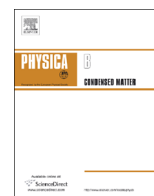




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Optical bandgap in various impurity-Si systems from the metal–insulator transition study

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ABSTRACT

In different impurity-Si systems, our expressions for spin-polarized ground-state energy, spin-polarized chemical potential energy, and spin susceptibility have been investigated and also compared with other theoretical-and-experimental results. That gives rise to a satisfactory description of some physical properties such as: metal–insulator transition of the first (or second) order, explored from the spin-polarized ground-state energy (or spin susceptibility), and optical bandgap, obtained from the spin-polarized chemical potential energy obtained in the metallic phase.

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1. Introduction

Doped indirect-bandgap Si is the basis of the modern electronics industry. Consequently, one would expect that its parameters are well understood. There exist two very important parameters observed in the n(p)-type doped Si (DS) at temperature $T=0$ K.

- (i) The first is the critical impurity density N_c [1–8], marking the metal-to-insulator transition (MIT) from the localized side ($N \leq N_c$) to the extended side ($N \geq N_c$), N being the total impurity density. Those values of N_c in various impurity-Si systems have been obtained from the theoretical conductivity study [1–5] or from measurements of temperature-dependent conductivity and Hall effect for $T > 1.7$ K [6–8].
- (ii) The second is the optical bandgap ($E_{g1n(p)}$) [or the reduced bandgap ($E_{g2n(p)}$)] defined in the heavily doped indirect-bandgap Si by: $E_{g1n(p)} \equiv E_{g2n(p)} + E_{Fn(p)}$. Here, $E_{Fn(p)}$ denotes the Fermi-energy level penetration into the majority-conduction (valence) band, and $E_{g2n(p)}$ the energy difference between the conduction-band edge and valence-band edge, being both perturbed by ionized donors (acceptors), respectively. Further, the observed values of $E_{g1n(p)}$ have been obtained from optical

absorption measurements [9]. Furthermore, the theoretical results of $E_{g2n(p)}$ have been obtained from chemical-potential energies, due to the majority carrier exchange-correlation, minority carrier correlation, and majority carrier-impurity interaction, obtained in a Thomas–Fermi screening model [10–15]. Of course, this model is only valid in the degenerate case ($N \gg N_c$) and wrong at low values of N , as that discussed in our previous work [16].

The purpose of the present paper is to investigate the numerical results of N_c and $E_{g1n(p)}$ in various impurity-Si systems. The treatment is based on our expressions for spin-polarized ground-state energy, spin susceptibility, and spin-polarized chemical potential energy, obtained from our accurate screening model, being valid at any N [16]. Moreover, our values of N_c are determined from the spin-susceptibility singularities at $N = N_c$, at which metal-to-insulator transitions (MITs) occur.

In Section 2, some values of band-structure parameters needed to our numerical calculations are presented. Then, in the heavily doped Si (HDS), some physical properties of the bandgap narrowing, reduced bandgap and optical bandgap in the n(p)-type HDS are presented and discussed in Section 3. In Section 4, our analytic expressions for spin-polarized ground-state energy, spin susceptibility, and spin-polarized chemical potential energy are investigated and applied to determine N_c and $E_{g1n(p)}$. Finally, numerical

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Table 1Band-structure parameters of the pure Si at 0 K. Here, $A = 10^{-8}$ cm.

E_{go} (meV)	$g_{c(v)}$	ϵ_0	m_n	m_p	a_{Bn} (Å)	a_{Bp} (Å)	Ry_n (meV)	Ry_p (meV)
1170	3(2)	11.4	0.3216	0.3664	18.76	16.465	33.666	38.36

results and concluding remarks are obtained and discussed in Sections 5 and 6, respectively.

2. Band-structure parameters

First of all, we present in the following Table 1 some band-structure parameters of the n(p)-type DS at 0 K, needed to the following numerical calculations, such as: the intrinsic bandgap: E_{go} [16], effective average number of equivalent conduction (valence)-band edge: $g_{c(v)}$, dielectric constant: ϵ_0 [2,12], effective electron (hole) mass to free electron mass m_0 : $m_{n(p)}$ [16,20,21], effective Bohr radius defined by

$$a_{Bn(p)} = a_{Bo} \times \frac{\epsilon_0}{m_{n(p)}}, \quad (1)$$

and effective Rydberg by

$$Ry_{n(p)} \equiv \frac{e^2}{2\epsilon_0 a_{Bn(p)}}. \quad (2)$$

Here, $a_{Bo} = (0.5292 \times A)$ is the Bohr radius obtained in the uniform three-dimensional electron gas (U3DEG) [22–27], $A \equiv (10^{-8} \text{ cm})$ being an angstrom.

In Table 1, our choice of $g_{c(v)} = 3(2)$ can be compared with the corresponding one by Rosenbaum et al. [2], 2(2), and also with its usual value: 6(2) given in the literature. Such a choice of $g_{c(v)}$ will be justified in Section 5.

Moreover, in the n(p)-type DS, the Wigner–Seitz radius, characteristic of interactions and related to the impurity density N , is defined by

$$r_{sn(p)} \equiv \frac{(3g_{c(v)}/4\pi N)^{(1/3)}}{a_{Bn(p)}} = r_{so} g_{c(v)}^{(1/3)} (a_{Bo}/a_{Bn(p)}), \quad (3)$$

where $r_{so} \equiv (3/4\pi N)^{(1/3)}/a_{Bo}$ is the one defined in the U3DEG. Therefore, when going from the U3DEG to the DS, one simply replaces r_{so} by $r_{sn(p)}$.

