Metal-insulator transitions in doped silicon and germanium

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The effect of including conduction-band minima into the calculation of metal-insulator transitions proposed for doped silicon is investigated with use of the variation of the effective wave function and the interference factor due to the minima. The calculations are extended for doped germanium. Good agreements with experiments are found.

In a recent paper, Park et al.[1] have used the Hubbard tight-binding Hamiltonian to investigate the metal-insulator (M-I) transitions in doped Si in the way of Berggren's[2] approach for doped Si and Ge. Berggren[2] considered the anisotropy of the host conduction band (HCB), replacing it by a spherical isotropic charge distribution, as well as the possibility of working with the isotropic HCB. For both cases an interference factor,[3,4] derived from the many-valley character of the HCB, is reduced to $v^{-1/2}$, v being the number of valleys (minima). Park et al.[1] have instead assumed, for Si, an average in this oscillating term, proposed by Bhatt,[5] as a better choice to investigate the transitions. They have also included in the calculation the concentration (N) dependence of the dielectric constant and the wave function. The purpose of this comment is to calculate the M-I transitions for both doped Si and Ge considering the N dependence of the effective Bohr radius and Berggren's[2] scheme for averaging the oscillatory factor. The N dependence of the effective dielectric constant will be neglected in the calculation. Such dependence was shown in Ref. 1 not changing results for transition much.

We describe the transition, as in the Hubbard tight-binding Hamiltonian, from an insulating to a metallic state when

$$W/U \approx 1 \qquad (1)$$

is satisfied. Here W is the unperturbed bandwidth of an array of one-electron states. It is related to the hopping integral T, with adjacent sites i and j, as

$$W = 2Z \, |T| \, , \qquad (2)$$

where Z is the coordination number for a particular arrangement of centers, and T is defined by

$$T = \int \psi_i^*(\mathbf{r})H_1\psi_j(\mathbf{r})d\mathbf{r} \, , \qquad (3)$$

where H_1 is the one-particle Hamiltonian including the kinetic energy operator and the electron-donor interactions. The wave function is written as[1-6]

$$\psi_i(\mathbf{r}) = \frac{1}{\sqrt{v}} \sum_{l=1}^{v} F_l(\mathbf{r})\phi_l(\mathbf{r}) \, , \qquad (4)$$

where $\phi_l(\mathbf{r})$ is the Bloch function associated with the lth of the v conduction-band minima of the HCB ($v=6$ for

silicon and $v=4$ for germanium), and $F_l(\mathbf{r})$ is a hydrogenic envelope function in which the effective mass at each of these minima has been assumed to be isotropic. Thus the calculation is simplified, since the envelope function can be written, in terms of a donor-concentration dependence $a_x^*(N)$, as

$$F_l[r,a_x^*(N)] = [\pi a_x^{*3}(N)]^{-1/2}\exp[-r/a_x^*(N)] \, , \qquad (5)$$

where a_x^* is the effective Bohr radius for a system like Si:X or Ge:X, with $X =$ Sb, P, or As. The term U represents the well-known intradonor Coulomb interactions, or correlation energy.[7] Equation (3) can be written as (from now on we will omit the a_x^* dependence in N)

$$T = -\frac{e^2}{\kappa a_x^*} \left[K + \frac{S}{2} \right] I \, , \qquad (6)$$

TABLE I. The critical concentration in doped Si and Ge.

Host	Donor	N_c (10^{18} cm^{-3}) Theor.	N_c (10^{18} cm^{-3}) Expt.	a_x^* (Å)[a,b]
Si	Sb	3.0[c]	3.0[d]	16.6
		2.8[e]		
		2.8[f]		
	P	3.9[c]	3.5[d]	15.2[b,g]
		3.6[d]	3.7[h]	
		3.6[e]		
	As	4.9[c]	6.4[d]	14.1
		4.8[d]	8.5[i]	
		4.6[e]		
Ge	P	0.23[e]	0.25[j]	38.7
	As	0.26	0.35	37

[a]$a_x^* = a_{Sb}^*$, a_P^*, or a_{As}^*.
[b]Reference 9.
[c]Calculation with constant Bohr radius a_x^* and dielectric constant ϵ_0, Ref. 1.
[d]Reference 11.
[e]Donor-concentration dependencies of $\epsilon_0(N)$ and $a_x^*(N)$, Ref. 1.
[f]Present calculation.
[g]Reference 15.
[h]Reference 12.
[i]Reference 13.
[j]Reference 14.

where S and K are the overlap and the transfer energy integrals,[7] respectively, between impurity sites and

$$I = \frac{1}{v} \sum_{l=1}^{v} \exp(i\mathbf{k}_l \cdot \mathbf{R}) \qquad (7)$$

is the interference factor, with $\mathbf{k}_l$ being the Bloch waves at the HCB minima. Such factor, following Berggren[2] and Miller and Abraham,[8] can be easily obtained for an isotropic HCB as $v^{-1/2}$ for both doped Si and Ge. Bhatt's[5] scheme, for Si, gives $\approx (v/2)^{-1}$. In our calculation we will adopt the former approach as well as the variational method to $a_x^*(N)$.

The calculations are performed assuming that the impurities are distributed over a regular lattice [simple cubic (sc), bcc, and diamond] of the host material (i.e., Si or Ge), averaging these different arrangement of the impurities and minimizing the energy with the many-valley correction.

In order to compare with previous works we adopt $\Delta W/U = 1.15$ as the criterion for the critical concentration N_c. The results are given in Table I. For the effective Bohr radii in Si and Ge, we adopt the values of Ref. 9. Such values do not differ much from the ratio between the ionization energies[10] scaled for the isochoric systems Si:P (Refs. 13, 16, and 17) and Ge:As, respectively, but for Si:As. Our results for Si are not much altered when compared to the results of Ref. 1.

Taking into account the variation of the dielectric constant in a straightforward calculation, which in addition involves other approximations, Park et al.[1] have shown that such additional variation has a minor quantitative effect on the transitions. Within our calculation the results for Si and Ge already show fair agreement when compared to the calculations for Si and available experimental data.

Owing to the effects of randomness,[18] anisotropic wave functions,[18,19] spin ordering, and central-cell effects[5] in real doped Si and Ge (which are neglected in our scheme) one should not expect the values of N_c be absolute values when comparing with experiments, but a good estimation for N_c. For instance in the particular case of Ge:Sb, which has a negligible central-cell effect,[20] the value of N_c increases by a factor of ≈ 2.2 by application of a rather modest stress,[19] i.e., N_c(stress, 1 valley)$\approx 2.2 N_c$(zero stress, 4 valleys).[19,20] In addition such stress on the isolated envelope function with the contribution of the valleys was found not to be enough to cause such large difference in N_c.[21] Bhatt[19] has shown that in such situation the anisotropy of the donor wave function is the main responsible for the increasing of N_c. Then, even with our value of $N_c \approx 1.3 \times 10^{17}$ cm^{-3} for Ge:Sb, with $a_{Sb}^* = 45.5$ Å,[9] compared to N_c(expt)$\approx 0.95 \times 10^{17}$ cm^{-3},[14] one has to account for such anisotropic effect, which certainly will affect the bandwidth of this system and directly affect the impurity critical concentration.

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