Brief Reports

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Concentration-dependent donor energies and Mott constant in heavily doped n-type silicon

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We have calculated, using the Krieger-Nightingale model, both the donor binding energy as a function of donor concentration and the Mott constant $aN_c^{1/3}$ in Si by numerically solving the Schrödinger equation. The Hubbard-Sham and effective Hubbard-Sham dielectric functions are used for the screening of the impurity potential. Our present results are compared with earlier theoretical and experimental results.

Doped semiconductors show metallic behavior at and beyond certain impurity concentrations. A number of experimental and theoretical estimates of the critical concentration N_c have been made in the recent past. Using simple arguments, Mott[1] predicted that the transition would take place when $aN_c^{1/3}=0.25$, where a is the effective Bohr radius in the material. Krieger and Nightingale[2] extended the Mott model to many-valley semiconductors. Greene, Aldrich, and Bajaj[3] have made variational estimates of the donor energies as a function of impurity concentration using the Krieger-Nightingale model. Aldrich[4] has considered the anisotropic nature of the electron masses in his variational estimate of the donor binding energies in Si and Ge. In all these works, the host semiconductor is assumed to have a static dielectric constant K.

The present authors[5,6] have incorporated the space-dependent or wave-vector–dependent nature of the host dielectric function in their effective dielectric function, and have made variational estimates of both the donor binding energies as a function of impurity concentration, and the Mott constant $aN_c^{1/3}$ in silicon, assuming isotropic and non-isotropic energy bands. However, in all these works, the values of the Mott constant $aN_c^{1/3}$ obtained are dependent on the type of trial wave function chosen in the variational procedure.

Martino, Lindell, and Berggren,[7] with a view to obtaining values of $aN_c^{1/3}$ with high numerical precision which do not depend on the type of trial wave function, have integrated the relevant Schrödinger equation numerically, and have pointed out that there is a considerable difference between the values of $aN_c^{1/3}$ obtained by variational calculations, and numerical integration for all semiconductors. They used an impurity potential $V(r)$ having the Fourier transform

$$V(q)=-4\pi e^2/K\epsilon(q)q^2 \quad , \tag{1}$$

where $\epsilon(q)$ is the Hubbard-Sham dielectric function, and obtained the value of $aN_c^{1/3}$.

In this paper, we present model calculations of both the donor binding energies as a function of $aN^{1/3}$, and the Mott constant $aN_c^{1/3}$ in silicon. Numerical integration of the relevant Schrödinger equation using both the Hubbard-Sham (in which the host material is assumed to have a static dielectric constant K) and effective Hubbard-Sham dielectric functions [in which the host material is assumed to have a wave-vector dependent dielectric function $\epsilon_h(q)$] in the impurity potential is performed. The wave-vector–dependent host dielectric function used is that of Azuma and Shindo.[8]

The radial part of the Schrödinger equation to be solved numerically is given by

$$-\frac{\hbar^2}{2m^*}\left(\frac{d^2F}{dr^2}+\frac{2}{r}\frac{dF}{dr}\right)+V(r)F(r)=EF(r) \quad , \tag{2}$$

where m^* is the effective mass in the conduction band, which here is assumed to be isotropic. The potential $V(r)$ has the Fourier transform

$$V(q)=-4\pi e^2/\epsilon_{\rm eff}(q)q^2 \quad , \tag{3}$$

where $\epsilon_{\rm eff}(q)$ is the effective dielectric function which is given by

$$\epsilon_{\rm eff}(q)=K[\epsilon_h(q)+\epsilon_l(q)-1] \quad , \tag{4}$$

where the host dielectic function $\epsilon_h(q)$ is given by

$$\epsilon_h(q)=\left(1+\frac{Kq^2}{q^2+\alpha^2}-\frac{KAq^2}{q^2+\beta^2}-\frac{KBq^2}{q^2+\gamma^2}\right)^{-1} \quad , \tag{5}$$

and the dielectric function of the impurity electrons $\epsilon_l(q)$ is

TABLE I. The values of Mott constant $aN_c^{1/3}$.

Method of calculation	Dielectric function used	Trial wave function	$aN_c^{1/3}$
Experimental	...	...	0.21 (Ref. 9)
Variational method	Hubbard-Sham	Hulthen	0.290 (Ref. 3)
	Effective Hubbard-Sham	Hulthen	0.317 (Ref. 5)
Numerical integration	Hubbard-Sham	...	0.295 (Ref. 7)
	Effective Hubbard-Sham	...	0.412 (Present work)

given by

$$\epsilon_I(q) = 1 + \frac{4\pi e^2}{Kq^2}\frac{3N}{2E_F}\left[\frac{1}{2}\frac{4k_F^2-q^2}{8k_Fq}\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right] \times \left[1-\frac{q^2}{2(q^2+k_F^2+\delta^2)}\right] , \tag{6}$$

where

$$k_F = (3\pi^2 N/\nu)^{1/3} , \tag{7}$$

and

$$\delta^2 = 4(3N/\nu\pi)^{1/3}/a . \tag{8}$$

ν is the number of the valleys of the semiconductor, which is 6 for silicon. $\epsilon_{\text{eff}}(q)$ reduces to $\epsilon(q)$ as used in Ref. 7 if we put $A = B = 0$ and $\alpha = \infty$. We choose the effective Rydberg $R^* = m^*e^4/2\hbar^2K^2$ and effective Bohr radius $a = K\hbar^2/m^*e^2$ as units of energy and distance, respectively. The numerical values of $m^*,K,A,B,\alpha,\beta,\gamma$ used in our work are the same as in Ref. 6. In order to solve Eq. (2) one needs $V(r)$ which may be generated by the anti-Fourier-transform of $V(q)$. For this purpose a fast-Fourier-transform routine is used.

