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Effect of disorder on the Mott constant in n-type semiconductors

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We have extended our calculation of the Mott constant in n-type semiconductors based on the Krieger-Nightingale model incorporating the effects of disorder through a model statistical impurity potential. Several impurity potentials are considered. Donor binding energies, $\langle r^2 \rangle$, and the radial probability density are presented as functions of the impurity concentration. The Mott constant obtained with disorder included agrees better with experimental results. The donor binding energy as a function of the impurity concentration is fitted to a power law, and the least-squares estimates of the fitting parameters are given.

I. INTRODUCTION

The metal-insulator (MI) transition in doped semiconductors has been a subject of intense study for over thirty years.[1] In the original Mott picture,[2] the transition was considered to be due to electron correlation and would occur when the interimpurity separation approached the effective Bohr radius a^*.

Mott's model was extended by Krieger-Nightingale[3] using screened impurity potentials and including the many-valley nature of the conduction band-minima in silicon and germanium. The present authors[4] used impurity potentials incorporating an effective dielectric function of the host crystal and impurity electrons and calculated variationally the donor binding energy for different impurity concentration, n, and obtained the Mott constant $a^* n_c^{1/3}$ in silicon. The effect of electron-mass anisotropy was also considered in a subsequent paper.[5] Numerical integration[6,7] of the relevant Schrödinger equation yielded values for the Mott constant much higher than the experimental value.

Another approach to estimate the critical concentration at which the MI transition occurs is based on the Hubbard model and the calculations involve the estimates of the on-site Coulomb repulsion between two electrons and the transfer integral in a lattice of impurities. The results obtained by Berggren's calculations,[8] using isotropic single-particle wave function yielded reasonable value for the critical concentration n_c. More exact calculations,[9] taking into account the anisotropy in the donor ground-state wave functions in Si, gave somewhat higher value for n_c.

In the Anderson model disorder plays the essential role in the MI transition. In this picture a sufficiently large random potential makes the system an insulator. Scaling ideas are used for MI transition in such disordered systems.[10] Assuming that the MI transition is arising due to topological disorder, Bauer *et al.*[11] estimated the Mott constant around 0.22 to 0.26 depending on the form of the off-diagonal matrix elements assumed.

The purpose of the present paper is to report the results of our calculations based on the Krieger-Nightingale model but incorporating disorder in the impurity distribution. In Sec. II we give the model used; Sec. III contains numerical results and Sec. IV gives discussions and conclusions.

II. THEORETICAL MODEL

The concentration-dependent donor binding energy is calculated by solving the Schrödinger equation in the effective-mass theory

$$[(-\hbar^2/2m^*)\nabla^2+v(\mathbf{r})]\psi(\mathbf{r})=E\psi(\mathbf{r}) , \tag{1}$$

where the potential energy $v(\mathbf{r})$ is the $3d$ Fourier transform (FT) of

$$V(\mathbf{q})=-4\pi e^2/K\epsilon_{\text{eff}}(\mathbf{q})q^2 . \tag{2}$$

$\epsilon_{\text{eff}}(\mathbf{q})$ in Eq. (2) is the effective dielectric function given by

$$\epsilon_{\text{eff}}(\mathbf{q})=\epsilon_h(\mathbf{q})+\epsilon_I(\mathbf{q})-1 , \tag{3}$$

where $\epsilon_h(\mathbf{q})$ is the dielectric function for the host semiconductor having a value K as $q \rightarrow 0$ and $\epsilon_I(\mathbf{q})$ is that due to the impurity electrons treated as a free-electron gas.

The disorder due to the random distribution of the impurities is introduced in the above potential as follows and the new potential is written as v_d. The impurity potential $v(r)$ is treated as a statistical quantity with $p(t)dt$ giving the probability of finding the given value of $v(r)$ within the interval t and $t+dt$, where $t=|v(r)|$. We take the probability density function[12] $p(t)$ as

$$p(t)=(1/\mu)\exp(-t/\mu) , \tag{4}$$

where μ is a parameter of the distribution. μ may be obtained as the first moment of the distribution:

$$\mu=n\int |v(r)|4\pi r^2 dr , \tag{5}$$

where n is the concentration of impurities. If the integral in Eq. (5) does not converge, μ is taken as the square root of the second moment σ given by

$$\sigma=n\int |v(r)|^2 4\pi r^2 dr . \tag{6}$$

We write

$$v_d = XP(|X|) \, , \tag{7}$$

where $X = v(r)$ at a given value of r and

$$P(|X|) = \int_0^{|X|} p(t)dt \, . \tag{8}$$

One gets the potential which incorporates the disorder of impurities, based on the distribution in Eq. (4):

$$v_d(r) = v(r)\{1 - \exp[-|v(r)|/\mu]\} \, . \tag{9}$$

III. NUMERICAL RESULTS

The unit of energy used is the effective rydberg $R^* = m^* e^4/2\hbar^2 K^2$ and the unit of distance is the effective Bohr radius $a^* = K\hbar^2/m^* e^2$. The energy eigenvalues of Eq. (1) are obtained by numerical integration of the resultant radial Schrödinger equation by the Runge-Kutta method with "matching in the middle."[13,14]

