Brief Reports

Brief Reports are short papers which report on completed research with no expectation of follow-up publication or are addenda to papers previously published in the **Physical Review** *by the same authors. A Brief Report may be no longer than 3½ printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Concentration-dependent donor ionization energy in silicon

A. Neethiulagarajan* and S. Balasubramanian
School of Physics, Madurai Kamaraj University, Madurai 625 021, India
(Received 26 January 1981)

Using 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 the impurity electrons. The Mott constants $aN_c^{1/3}$ obtained are higher than those published earlier.

It is well known that as the density of the donors in a semiconductor increases, the donor binding energy decreases and becomes zero for sufficiently high concentration. A number of workers have theoretically estimated the value of the critical concentration at which the binding energy goes to zero. Krieger and Nightingale[1] have variationally estimated the binding energies using the simple effective-mass theory for hydrogenlike impurities. Recently Greene *et al.*[2] have made variational estimates of the binding energies of donors bound in Lindhard potentials and Hubbard-Sham potentials using Hulthen trial functions. In all the above work, the screening of the impurity potential due to the host semiconductor is assumed to be due to the static dielectric constant K. More recently Resta[3] has introduced the q-dependent nature of the host dielectric function in generalizing the Thomas-Fermi screened potential in semiconductors. The effect of this generalization on the electron mobilities has been shown in a subsequent paper[4] to be not appreciable. When one studies the impurity binding in semiconductors, high q values are important.

In the present work we study the concentration-dependent donor ionization energy following the Krieger-Nightingale model but with the impurity potential screened by an effective dielectric function. If one assumes that the valence charge distribution of the host semiconductor and the impurity electrons independently contribute to the polarization, the Maxwell displacement in the medium may be written as

$$\vec{D}=\vec{E}+4\Pi(\vec{P}_h+\vec{P}_I)\,, \tag{1}$$

which gives

$$\epsilon_{\rm eff}(\vec{q})=\epsilon_h(\vec{q})+\epsilon_I(\vec{q})-1\,, \tag{2}$$

where $\epsilon_{\rm eff}(\vec{q})$ is defined as

$$\vec{D}(\vec{q})=\epsilon_{\rm eff}(\vec{q})\,\vec{E}(\vec{q})\,, \tag{3}$$

and $\epsilon_h(\vec{q})$ is the host dielectric function and $\epsilon_I(\vec{q})$ is that due to the impurity electrons treated as an electron gas.

A donor electron is taken to be moving with potential energy $V(\vec{r})$ which is the Fourier transform of $V(\vec{q})$ given in the point-charge model as

$$V(\vec{q})=-\frac{4\pi Ze^2}{q^2\epsilon_{\rm eff}(q)}\,, \tag{4}$$

where Ze is the charge on the impurity ion. Using the usual effective-mass theory, the variational expression for the donor ground-state energy in units of $(m^*e^4\,2\hbar^2)$ with hydrogenlike[1] trial function is given by

$$E_d=\frac{a_0^2}{\rho^2}-\frac{8\mu}{\pi}\int_0^\infty\frac{dx}{[1+(\mu\rho x/a_0)^2]^2\epsilon_{\rm eff}(x)}\,, \tag{5}$$

where

$$\mu=\hbar^2k_F/m^*e^2=a_0k_F\,,\quad x=a_0q/2\mu\,,$$

and ρ is the variational parameter. With Hulthen-type trial functions,[2] the energy expression turns out to be

$$E_d=(1-\eta^2/4)/K^2-(4/\eta^2-1)(4I/K\pi)\,, \tag{6}$$

where

$$I=\int_0^\infty\left\{\left[\tan^{-1}\left(\frac{2\mu Kx}{2-\eta}\right)+\tan^{-1}\left(\frac{2\mu Kx}{2+\eta}\right)-2\tan^{-1}(\mu Kx)\right]\Big/x\epsilon_{\rm eff}(x)\right\} \tag{7}$$

