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NEW DONOR STATE OF *S* SYMMETRY*

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The influence of the short-range potential and the electron–phonon coupling on the donor spectrum is discussed. It is shown that the attractive short-range potential leads to a formation of a single additional state of s symmetry and with energy lying below a weakly perturbed hydrogen-like spectrum, which includes the $1s$ level. The new state can be called the $0s$ state. With decreasing short-range attraction, the energy of this state increases crossing over the hydrogen-like levels and, for weak short-range potential, the $0s$ state disappears. If the electron–phonon coupling is sufficiently strong, the donor hydrogen-like spectrum is perturbed only in a very narrow region of the level crossing.

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The donor states in semiconductors exhibit a variety of properties: they can be weakly (strongly) localized, which yields shallow (deep) energy levels, moreover, the same donor atom can possess both types of states coexisting with each other, which is known as a metastability (bistability). If the localization of the donor state exceeds the size of the elementary cell, this state can be described in frames of the one-band approximation. In the present paper the energy of few lowest donor states was calculated by variational method taking into account the coupling with LO phonons and both the Coulomb and short-range (SR) donor potentials. According to the one-band approximation, the donor states are formed from the states of the conduction band, which is assumed to have a finite width, moreover, it is analytically parametrized and takes a form similar to our previous choice [1, 2]. The variational calculations are performed in the $\boldsymbol{k}$-vector space. To this purpose, the summation over the first Brillouin zone is replaced by the integration over the Debye sphere of the same volume.

The variational basis is proposed in the form $\psi_i = \varphi(\alpha_i)\chi(\beta_i)$, where φ and χ are the electron and phonon parts of the wave function, respectively, and α_i and β_i are the nonlinear variational parameters ($i = 1, \ldots, N$). The phonon wave functions χ were taken in the generalized Lee–Low–Pines form [3–5]. The convergence for the three lowest s states was obtained with $N = 6$-element basis. Therefore, the minimization is performed over the 12 nonlinear variational parameters, and the 6 linear variational parameters are determined by the diagonalization procedure.

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The potential of the donor consists of the long-range and short-range components. The long-range donor potential is approximated by the Coulomb potential, which is statically screened by the high-frequency dielectric constant ε_∞. The additional screening of this potential results from the coupling with phonons, which is included in the present work. The short-range potential results from the difference between the core states of the impurity and host crystal atoms and allows us to reproduce the actual donor energy levels. This potential takes on different values for different donor species. We assume that this is a local potential with the Fourier transform being constant in the k-space, i.e. $V_{\rm SR}(k) = {\rm const} = \gamma$, where $\gamma < 0$. If the potential of the defect only includes the short-range component, one energy level can at most appear. Similar model has been applied to the vacancy in Si by Pantelides et al. [6]. If the short-range potential acts together with the Coulomb potential, the ground-state ($1s$) energy level is lowered with increasing short-range attraction (decreasing γ) and becomes deep. However, other hydrogen-like energy levels are only slightly lowered and do not exceed the unperturbed $1s$ level. This effect is similar to the shallow-deep instability described by Altarelli [7] and Resca [8].

After taking into account the interaction with phonons, e.g. in the Fröhlich form, the picture undergoes an essential qualitative change. If γ decreases, the energy levels for both the ground state and excited s states are lowered. Moreover,

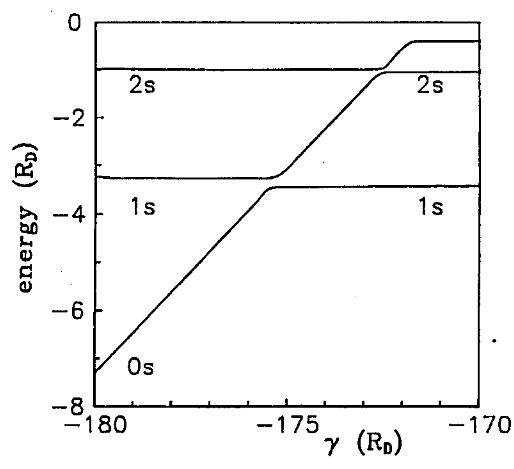

Fig. 1. Calculated donor energy levels of s symmetry as functions of the strength γ of the short-range potential. The energy is measured with respect to the bottom of the polaronic conduction band. The energy and the parameter γ are expressed in donor rydbergs, i.e. $R_{\rm D} = (m_e/m_{e0})Ry/\varepsilon_0^2$, where m_e is the electron conduction band mass, m_{e0} is the electron rest mass, ε_0 is the static dielectric constant, and Ry is the atomic rydberg.

they in turn go over one into another, i.e. $E_{ns} \rightarrow E_{(n-1)s}$, again giving the hydrogen-like spectrum. As a result, we obtain identical hydrogen-like spectra for both the weak and strong short-range potentials; besides, for sufficiently strong short-range potential, there appears one additional donor state. This new donor state possesses the *s* symmetry and coexists with all the hydrogen-like donor states. Therefore, we call it the 0*s* state.

The transition region between both the spectra occurs for the intermediate values of γ and possesses a different character depending on the electron–phonon coupling. For weak coupling, we obtain a typical level repulsion picture, i.e. the repulsing energy levels are smooth functions of γ. If the electron–phonon coupling is sufficiently large, the transition region of γ becomes very narrow and the unusual level crossing ("anticrossing") appears (see Fig. 1). For the material parameters corresponding to the anticrossing, the metastability of donors is possible. If γ_c is the strength of the short-range potential corresponding to the anticrossing between the energy levels E_{0s} and E_{1s}, then the donors with $\gamma < \gamma_c$ are metastable, while the donors with $\gamma > \gamma_c$ are stable. For the metastable donors, the deep 0*s* state can coexist with all the shallow states.

The nature of the new 0*s* state is the same as that of the "self-trapped" state discussed by Toyozawa [9]. The variational calculations [9] have been performed with the one-element basis, which does not describe the excited states.

The present work has shown that the new 0*s* donor state can coexist with the hydrogen-like shallow donor states. The 0*s* state is generated by the short-range donor potential of the atomic nature. The calculations were performed with the many-element variational basis, which was used to construct the orthogonal wave functions for the considered states. The calculated energy levels show the characteristic anticrossing structure, which results from the interplay between the three interactions involved, namely, the Coulomb, the short-range and the electron–phonon one.

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