The potentials $v(r)$ used in our present work are listed in Table I with relevant typical values of μ. The donor energies are obtained for various values of $a^* n^{1/3}$ until the energy becomes very near to zero, thus finding the value of Mott constant $a^* n_c^{1/3}$.

Calculations are done with $v_d(r)$ of Eq. (9) in the radial Schrödinger equation and also with $v(r)$ $[v_d(r) \rightarrow v(r)$

TABLE I. Potentials used in this work.

1. Thomas-Fermi potential

$V(r) = (-2/r)\exp(-r/L)$, $\mu = 8\pi n L^2$

$L^2 = (3\pi^2/\nu)^{1/3}/(12\pi a^* n^{1/3})$

ν is the number of valleys

$a^* n^{1/3}$	0.05	0.10	0.15	0.20	0.24
μ ($\nu=1$)	0.0051	0.0206	0.0464	0.0824	0.1187

2. Hubbard-Sham potential

$v(r)$ is the Fourier transform of $\{-8\pi/q^2[\epsilon_h(q) + \epsilon_I(q) - 1]\}$

$\epsilon_h(q)$ is taken as a constant $= 1$

$$\epsilon_I(q) - 1 = \frac{\nu\delta^2}{q^2}\left[1 - \frac{q^2}{2(q^2 + k_F^2 + \delta^2)}\right] f(q, k_F)$$

$$f(q, k_F) = \tfrac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln\left|\frac{2k_F + q}{2k_F - q}\right|$$

$\delta^2 = 4(3n/\nu\pi)^{1/3}/a^*$, $k_F = (3\pi^2 n/\nu)^{1/3}$

k_F is the Fermi wave number

$a^* n^{1/3}$	0.05	0.10	0.15	0.20	0.25
μ ($\nu=1$)	0.1256	0.2740	0.4324	0.5981	0.7699
μ ($\nu=4$)	0.1134	0.2475	0.3905	0.5399	0.6941
μ ($\nu=6$)	0.1112	0.2429	0.3833	0.5298	

3. Effective Hubbard-Sham potential $v(r)$ as is defined in part 2 and $\epsilon_I(q) - 1$ as is given in part 2.

$$\frac{1}{\epsilon_h(q)} = 1 + \frac{Kq^2}{q^2 + \alpha^2} - \frac{KAq^2}{q^2 + \beta^2} - \frac{KBq^2}{q^2 + \gamma^2}$$

K	A	B	α	β	γ
12.0	0.0726	0.0107	26.635	36.674	12.132

$a^* n^{1/3}$	0.05	0.10	0.15	0.20	0.25
μ ($\nu=6$)	0.1858	0.4737	0.8633	1.3032	1.7973

TABLE II. Values of Mott constant $a^*n_c^{1/3}$.

Potential $v(r)$	No. of valleys ν	$a^*n_c^{1/3}$ with disorder	without disorder
Thomas-Fermi	1	0.24	0.35[a]
	4	0.09	0.13
	6	0.07	0.10
Hubbard-Sham	1	0.29	0.43[a]
	4	0.25	0.30[a]
	6	0.24	0.29[a]
Effective Hubbard-Sham	6 (Silicon)	0.25	0.41[b]

Experimental value of $a^*n_c^{1/3}=0.26$[c]

[a] Reference 7.
[b] Reference 6.
[c] Reference 15.

when $\mu \to 0$]. In the case of Thomas-Fermi potential, if the value of the Mott constant for a semiconductor with ν_1 valleys is obtained, the value of the Mott constant for another semiconductor with ν_2 valleys can be calculated using the relation

$$a^*n_c^{1/3}|_{\text{with } \nu_2 \text{ valleys}} = (\nu_1/\nu_2)^{2/3} a^*n_c^{1/3}|_{\text{with } \nu_1 \text{ valleys}} . \quad (10)$$

Our results for $a^*n_c^{1/3}$ are presented in Table II which also shows earlier estimates. Typical results of donor binding energies as functions of $a^*n^{1/3}$ for the semiconductors using the above-mentioned potentials with and without disorder obtained are presented in Figs. 1–3.