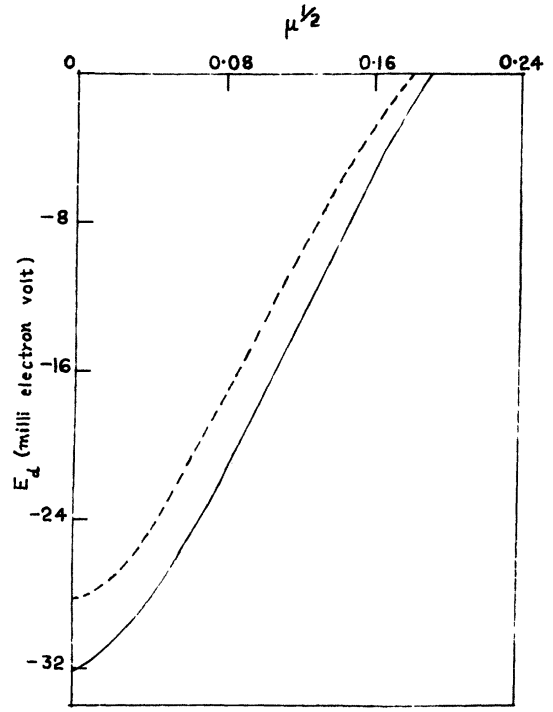

FIG. 1. Donor ground-state energy as a function of concentration expressed as μ. Hydrogenic trial function; ----, Lindhard form (Krieger-Nightingale). —— Effective Lindhard form (present work).

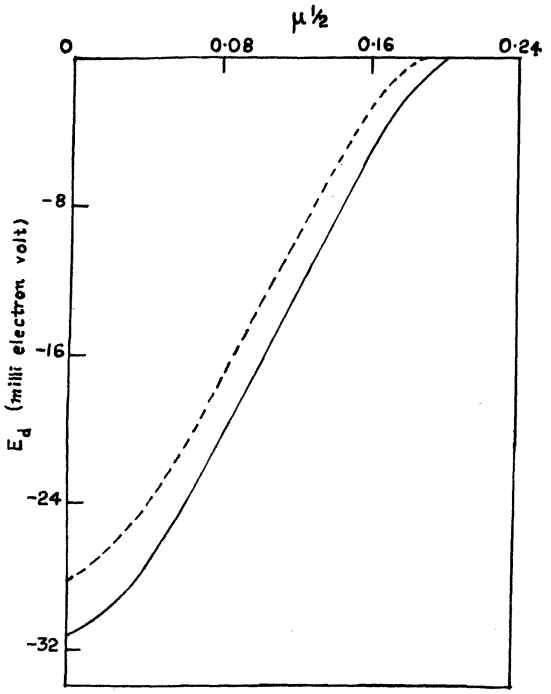

FIG. 2. Donor ground-state energy as a function of concentration expressed as μ. Hulthen trial function; ---- Lindhard form (Greene *et al.*). —— Effective Lindhard form (present work).

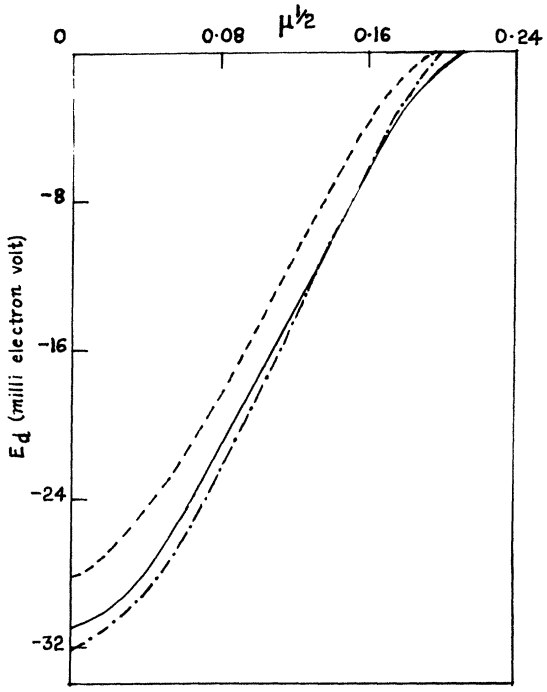

FIG. 3. Donor ground-state energy as a function of concentration expressed as μ. --- Hubbard-Sham form; Hulthen (Greene *et al.*). —— Effective Hubbard-Sham form; Hulthen-type (present work). -·-·- Effective Hubbard-Sham form; hydrogenlike (present work).

and η is a variational parameter.

