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Spin susceptibility and effective mass in shallow doubly doped semiconductor systems

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In light of a recent investigation of the conductivity and metal-insulator transition in the shallow double donor Si:P,As, the spin susceptibility χ_s and effective mass m^* of the systems Si:P,As and Si:P,Sb have been calculated. The electronic systems are described by a Gutzwiller scheme to finite temperature. The results for the doubly doped systems predict an enhancement of m^* and χ_s similar to that of the single-donor system Si:P in the vicinity of the transition.

The spin susceptibility χ_s, effective mass m^*, and metal-insulator (MI) transition have been widely studied in recent years for single-donor states in doped semiconductors,[1] and yet the nature of the state near the transition remains unclear.[2-4] Recently Newman and Holcomb[5] (NH) reported measurements of electrical conductivity in the shallow double-donor system Si:P,As and found its critical concentration N_c for the MI transition between the N_c of the shallow single-donor system Si:P and Si:As. In the wake of their measurements we have worked out a single method that provides an N_c for the MI transition, a first step to study further these doubly doped systems, which have a merit of increasing disorder because of the different impurity binding energies present in them.[6] In a real system the impurities will, of course, be randomly distributed, but we shall ignore this randomness and assume that the impurities are distributed over a regular lattice (sc, fcc, bcc, and diamond) (Refs. 7–11) of the host material (i.e., silicon in our case), and then average these different arrangements of the impurities as well as the different type of hopping integrals $T_{ij}^{\alpha,\beta}$, which appear in the calculation.[6] The randomness produces band tailing[12] and as a result the MI transition will be at a lower concentration.

The method used in our calculation for χ_s and effective mass was illuminated in part by the Chao and Berggren[13] (CB) formulation for spin susceptibility in the shallow single-donor system Si:P in terms of the Gutzwiller variational treatment[14-20] to finite temperature.[21] Such formulation has led Ferreira da Silva[22] to find a good scheme for χ_s, which gives a satisfactory agreement between theory and experiment.

Following the CB scheme[13] we may find the spin susceptibility at finite temperature $\chi_s(T)$ as

$$\chi_s(T)=\eta_x(T)\chi_0(T) , \tag{1}$$

where $\chi_0(T)$ is the Pauli spin susceptibility[13] and $\eta_x(T)$ is

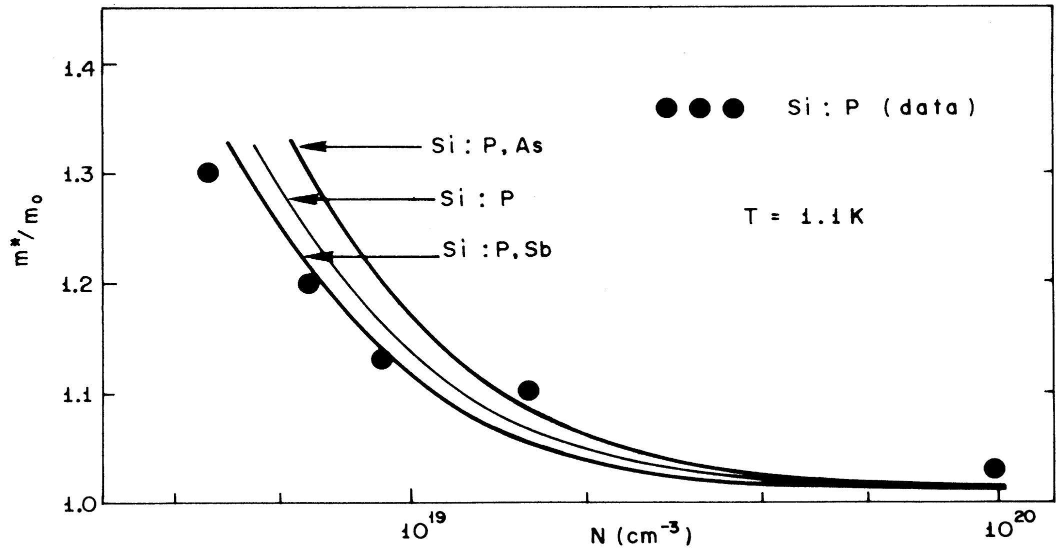

FIG. 1. Effective mass m^*/m_0 as a function of concentration N at $T=1.1$ K. Solid curves correspond to the present calculations. Solid circles correspond to observed values of Ref. 26.