We have also plotted $r^2|R(r)|^2$ for different concentration using potentials listed in Table I. Typical results for silicon ($\nu=6$) are presented in Fig. 4. $\langle r^2 \rangle$ for silicon as functions of $a^*n^{1/3}$ are also obtained and presented in Fig. 5.

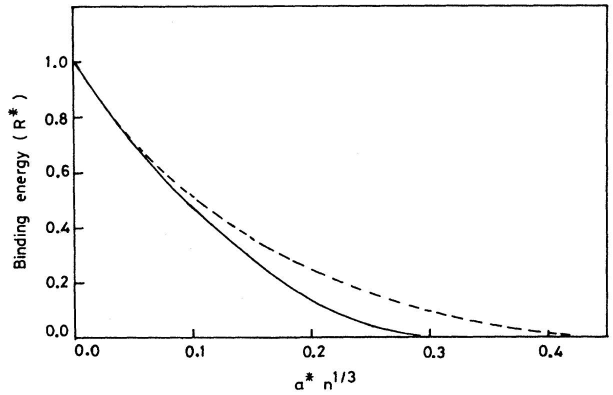

FIG. 1. Variation of donor binding energy with impurity concentration in a single-valley semiconductor for the Hubbard-Sham potential; dashed curve denotes no disorder; solid curve denotes disorder.

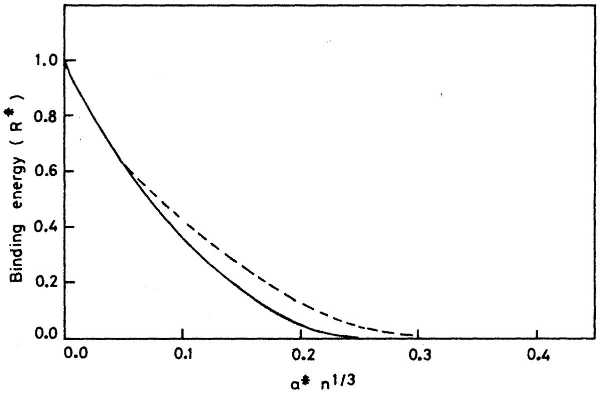

FIG. 2. Variation of donor binding energy with impurity concentration in a four-valley semiconductor for the Hubbard-Sham potential; dashed curve denotes no disorder; solid curve denotes disorder.

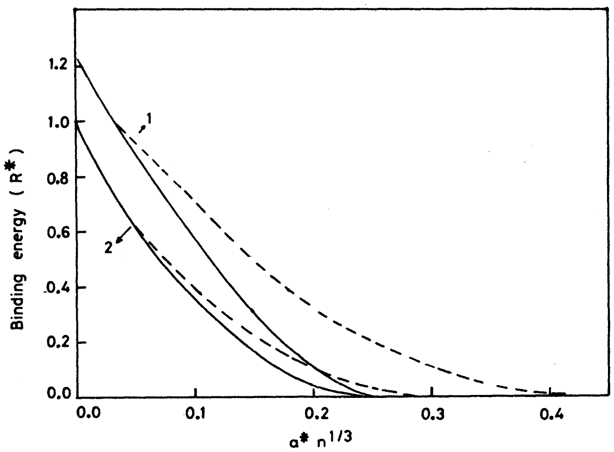

FIG. 3. Variation of donor binding energy with impurity concentration in a six-valley semiconductor. Curve 1 represents the effective Hubbard-Sham potential. Curve 2 represents the Hubbard-Sham potential. Dashed curve denotes no disorder. Solid curve denotes disorder.

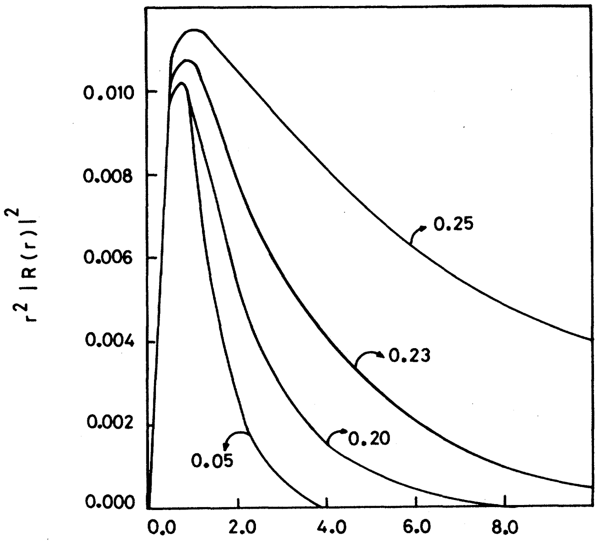

FIG. 4. Radial probability density vs radial distance r in silicon. The numbers by the side of a curve give the value of $a^*n^{1/3}$. The results are for the effective Hubbard-Sham potential with disorder.

