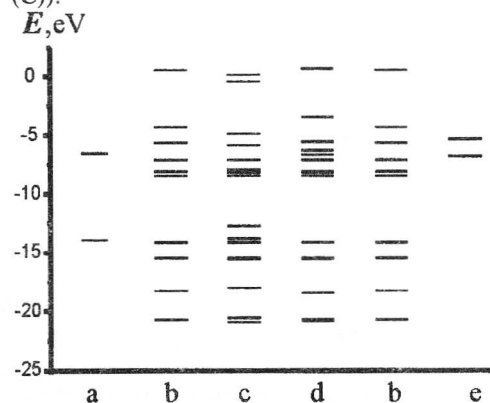


Fig. 2. Energies of one-electron MO's for a zirconia cell as a function of substitutional impurities. It shows that (A) is Cr, (B) is Zr₄O₈, (C) is Cr+Zr₃O₈, (D) is Y+Zr₃O₈, (E) is Y

Orbitals connected with yttrium are absent in the forbidden gap and appear in the conduction band. Two doubly degenerate and one non-degenerate levels appear in the conduction band. This orbitals are unoccupied. An unpaired electron of yttrium is not localized at the yttrium. Thus, the substitutional yttrium must be shallow acceptor (Fig. 2 (D)).

6. General conclusions

From the results of calculation presented in Fig. 1 we can see that lithium in interstitial positions of diamond insulator forms donor levels (a shallow donor in H-site and a deep level in T-site). Lithium in the substitutional position forms acceptor levels. From the results of calculation presented in Fig. 2 we can see that chromium and yttrium in the substitutional positions of zirconium form deep donor and shallow acceptor levels, respectively.