Further, the Fermi wave number is defined by

$$k_{Fn(p)} \equiv \frac{1}{\alpha(3g_{c(v)}/4\pi N)^{(1/3)}} = \frac{k_{Fo}}{g_{c(v)}^{(1/3)}}, \quad \alpha = \left(\frac{4}{9\pi}\right)^{(1/3)}, \quad (4)$$

where $k_{Fo} \equiv (1/\alpha(3/4\pi N)^{(1/3)})$ is defined in such the U3DEG.

From Eqs. (3) and (4), we can thus establish the universal relations in both DS and U3DEG as

$$\alpha r_{sn(p)} k_{Fn(p)} a_{Bn(p)} = \alpha r_{so} k_{Fo} a_{Bo} = 1. \quad (5)$$

Furthermore, the relative spin polarization is defined by

$$-1 \leq \zeta \equiv (n^\uparrow - n^\downarrow)/N \leq 1. \quad (6)$$

Here, $N = (n^\uparrow + n^\downarrow)$, and n^\uparrow and n^\downarrow being the up-and down-spin carrier densities, noting that the particular values of ζ ($=0$ and ± 1) respectively denote the paramagnetic-and-ferromagnetic states in the U3DEG, corresponding also to the metal-and-insulator phases in the DS.

3. Physical properties of the bandgap narrowing, reduced bandgap and optical bandgap

Some physical properties of the optical bandgap $E_{g1n(p)}$ for $N \geq N_c$ given in the n(p)-type HDS and defined in Section 1, are further discussed as follows.

- Since, by the Fermi–Dirac statistics, the states below (or above) the Fermi-energy level are filled (or empty), the fundamental optical transitions to states below (or above) the Fermi-energy level are thus forbidden, according to the photon energy: $h\nu \leq E_{g1n(p)}$. That can thus explain such the above definition of “the optical bandgap” [18]. Hence, the absorption edge should shift to higher energies by $h\nu \geq E_{g1n(p)}$.
- Further, it should be noted that the absorption coefficient for a transition with phonon absorption is proportional to the phonon number, $N_p \equiv (e^{E_p/k_b T} - 1)^{-1}$, defined by the Bose–Einstein statistics for any longitudinal-or transverse-acoustic phonon energy E_p . So, $N_p = 0$ at $T=0$ K, according to the vanishing phonon-absorption coefficient.
- Furthermore, it is possible to conserve momentum by a scattering process such as: carrier–carrier scattering or by impurity scattering [18]. Thus, in those cases, the scattering probability is proportional to N , and the phonon assistance is not needed as discussed in (b). The optical absorption coefficient at $T=0$ K is defined by [18]:

$$\alpha_{n(p)}(h\nu) \equiv CN(h\nu - E_{g1n(p)})^2 \geq 0,$$

at the photon energy $h\nu \geq E_{g1n(p)}$ and for any N , where C is a constant [9,12,18]. So, $\alpha_{n(p)}(h\nu) = 0$ at the optical bandgap $h\nu = E_{g1n(p)} \equiv E_{g2n(p)} + E_{Fn(p)}$.

- A high doping perturbs both the conduction-and-valence bands [10–18] by forming respective exponential band tails, at perturbed majority conduction (valence) band-edge (or at mobility conduction (valence) band-edge [2]),

$$E_{cn(vp)} \equiv E_{co(vo)} \mp \Delta E_{cn(vp)}, \quad \Delta E_{cn(vp)} > 0,$$

and at perturbed minority valence (conduction) band-edge,

$$E_{vn(cp)} \equiv E_{co(vo)} \pm \Delta E_{vn(cp)}, \quad \Delta E_{vn(cp)} > 0.$$

As a result, the unperturbed conduction (valence) band-edge $E_{co}(E_{vo})$ is shifted downwards (upwards) by an amount equal to $\Delta E_{cn(vp)}$ ($\Delta E_{vn(cp)}$). In particular, for carrier-impurity interactions, those amount are found to be represented by:

$$\Delta E_{cn(vp)}^{e(h)-D(A)} (\Delta E_{vn(cp)}^{h(e)-D(A)}) \equiv -\mu_{n(p)}^{e(h)-D(A)} (-\mu_{n(p)}^{h(e)-D(A)}).$$

Here, in the n(p)-type HDS, $-\mu_{n(p)}^{e(h)-D(A)}$ physically represents the contribution of spin-polarized chemical potential energy due to the majority electron (hole)-ionized donor (acceptor) [e(h)-D(A)]-interaction screened Coulomb potential energy. Then, $-\mu_{n(p)}^{h(e)-D(A)}$ is that due to the minority hole (electron)-ionized donor (acceptor) [h(e)-D(A)]-interaction screened Coulomb potential energy, being assumed to be here equal to: $-\mu_{p(n)}^{h(e)-D(A)}$ given in the p(n)-type HDS. It should be noted that those assumptions due to the high-doping effect have been used also in our previous works [19] to study the n(p)-type photoluminescence and electroluminescence in doped GaAs crystals by band (tail)–tail (band) and tail–tail transitions, respectively.

So, the reduced bandgap (RBG) in the n(p)-type HDS is defined by

$$RBG \equiv E_{g2n(p)} \equiv E_{cn(p)} - E_{vn(p)} \equiv E_{go} - \Delta E_{gn(p)} \leq E_{go}. \quad (7)$$

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