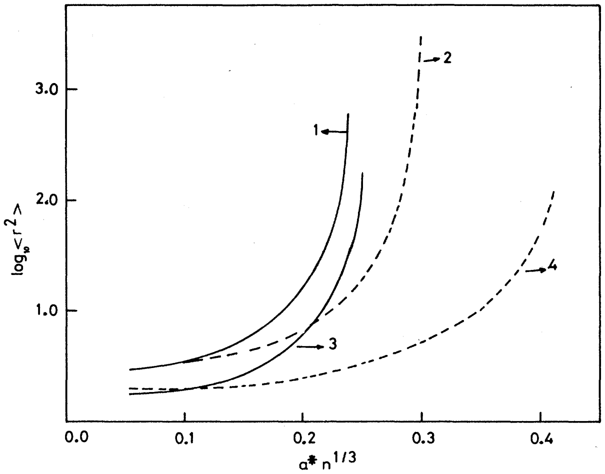

FIG. 5. Variation of $\langle r^2 \rangle$ with impurity concentration expressed as $a^*n^{1/3}$. Curves 1 and 2 represent the Hubbard-Sham potential. Curves 3 and 4 represent the effective Hubbard-Sham potential. Solid curves denote disorder. Dashed curves denote no disorder. The results are for silicon, a six-valley semiconductor.

The concentration-dependent donor binding energies are fitted to a form

$$\frac{E}{E_0-E}=\eta\left[\frac{n_c}{n}-1\right]^{\zeta}, \tag{11}$$

where E_0 is the binding energy for $n=0$ and n_c is the critical concentration. The least-squares estimates of η and ζ are given in Table III.

IV. DISCUSSIONS AND CONCLUSIONS

From Table II we find that when disorder is included the Mott constant $a^*n_c^{1/3}$ at which E is zero is in good agreement with the experimental value[15] of 0.26, for the Thomas-Fermi potential for the single-valley semiconductor, for the Hubbard-Sham potential for multivalley semiconductors, and for the effective Hubbard-Sham potential for silicon. However, in the case of the Hubbard-Sham potential for the single-valley semiconductor, $a^*n_c^{1/3}$ comes out as 0.29 while without disorder the value was 0.43. For $\nu=4$ and 6 the Thomas-Fermi potential does not yield acceptable values for the Mott constant even when disorder is included.

Figures 1–3 show that the effect of disorder becomes important as the impurity concentration is large. In the case of extreme dilution there is no difference in the binding energies with and without disorder. Once the disor-

TABLE III. Values of fitting parameters η and ζ. The values given within the parentheses are for the potentials without disorder.

Potential and No. of valleys	η (10^{-3})	ζ
Thomas-Fermi		
$\nu=1$	26.5 ±1.1	1.21 ±0.05
	(13.16±0.06)	(0.901±0.004)
Hubbard-Sham		
$\nu=1$	70.18±0.41	0.972±0.005
	(37.76±0.03)	(0.972±0.001)
$\nu=4$	56.9 ±1.1	1.21 ±0.02
	(47.59±0.29)	(1.109±0.006)
$\nu=6$	56.5 ±1.4	1.21 ±0.03
	(46.37±0.43)	(1.153±0.009)
Effective Hubbard-Sham		
$\nu=6$	91.1 ±1.1	1.07 ±0.02
	(55.96±0.09)	(0.985±0.001)

der becomes important (as seen from the large difference in the binding energies with and without disorder) the nature of the potential used seems to be not so important.

The radial probability distribution plotted in Fig. 4 indicates the delocalization of the electron near the critical concentration. The radial probability density, however, has its peak value at about the same radial distance for all concentration. The results are qualitatively the same for all the potentials used.

Figure 5 shows the divergence of $\langle r^2 \rangle$ near the critical concentration n_c. Since $\langle r^2 \rangle$ is qualitatively related to the donor polarizability,[16] our results indicate the nonlinear increase of donor polarizability.

Table III shows that the value of ζ is around 1.0. With the effective Hubbard-Sham potential, ζ turns out to be 1.07. The value of η is systematically larger for the disordered case than for the case neglecting disorder. Critical exponents for the binding energies have not been reported earlier. The exponents for the conductivity data and the dielectric susceptibility[1] are, respectively, 0.55 and 1.15.

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