We have used in the numerical estimates of E_d both the Lindhard form and the Hubbard-Sham form for $\epsilon_I(\vec{q})$. The Lindhard form for $\epsilon_I(x)$ is[5]

$$1+(\nu/\pi\mu x^2)\left[\frac{1}{2}+\left(\frac{1-x^2}{4x}\right)\ln\left|\frac{1+x}{1-x}\right|\right]. \qquad (8)$$

The Hubbard-Sham form for $\epsilon_I(x)$ is[6]

TABLE I. Values of $aN_c^{1/3}$.

Particulars of dielectric function of the impurity electrons and trial wave function	$aN_c^{1/3}$ Present work	Earlier work
Lindhard form for ϵ_I		
hydrogenlike trial function	0.257	0.23, Ref. 1
Hulthen trial function	0.288	0.263, Ref. 2
Hubbard-Sham form for ϵ_I		
hydrogenlike trial function	0.279	
Hulthen trial function	0.317	0.290, Ref. 2

$$1+(\nu/\pi\mu x^2)\left[\frac{1}{2}+\left(\frac{1-x^2}{4x}\right)\ln\left|\frac{1+x}{1-x}\right|\right]$$

$$\times[1-(2\mu^2x^2)/(4\mu^2x^2+\mu^2+4\mu/K\pi)], \quad (9)$$

where ν is the number of equivalent conduction-band minima (six in Si). For $\epsilon_h(\vec{q})$, the dielectric function obtained by Nara[7] is used:

$$\epsilon_h(x)=\left[\frac{1}{K}+1\Big/\left(1+\frac{\alpha_1^2}{\mu^2x^2}\right)\right.$$

$$\left.-A\Big/\left(1+\frac{\beta_1^2}{\mu^2x^2}\right)-B\Big/\left(1+\frac{\gamma_1^2}{\mu^2x^2}\right)\right]^{-1} \quad (10)$$

where $\alpha_1=1.1098$, $\beta_1=1.5281$, $\gamma_1=0.5055$, $A=0.0726$, and $B=0.0107$. It may be noted that the constants α_1, β_1, and γ_1 are now dimensionless and are obtained from the constants given in Ref. 7 by multiplying by $a_0/2$, a_0 given under Eq. (5).

The value of m^* used is $0.2987m_0$ and $K=12$.

The integrals in Eqs. (5) and (6) are evaluated for various concentrations and for different variational parameters. For each concentration, the minimum of E_d with respect to the variational parameter is obtained. The donor ground-state energies obtained in the present work are given in Figs. 1–3 in which the specification, "effective Lindhard" or "effective Hubbard-Sham" means use of $\epsilon_{\text{eff}}(x)$ with ϵ_I either as in Eq. (8) or Eq. (9). For all concentrations the donor binding energy obtained using the effective dielectric function is higher than the corresponding results of the earlier workers. The Mott constant $aN_c^{1/3}$ (a being effective Bohr radius, a_0K) obtained from the figures is presented in Table I. These values are higher than the corresponding results of earlier workers, thus showing the importance of taking into account the q-dependent nature of the ϵ_h.

---

*Permanent address: Department of Physics, V.H.N.S.N. College, Virudhunagar 626 002, India.

[1]J. B. Krieger and M. Nightingale, Phys. Rev. B 4, 1266 (1971).
[2]R. L. Greene, C. Aldrich and K. K. Bajaj, Phys. Rev. B 15, 2217 (1977).
[3]R. Resta, Phys. Rev. B 19, 3022 (1979).
[4]R. Resta and L. Resca, Phys. Rev. B 20, 3254 (1979).
[5]J. Lindhard, K. Dan Vidensk. Selsk. Mat. Fys. Medd. 28, 8 (1954).
[6]L. Sham, Proc. Phys. Soc. London Sect. A 283, 33 (1965).
[7]H. Nara, J. Phys. Soc. Jpn. 20, 778 (1965).