the enhancement factor

$$\eta_x(T)=D(T)^{-1}\left[1-\frac{\chi_0(T)U[1+U/2U_0(T)]}{2\mu_B^2[1+U/U_0(T)]}\right]^{-1} . \tag{2}$$

In Eq. (2) U is the intradonor Coulomb interaction or correlation energy, given by the experimental value $U=0.96E_B$ (E_B being the ionization energy of the system considered),[22] μ_B is the Bohr magnetron, $U_0(T)$ is a critical correlation energy as a function of the free energy at $U=0$,[13] and $D(T)^{-1}$ is identified as the effective mass[15,17]

$$m^*/m_0=D(T)^{-1}=\{1-[U/U_0(T)]^2\}^{-1} , \tag{3}$$

where m_0 is the bare band mass.

The electronic effective mass will enhance $\chi_s(T)$ as the MI is approached from the metallic side, with a dependence on the Hubbard U.[22] The quantities $\chi_0(T)$ and $U_0(T)$ are also dependent on the hopping energy.[13] In our scheme we define the hopping integrals for doubly doped systems as $T_{ij}^{\alpha,\beta}$, with adjacent sites i and j and screened parameters α and β. These latest parameters, α and β, are defined for two different kinds of donors, with differing values of the impurity binding energy, E_B, i.e., $\alpha=1/a_p^*$ and $\beta=1/a_x^*$, where $a_x^*=e^2/2\kappa E_B^x$ is the effective Bohr radius for a system like Si:X, with $X=$Sb, P, or As. $T_{ij}^{\alpha,\beta}$ are defined by

$$T_{ij}^{\alpha,\beta}=\int \psi_i^{\alpha *}(\mathbf{r})H_1\psi_j^{\beta}(\mathbf{r})d\mathbf{r} , \tag{4}$$

where H_1 is the one-particle Hamiltonian including the kinetic-energy operator and the electron-donor interactions. Here the wave function is written as[6–9,11,23,24]

$$\psi_i^{\alpha}(\mathbf{r})=\frac{1}{\sqrt{\nu}}\sum_{l=1}^{\nu}F_l^{\alpha}(\mathbf{r}-\mathbf{R}_i)\phi_l(\mathbf{r}) , \tag{5}$$

for the ground state associated with ν equivalent conduction-band minima ($\nu=6$ for Si). ϕ_l is the Bloch function at the lth minima and $F_l(\mathbf{r})$ are the screened hydrogenic wave functions. Equation (4) can be scaled to the binding energy E_B of Si:P and written as

$$T_{ij}^{\alpha\beta}=-\frac{e^2}{\kappa a_p^*}\left[K_{ij}^{\alpha,\beta}+\frac{S_{ij}^{\alpha,\beta}}{2}\right]I , \tag{6}$$

where κ is the dielectric constant, $S_{ij}^{\alpha,\beta}$ and $K_{ij}^{\alpha,\beta}$ (from now on we will omit the subscripts i and j) are, respectively, the overlap and the transfer energy integrals between impurity sites and

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

where $\mathbf{k}_l$ are the wave vectors at the CB minima.

