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Effect of electron-mass anisotropy and effective dielectric function on the donor binding energies in silicon

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With the use of the Krieger-Nightingale model, the donor binding energy in Si is calculated variationally as a function of donor concentration. The impurity potential incorporates an effective dielectric function of the host and impurity electrons. The mass anisotropy of the electron is also included. The Mott constant, $aN_c^{1/3}$, obtained is compared with the earlier results.

It is well known that the donor binding energy decreases as the impurity concentration increases and becomes zero at a critical concentration N_c in semiconductors. A number of theoretical investigations were made in the recent past to estimate the Mott constant $aN_c^{1/3}$, where a is the effective Bohr radius in the material.

Krieger and Nightingale[1] have made a variational estimate of donor binding energy as a function of impurity concentration in many valley semiconductors using a hydrogenlike trial function. Greene, Aldrich, and Bajaj[2] have improved the Krieger-Nightingale model by using the Hulthén function as a trial wave function. Martino, Lindell, and Berggren[3] have solved the relevant Schrödinger equation numerically and estimated $aN_c^{1/3}$. In these works the impurity potential in the Hamiltonian is the Coulomb potential screened by the Lindhard[4] or Hubbard-Sham[5] dielectric function in which the screening due to the valence-charge distribution of the host material is included in the form of the static dielectric constant K. The present authors[6] have extended the variational calculations using an effective dielectric function in the impurity potential which takes into account the spatial variation of the dielectric function of the host material. In all these works the effective mass of the electron is assumed to be isotropic while it is known that the constant energy surfaces corresponding to the conduction-band minima in Si and Ge are spheroids.

Aldrich[7] has considered the anisotropic nature of the electron masses in Ge and Si in his variational estimate of donor binding energies in these materials. However, in his work the spatial dispersion of the host dielectric constant was also neglected.

In the present paper we make variational estimates of the donor binding energies in silicon taking into account the mass anisotropy of the conduction electrons and the spatial variation of the host dielectric function as in Ref. 6. The nonisotropic nature of the electron mass is included along the lines of Aldrich.[7]

The trial wave function for the donor electron is chosen as

$$\psi(r) = [(4-\mu^2)/4\pi\mu^2\beta^3]^{1/2} \times (e^{-(1-\mu/2)\rho} - e^{-(1+\mu/2)\rho})/\rho \ , \quad (1)$$

where

$$\rho = \left[\frac{M_\parallel}{M^*}\left(\frac{x}{a_\parallel}\right)^2 + \frac{M_\perp}{M^*}\left(\frac{y}{a_\perp}\right)^2 + \frac{M_\perp}{M^*}\left(\frac{z}{a_\perp}\right)^2 \right]^{1/2} , \quad (2)$$

with

$$a_\parallel = \beta\epsilon^{2/3},\ a_\perp = \beta/\epsilon^{1/3},\ \text{and}\ M^* = (M_\parallel M_\perp^2)^{1/3} \ . \quad (3)$$

μ, β, and ϵ are variational parameters chosen to minimize energy. Equation (2) is different from the one given by Aldrich,[7] but ensures correct normalization for ψ.

The Hamiltonian for the system is

$$H = -\frac{\hbar^2}{2}\left[\frac{1}{M_\parallel}\frac{\partial^2}{\partial x^2} + \frac{1}{M_\perp}\frac{\partial^2}{\partial y^2} + \frac{1}{M_\perp}\frac{\partial^2}{\partial z^2} \right] + V(r) \ , \quad (4)$$

where the potential $V(r)$ has the Fourier transform

$$V(\vec{q}) = -\frac{4\pi e^2}{q^2 \epsilon_{\mathrm{eff}}(\vec{q})} \ , \quad (5)$$

where $\epsilon_{\mathrm{eff}}(\vec{q})$ is the effective dielectric function.[6] We use for the host dielectric function $\epsilon_h(q)$ the modified dielectric function of Azuma and Shindo,[8] the modification incorporating the electron-mass anisotropy,

$$\epsilon_h(q) = \left[\frac{1}{K} + \frac{s^2}{s^2+\alpha_1^2} - \frac{As^2}{s^2+\alpha_2^2} - \frac{Bs^2}{s^2+\alpha_3^2} \right]^{-1} , \quad (6)$$

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where A, B, α_1, α_2, and α_3 are numerical constants and

$$s=\left[\frac{M^*}{M_\parallel}q_x^2+\frac{M^*}{M_\perp}q_y^2+\frac{M^*}{M_\perp}q_z^2\right]^{1/2} . \tag{7}$$

