Impurity conductivities in compensated semiconductor systems

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In light of recent measurements of the transport properties in compensated semiconductor systems, we report a calculation for the low-temperature dc electrical conductivity of the systems Si:P and Ge:Sb as a function of concentration and compensation. The effects of disorder are taken into account in the calculation. With increasing compensation the conductivity follows the trend of the experimental results. For uncompensated systems the results agree fairly well with experiments.

In the past few years, much attention has been paid to the measurements of the transport properties of compensated semiconductor systems.[1-8] Adding compensation, for instance, results in a higher impurity critical concentration N_c for the metal-insulator (MI) transition,[3,4] lowering the conductivity σ, which produces a broader σ as a function of concentration.[1-7] The lowering of σ provides a better description of the scaling theories of localization above the Mott minimum metallic conductivity.[1,9]

Bearing in mind these recent measurements, we report here a calculation of the low-temperature dc electric conductivity for the uncompensated and compensated Si and Ge doped with P and Sb, respectively, using no adjustable parameters as explained below. The compensation is related to the donor and acceptor concentration N_D and N_A, according to $K=N_A/N_D$. The net donor concentration is defined as $N=N_D-N_A$.

The impurity conductivity has been investigated by a one-band Matsubara-Toyozawa (MT) configuration-average model[10] and a two Hubbard-MT bands scheme,[11-15] which combine the electron-correlation and disorder effects. The MT model has been used recently, for instance, to study the impurity states in low dimensional disordered systems.[16-18].

Following the argument of MT to approximate the average of the two-particle Green's function into a product of one-particle Green's functions, Lü *et al.*[13] calculated the conductivity for a Hubbard-type Hamiltonian with correlated operators representing electron transfers with four different local environments, and a Chandrasekhar's correlated two-particle wave function for the D^- state. This wave function also has been used in computer simulation.[19] In a recent numerical calculation for the density of states, a shift in energy of the D^- state has shown a similar result.[20] It was observed that both analytical and numerical results show a reasonable agreement for the density of states. The result obtained by Lü *et al.*[13] for the conductivity is similar to previous works on the Hubbard-MT (two-band) and one-band MT schemes. In the wake of all these above results, we will ignore the effects of electron-electron interactions as well as the vertex correction, keeping the random nature of the impurity in the sense of the MT model. Although this correction has not been justified rigorously, the decoupling approximation has been commonly accepted by almost every author to study the impurity conductivity in disordered semiconductor systems.[10-15,24]

The one-band MT model has been improved through the introduction of the alternant-molecular-orbital (AMO) method calculation for the matrix elements in the MT–Green's-function results.[21-23] This AMO-MT scheme yields an enhanced density of states[21] of the impurity bands and gives rough agreement between the calculated and the measured electric conductivities, above the MI transition,[23] when compared to the Hubbard-MT scheme.[12-15]

The AMO-MT (Refs. 21 and 23) scheme starts from a one-body tight-binding Hamiltonian

$$H=E_d\sum_i |i\rangle\langle i|+\sum_{i\neq j} V_{ij}|i\rangle\langle j| , \tag{1}$$

where E_d is the donor ionization energy, which is taken as our energy origin, V_{ij} is the energy integral for the transfer of an electron from the ith site to the jth site (i.e., a hopping matrix). This V_{ij} matrix will be calculated by the AMO method.[21,23] The reader should refer to the previous works for details.

