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Relaxation time for ionized impurity scattering in compensated n-type $Hg_{1-x}Cd_xTe$ near $x = 0.2$

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The electron relaxation time, τ_I, for ionized impurity scattering in heavily compensated $Hg_{1-x}Cd_xTe$ ($x \sim 0.2$) is calculated. The Kane model of band structure is used. The τ_I expression differs from that of Szymanska–Dietl because in heavily compensated materials the Brooks–Herring scattering potential is not adapted. The relaxation time depends essentially on the pair correlation function between acceptors and donors. Acceptor and donor concentrations using the Szymanska–Dietl model and our model have been determined for two samples.

1. Introduction

$Hg_{1-x}Cd_xTe$ (MCT), $Hg_{1-x}Zn_xTe$ or $Hg_{1-x}Cd_xSe$ are II–VI compound semiconductors whose energy gaps vary with the content, x, of cadmium or zinc [1,2]. MCT ($x \sim 0.2$) can be used to make infrared detectors operating in the 8–12 μm atmospheric window [3–4]. The efficiency of these detectors is conditioned by the quality of the active layer. Characterization of this active layer can be done using Hall and resistivity measurements at low temperature ($T < 60$K). Carrier mobility can then be deduced in this temperature range where the effects of phonons are weak and carriers are mainly scattered by the electric field of ionized impurities. A compensated n-type semiconductor contains donors (concentration: N_D^+) and acceptors (N_A^-), so the corresponding mobility is a function of $N_D^+ + N_A^-$, whereas $N_D^+ - N_A^-$ occurs in the neutrality equation. We can thus obtain N_D^+ and N_A^- separately by solving both equations simultaneously. We will therefore be able to obtain the total concentrations and energy levels of the doping impurities from thermal variation of their ionic concentrations.

$Hg_{1-x}Cd_xTe$ with $x \leqslant 0.2$ is a narrow or zero gap semiconductor (NGS or ZGS). One of the consequences of this situation is the non-parabolicity of the bands studied by Groves *et al.* in HgTe [5] and by Pidgeon and Brown in InSb [6]. Kane's model [7] is generally used to describe the conduction band of NGS or ZGS. The small effective density of states in the conduction band very often induces degeneracy for n-type materials.

Several papers have reported experimental and theoretical studies of carrier mobility in NGS or ZGS [8–13]. Szymanska and Dietl [11] established the relaxation time due to ionized impurity scattering for NGS or ZGS. Their expression rests on the Brooks–Herring type Fourier transform of the diffusing potential [14]. We show, in Section 2, that this treatment is not applicable in heavily compensated n-type $Hg_{1-x}Cd_xTe$ ($0.19 \leqslant x \leqslant 0.21$). Considering this situation in Section 3, we develop an expression of the electron relaxation time for ionized impurity scattering. We follow the Szymanska–Dietl calculation but modify the Fourier transform of the diffusion potential as proposed by Falicov and Cuevas [15]. In Section 4, we compare experimental results with both theories. A final conclusion is given in Section 5.

2. Existing theory and validity range

In the following, we consider elastic electron scattering and suppose that the impurities are singly ionized.

2.1. Existing theory

For a semiconductor with non-parabolic bands (NGS or ZGS) Szymanska and Dietl [11] used properly mixed s-type and p-type electron wave functions given by Kane [7] and obtained for the relaxation time

$$\frac{1}{\tau_I} = \frac{2\pi e^4 N_I}{\hbar^3 \kappa^2} \frac{m^*}{k^3} F_{imp} \tag{1}$$

where $\kappa = 4\pi\varepsilon_0\varepsilon_L$ (ε_L is the lattice constant), $\hbar = h/(2\pi)$, h: Planck's constant, m^* the electron effective mass, e the electron change, $k = \|\mathbf{k}\|$ with $\mathbf{k}$ the electron wave vector and F_{imp} is given by

$$F_{imp} =$$

$$\ln(1+\xi) - \frac{\xi}{1+\xi} + 4A'\left[1 + \frac{1}{1+\xi} - \frac{2}{\xi}\ln(1+\xi)\right]$$

$$+ 2B'\left[1 - \frac{4}{\xi} + \frac{6}{\xi^2}\ln(1+\xi) - \frac{2}{\xi(1+\xi)}\right] \quad (2)$$

For F_{imp} we have only considered the first term F'_{imp} (Equations 4.5a and b in [11]) because the second term F''_{imp} becomes significant only for intrinsic ZGS, which is not the case of interest. A' and B' are given by Equation 2.7d in [11]. $\xi = 4k^2\lambda^2$, where λ is the screening length of the screened Coulomb potential $\phi(\boldsymbol{r}) = q/\kappa r \exp(-r/\lambda)$ where q is the charge of the considered impurity, and $\mathbf{r} = \|\mathbf{r}\|$ is the distance from the impurity.

To obtain the expression F_{imp}, Szymanska and Dietl followed the procedure described by Zawadzki and Szymanska [9]. In this procedure, the Brooks–Herring type Fourier transform of the diffusing potential is used. This treatment is based on calculating the charge density around a given impurity as a function of the distance. The solution of Poisson's equation is then obtained after linearization in $q\phi/k_BT$, where k_B is the Boltzmann constant and T is the temperature. For an energy band described by Kane's model [7], this linearization leads to the screening length (Equation A7 in [9])

$$\left(\frac{1}{\lambda}\right)^2 = \frac{2}{\pi}\frac{e^2}{\kappa k_B T}\left(\frac{2m_0^* k_B T}{\hbar^2}\right)^{3/2} {}^{\circ}L_1^{1/2}(\alpha,\beta) = \frac{4\pi e^2}{\kappa}\frac{\partial n}{\partial E_F} \quad (3)$$

where ${}^{\circ}L_1^{1/2}$ is a generalized Fermi integral; $\alpha = E_F/k_BT$, $\beta = k_BT/E_g$, E_F: Fermi energy and E_g: energy gap.