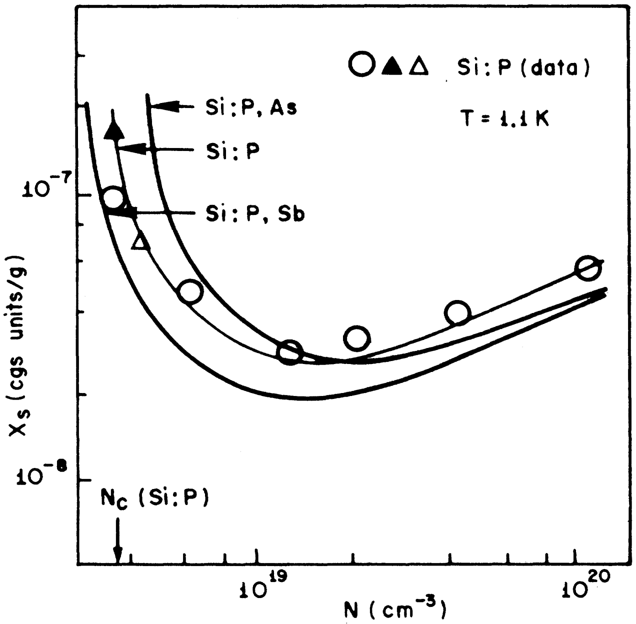

FIG. 2. The spin susceptibility χ_s as a function of concentration N at $T=1.1$ K. Solid curves correspond to the present calculations. Symbols correspond to the measured samples; ○, Ref. 27; ▲, Ref. 28; △, Ref. 29.

The expressions for the matrix elements of S and K are obtained as

$$S^{\alpha,\beta}=S^{\beta,\alpha}=\frac{8y^{5/2}}{(1-y^2)^2}\left[1+\exp(1-y)R^*+\frac{1-\exp(1-y)R^*}{(1-y^2)R^*}\right]\exp(-R^*) , \tag{8}$$

$$K^{\alpha,\beta}=\frac{4y^{1/2}}{(1-y^2)}\left[1+\frac{2[1-\exp(1-y)]R^*}{(1-y^2)R^*}\right]\exp(-R^*) , \tag{9}$$

and

$$K^{\beta,\alpha}=\frac{4y^{1/2}}{(y^2-1)}\left[1+\frac{2y[1-\exp(y-1)R^*]}{(y^2-1)R^*}\right]\exp(-R') , \tag{10}$$

where $y=a_x^*/a_p^*$ (i.e., the ratio of the different impurity binding energies), $R^*=R/a_x$, and $R'=R/a_p$, R being the separation between donor states.

For $y\rightarrow 1$ Eqs. (8) and (9) reduce to the very well known Slater's integrals[25] $S=(1+w+w^2/3)\exp(-w)$ and $K=(1+w)\exp(-w)$, where $w=R/a_x^*$. Then the calculation turns out to be for a single-donor system like Si:P or Si:As.

The calculations are performed, for both Si:P,As and Si:P,Sb (as well as for Si:P) assuming an average in Eq. (6)

due to the oscillating term I,[11] as well as the different arrangements of the donors and differents types of hoppings (i.e., $T^{\alpha,\alpha}$, $T^{\alpha,\beta}$, $T^{\beta,\alpha}$, $T^{\beta,\beta}$). It is worth mentioning that the different binding energies introduced by a double-donor system give a different hopping energy when compared to a single-donor system, e.g., at a certain concentration the bandwidths are different and certainly will be the shape of the impurity bands for both systems, which lead to different $\chi_s(T)$, m/m^*, and N_c.

The results for the effective mass m^*/m_0 at $T=1.1$ K are shown in Fig. 1 for different systems. The qualitative agreement between theory and experiment[26] for Si:P is satisfactory. In Fig. 2 we show the spin susceptibility $\chi_s(T)$ for the same systems presented in Fig. 1. A good agreement with the existing data for $T=1.1$ K is found for Si:P. The MI transitions take place at N_c(Si:P,Sb)$=3.2\times10^{18}$ cm^{-3}, N_c(Si:P)$=3.5\times10^{18}$ cm^{-3}, and N_c(Si:P,As)$=4.5\times10^{18}$ cm^{-3}. The experimental values for the two latest N_c are 3.7×10^{18} cm^{-3} and 5.1×10^{18} cm^{-3}, respectively.[5] In a Mott-Hubbard picture[6] we found 3.4×10^{18} cm^{-3} and 4.6×10^{18} cm^{-3}, respectively. These quantities lead to a transition in the following order: N_c(Si:P,Sb)$<N_c$(Si:P)$<N_c$(Si:P,As). For χ_s and m^*/m_0 we also observe an enhancement around N_c as (m^*/m_0)(Si:P,Sb)$<(m^*/m_0)$(Si:P)$<(m^*/m_0)$(Si:P,As) and χ_s(Si:P,Sb)$<\chi_s$(Si:P)$<\chi_s$(Si:P,As). The parameters used in the calculation were compiled from Refs. 6, 11, and 30. Further experimental and theoretical works on these doubly doped systems could be of interest to test the model.

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