To find the Mott constant $aN_c^{1/3}$ the following numerical procedure was adopted. Because of the dielectric screening, the potential $V(r)$ goes to zero for large values of r. Thus, outside some radius R the potential is put equal to zero. The radial equation is integrated numerically out to this radius with $E = 0$, and then matched to the solution of the outer region through the continuity condition

$$R\left[\frac{d}{dr}\ln F(r)\right]_{r=R} = -1 , \tag{9}$$

for different values of $aN^{1/3}$. The value of $aN^{1/3}$, which satisfies the continuity condition, Eq. (9), for a wide range of R, is chosen as the value of the Mott constant $aN_c^{1/3}$.

The donor ground-state energies for all concentrations were determined by the following procedure. Since we are interested in the bound states only, we put $E = -|E|$. The continuity condition for finite values of $aN^{1/3}$ is given by

$$R\left[\frac{d}{dr}\ln F(r)\right]_{r=R} + R\sqrt{|E|} = -1 , \tag{10}$$

and for $aN^{1/3} = 0$, it becomes

$$\left[\frac{d}{dr}\ln F(r)\right]_{r=R} = -1 , \tag{11}$$

since, in the latter case, the potential does not go to zero, but varies as $1/r$ for large values of r.

For a given value of $aN^{1/3}$, the relevant Eq. (2) is integrated numerically out to a large radius R for different values of $|E|$. The value of $|E|$ for which the continuity condition, Eq. (10) or Eq. (11), is satisfied for a wide range of R, is chosen as the energy eigenvalue.

The value of $aN_c^{1/3}$ obtained by using the effective Hubbard-Sham dielectric function in Eq. (2) is given in Table I along with earlier theoretical and experimental estimates. We find that the inclusion of the spatial variation of the host dielectric function increases the value of $aN_c^{1/3}$. This increase in the value of $aN_c^{1/3}$ observed in the numerical method is larger than the increase in the value of $aN_c^{1/3}$ observed in the variational method.

The ground-state energies are estimated as functions of $aN^{1/3}$ using both the Hubbard-Sham and effective Hubbard-Sham dielectric functions in Eq. (2). The results are presented in Fig. 1. The donor binding energies calculated using the effective Hubbard-Sham dielectric function in Eq. (2) are larger than the energies calculated using the

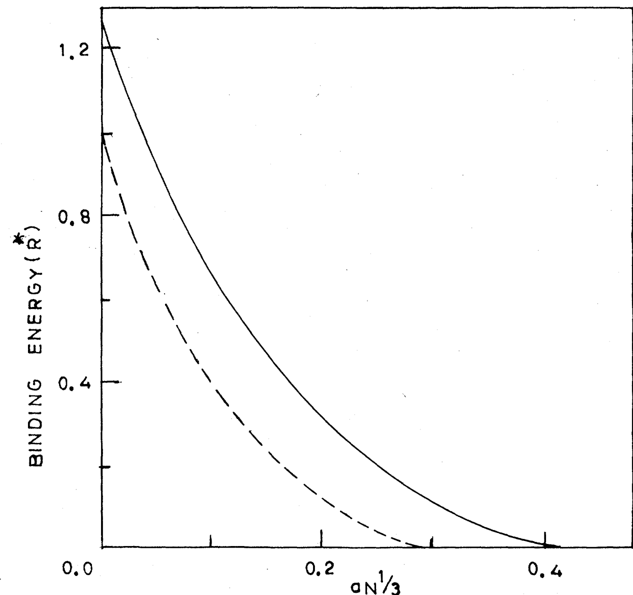

FIG. 1. Variation of donor binding energy in Si, with impurity concentration expressed as $aN^{1/3}$. (— — —), Hubbard-Sham screening; (——), effective Hubbard-Sham screening.

Hubbard-Sham dielectric function in Eq. (2) for all impurity concentrations.

When we compare the results based on the variational method using Hulthen-type trial function[3] and the result obtained by Martino *et al.*,[7] the variational estimates look reasonably accurate, thus showing the merit in the choice of trial function. With the effective Hubbard-Sham dielectric function, the results based on our variational calculation[5] and the present work show considerable difference in the critical constant, thus possibly showing that the choice of trial function in Ref. 5 may have to be better. It appears hard to solve the relevant Schrödinger equation with the mass anisotropy included.

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