The impurity density of states $D(E)$ is calculated from the Green's functions

$$G_{ij}^{(\pm)}(E)=\langle 0|a_i[1/(E-H\pm i\varepsilon)]a_j|0\rangle , \tag{2}$$

with configuration averaging over the random distribution of impurities. Defining[10,16,21,23]

$$\xi^{(\pm)}(E)=Z_\pm\langle G_{ij}^{(\pm)}(E)\rangle , \tag{3}$$

where $\langle\cdots\rangle$ refers to the configuration averaging and $Z_\pm=E\pm i\varepsilon$, we arrive at the coupled equations

$$\xi^{\pm}=(1-\eta)^{-1} \tag{4}$$

and

$$\eta=1-\frac{1}{\xi^{\pm}(E)}=\frac{N\xi^{\pm}(E)}{(2\pi)^3 Z_+^2} =\int\frac{v(\mathbf{K})^2 d\mathbf{K}}{1-[N\xi^{\pm}(E)v(\mathbf{K})/Z_+]} , \tag{5}$$

where N is the impurity concentration given by $N_D - N_A$, and $V(\mathbf{K})$ is the Fourier transform of V_{ij}. The density of states is then

$$D(E) = iN(\xi^+ - \xi^-)/2\pi E \ . \tag{6}$$

The low-temperature impurity dc conductivity σ_{LT} is calculated making use of the equation derived by Kubo[10,23–25]

$$\sigma = \lim_{\eta \to 0^+} \int_0^\infty dt \int_0^\beta d\lambda \exp(-\eta t) \langle \mathbf{J}(-it\lambda)\mathbf{J}(t) \rangle \ , \tag{7}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant and $\mathbf{J}$ is the current operator. Decoupling the current-current Green's function into a sum of products of Green's functions connecting impurity sites, evaluated at the Fermi energy E_F for different compensation $K = N_A/N_D$, the equation for σ then reads[15,22,24–27]

$$\sigma = \frac{e^2\gamma}{3\hbar} = \int \Xi(E) \left\{ \frac{-df(E)}{dE} \right\} dE \ . \tag{8}$$

Here $f(E)$ is the Fermi distribution function, γ is the number of valleys of the conduction band ($\gamma = 6$ for Si, $\gamma = 4$ for Ge),[26] and

$$\Xi(E) = \Xi_1(E) + \Xi_2(E) \ , \tag{9}$$

where

$$\Xi_1(E) = \frac{1}{32\pi^5} \int \left[\frac{1}{V(\mathbf{K})} \frac{dV(\mathbf{K})}{d\mathbf{K}} \right]^2 \left[2\mathrm{Im} \left[\frac{N\xi^+}{N\xi^+ - Z_+/V(\mathbf{K})^{-1}} \right] \right]^2 d\mathbf{k} - \frac{1}{(2\pi)^2} \times \int R^2 V(\mathbf{R})^2 \left[\frac{1}{(2\pi)^2} \int e^{i\mathbf{K}\cdot\mathbf{R}} \mathrm{Im} \left[\frac{\xi^+}{Z_+} \frac{N\xi^+}{N\xi^+ - Z_+/V(\mathbf{K})} \right] d\mathbf{K} \right]^2 d\mathbf{R} \tag{10}$$

and

$$\Xi_z(E) = \frac{1}{4\pi^2} \int R^2 V(R)^2 d\mathbf{R} \left[\frac{1}{8\pi^3} \int d\mathbf{K}\, e^{i\mathbf{K}\cdot\mathbf{R}} \left\{ \frac{\xi}{Z_+} \frac{N\xi^+}{N\xi^+ - Z_+/V(\mathbf{K})} - \frac{\xi^+}{Z_-} \frac{N\xi^-}{N\xi^- - Z_-/V(\mathbf{K})} \right\} \right] . \tag{11}$$

From. Eq. (8), we can use the low-temperature expansion to obtain

$$\sigma_{LT} = \sigma + \Delta\sigma \ , \tag{12}$$

where

$$\Delta\sigma = \frac{\pi^3}{18} (K_B T)^2 \left[\frac{1}{D(E_F)} - \left[\frac{dD(E)}{dE} \frac{d\Xi(E)}{dE} \right]_{E=E_F} - \frac{d^2\Xi(E)}{dE^2} \bigg|_{E=E_F} \right] . \tag{13}$$