For the screening due to impurity electrons the modified Lindhard dielectric function is used. This is given by

$$\epsilon_I(\vec{q})=1+\frac{4\pi e^2}{q^2}\left[\frac{3N}{2E_F}\right]\left[\frac{1}{2}+\frac{4k_F^2-s^2}{8k_F s}\ln\left|\frac{2k_F+s}{2k_F-s}\right|\right] , \tag{8}$$

where k_F is the magnitude of the Fermi wave vector. Now

$$\epsilon_{\rm eff}(\vec{q})=K\left[\left[1+\frac{Ks^2}{s^2+\alpha_1^2}-\frac{KAs^2}{s^2+\alpha_2^2}-\frac{KBs^2}{s^2+\alpha_3^2}\right]^{-1}+\frac{4\pi e^2}{Kq^2}\left[\frac{3N}{2E_F}\right]\left[\frac{1}{2}+\frac{4K_F^2-s^2}{8k_F s}\ln\left|\frac{2k_F+s}{2k_F-s}\right|\right]\right] . \tag{9}$$

Equation (5) with $\epsilon_{\rm eff}(q)$ in Eq. (9) with $A=B=0$ and $\alpha_1=\infty$ yields the impurity potential used by other authors.[1–3,7] The screened potential for a point charge with $\epsilon_{\rm eff}$ as the screening function has been presented recently in the r space by Geetha and Balasubramanian.[9]

The units of energy and distance in our calculations are the effective Rydberg $R^*=M^*e^4/2\hbar^2K^2$ and effective Bohr radius $a=K\hbar^2/M^*e^2$, respectively. The numerical values of M^*, $M_\parallel/M_\perp$, K, A, B, α_1, α_2, α_3 used are 0.2981, 5.16, 12, 0.0726, 0.0107, 26.635, 36.674, 12.132.

The expectation value of H in Eq. (4), in the present units of energy, is

$$E=\frac{1}{3}\left[\frac{1}{a_\parallel^2}+\frac{2}{a_\perp^2}\right]\frac{1}{4}(4-\mu^2)-8\pi\int\frac{F(\vec{q})\,d^3q}{q^2\epsilon_{\rm eff}(\vec{q})} , \tag{10}$$

where $F(\vec{q})$ is the Fourier transform of $\psi\psi^*$ given by

$$F(\vec{q})=\frac{1}{(2\pi)^3}\left[\frac{4}{\mu^2}-1\right]\times 1/t\left[\tan^{-1}\frac{t}{2-\mu}+\tan^{-1}\frac{t}{2+\mu}-2\tan^{-1}\frac{t}{2}\right] , \tag{11}$$

where

$$t=\left[\frac{M^*}{M_\parallel}(a_\parallel q_x)^2+\frac{M^*}{M_\perp}(a_\perp q_y)^2+\frac{M^*}{M_\perp}(a_\perp q_z)^2\right]^{1/2} . \tag{12}$$

The energy value for a given concentration is numerically evaluated by locating the minimum of E with respect to μ, β, and ϵ. This is repeated for various concentrations. The results are presented in Fig. 1 in which the binding energy is plotted as a function of impurity concentration. Our[6] earlier results and the results of Aldrich[7] are also given for comparison. The values of the Mott constant $aN_c^{1/3}$ are given in Table I, along with earlier theoretical and experimental values.

We find that the introduction of the mass anisotro-

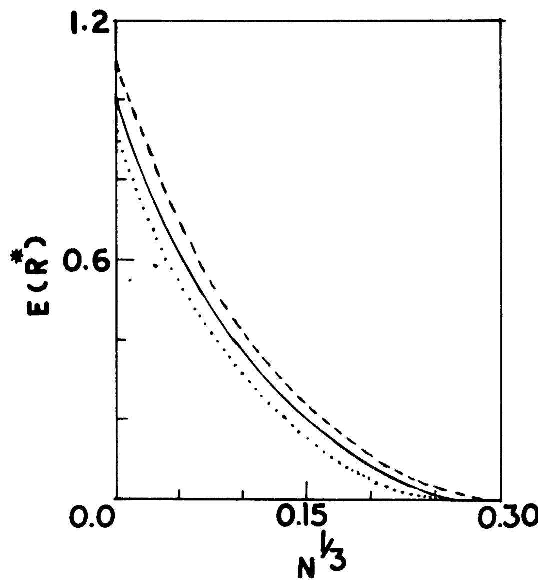

FIG. 1. Donor binding energy in Si vs impurity concentration. – – –, present authors' earlier work (Ref. 6); ——, present authors' current work; · · · ·, Aldrich's work (Ref. 7).

TABLE I. Values of Mott constant. Experimental value of Mott constant =0.21 (Ref. 1).

Dielectric function	Electron mass	$aN_c^{1/3}$
$\epsilon_{\rm eff}$ with $\epsilon_h=K$	Isotropic	0.263 (Ref. 2)
	Anisotropic	0.25 (Ref. 7)
$\epsilon_{\rm eff}$ as in Eq. (9)	Isotropic	0.288 (Ref. 6)
	Anisotropic	0.27 (present work)

py decreases the binding energy and critical density, whereas the inclusion of the spatial variation of the host dielectric function increases these quantities. Thus the error in the spherical band approximation and the error due to the neglect of spatial dispersion partially cancel each other.

It may be emphasized that the results presented are of model calculations, since the valley-orbit interaction and "umklapp processes" have not been included. These effects are known to be important for the electronic ground states of shallow donors in Si and Ge.[10] The importance of these effects at high impurity concentration may have to be investigated.

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