The decoupling approximation, to which we referred above, has gone into obtaining the latter expressions. In deriving the ensemble average of Eq. (9), we are required to calculate the average of a product of two Green's functions as

$$\langle G_{kl}(E) G_{mn}(E) \rangle \cong \langle G_{kl}(E) \rangle \langle G_{mn}(E) \rangle \ . \tag{14}$$

This means that certain terms, arising from the correlated diagrams of the two Green's functions, are neglected. It is difficult to estimate the effects of such terms in the calculation, although MT claim that they are less important at high concentrations.[10,14,15] It is worthwhile to say that, by performing impurity averaging only in $\langle G \rangle$ and not $\langle GG \rangle$, the possibility of localization is lost. Since the model does not localize, the comparison of the conductivity with experiments must break down on the insulating side of the MI transition.

In Fig. 1, we show the low-temperature dc conductivi-

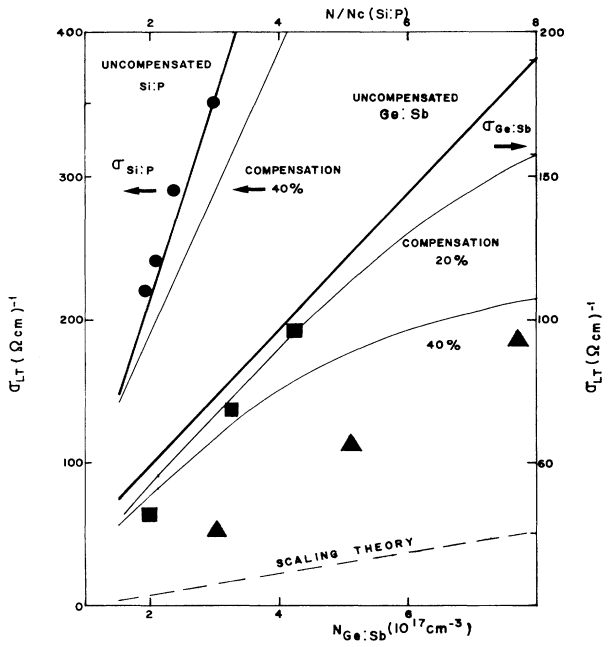

FIG. 1. Theoretical and experimental low-temperature conductivity σ_{LT} as a function of concentration, for uncompensated and compensated Si:P and Ge:Sb systems. Solid curves correspond to the present model. Solid circles represent the data for Si:P (upper scale), Refs. 3–6 and 28. Solid squares ($\leq 5\%$) and triangles ($\sim 36\%$) represent the data for Ge:Sb, Ref. 1.

ty for Si:P and Ge:Sb as a function of concentration and compensation for $T=4$ K. For uncompensated systems, we find rough agreement with the experiments above $N_c \cong 4.0\times10^{18}$ cm^{-3} for Si:P,[3-6,28] and $N_c \cong 1.6\times10^{17}$ cm^{-3} for Ge:Sb.[1,2,7] For compensated samples, we find the same behavior as observed in the experimental results for Ge:Sb (Refs. 1 and 2) and Si:P, respectively.[3,5-7] The Bohr radii used in the calculation are obtained from the experimental ionization energy as 15.2 Å for Si:P and 45.5 Å for Ge:Sb.[29]

As the increasing values of the compensation suggest a trending of σ_{LT} toward the estimated sealing theory, we plot this latter result for a visual comparison.[1,9]

A calculation of zero-temperature conductivity also has been carried out by Berggren by means of a diffusion model[30] and a memory-function approach.[31,32] The former model for the uncompensated Si:P system presents a very good agreement with experiment above N_c. The latter approach presents rough agreement with experiment only when the theoretical results are rigidly shifted to experimental N_c.

In summary, our theoretical model for conductivity, valid for above N_c, supports recent investigations of uncompensated and compensated semiconductor systems.[1-8] It is worth pointing out that our scheme does not include localization in the Anderson sense. To incorporate the Anderson localization to the present model, we may apply the scheme introduced by Kamimura.[33,34] But it still is a very intricate problem to be considered.

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