2.2. Validity range of the screening length λ

For an NGS or ZGS, the linearization is valid only if $q\phi \ll E_F$ [9]. This inequality cannot be satisfied at sufficiently small values of r due to the divergence of ϕ. For $r = \lambda$, the condition requires

$$q^2/(2.72\kappa\lambda) \ll E_F \text{ or } \lambda(\text{nm}) \gg \lambda_1 = 528.69/\varepsilon_F E_F(\text{meV}) \quad (4)$$

Moreover, the use of Equation 3 implies that the scattering potential is only screened by electrons. In this case, it is necessary to neglect the interaction of the charged atmosphere about a given ionized impurity with a neighbouring impurity. This means that the screening length is small compared with the distance between ionized impurities. In other words, and if spherical symmetry is assumed, it is valid only if Equation 3 leads to a screening length, λ, that verifies

$$\lambda < \lambda_2 = \left(\frac{3}{4\pi}\right)^{1/3}\left(\frac{1}{N_I}\right)^{1/3} \quad (5)$$

where N_I is the concentration of charged ions.

At low temperatures and for an uncompensated degenerate semiconductor, the number of electrons equals the number of singly ionized impurities and $\lambda_2 = (3/4\pi)^{1/3}(1/n)^{1/3}$, which is the greatest value of λ_2 for a given n. A comparison of λ with λ_1 and λ_2 is shown in Fig. 1a and b for $Hg_{1-x}Cd_xTe$ (x = 19, 20 and 21%) at T = 20 K. Values of E_F are obtained from the well known relation between n and E_F in Kane's band model; the parameters used for calculation are summarized in Table I. We see that $\lambda_1/\lambda < 0.1$ ($\lambda \gg \lambda_1$) only for $n > 3 \times 10^{20}\ \text{m}^{-3}$, $n > 6 \times 10^{20}\ \text{m}^{-3}$ and $n > 10^{21}\ \text{m}^{-3}$ for x = 19, 20 and 21%, respectively. Equation 4 is then verified. But the $N_I = n$ screened ions can be treated as independent scattering centres ($\lambda < \lambda_2$) only for x = 21% and in the concentration range 2×10^{20} to $10^{21}\ \text{m}^{-3}$.

In conclusion, for uncompensated materials, Equations 4 and 5 cannot be simultaneously satisfied.

For a compensated degenerate semiconductor the screening length, λ, is still given by Equation 3 and λ_2 by Equation 5, but with $N_I > n$. If the two conditions

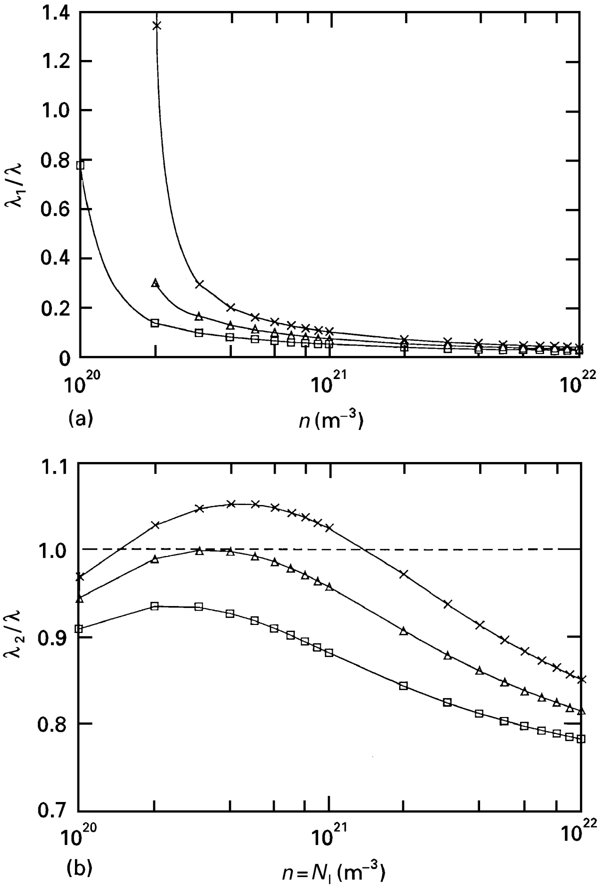

Figure 1 Variation (a) λ_1/λ versus electron concentration, n, and (b) λ_2/λ versus concentration of ionized impurities, $N_I = n$, for $Hg_{1-x}Cd_xTe$ at T = 20 K: (□) x = 0.19, (△) x = 0.2, (×) x = 0.21.

TABLE I Values of parameters for $Hg_{1-x}Cd_xTe$

Quantity	Value	Reference
Γ_6–Γ_8 energy gap $E_g(x, T)$ (eV)	$-0.302 + 1.93x$ $+ 5.35 \times 10^{-4}(1-2x)T$ $- 0.81x^2 + 0.832x^3$	[16]
Lattice constant, ε_L	$20.5 - 15.6x + 5.7x^2$	[13]
Momentum matrix element coupling, P, between conduction and valence band, eV cm	$1.953 \times 10^{-5}(18 + 3x)^{1/2}$	[17]
Spin-orbit splitting, Δ, eV	$-0.53x + 0.37x^3 + 1.08$	Fit with data in [18]

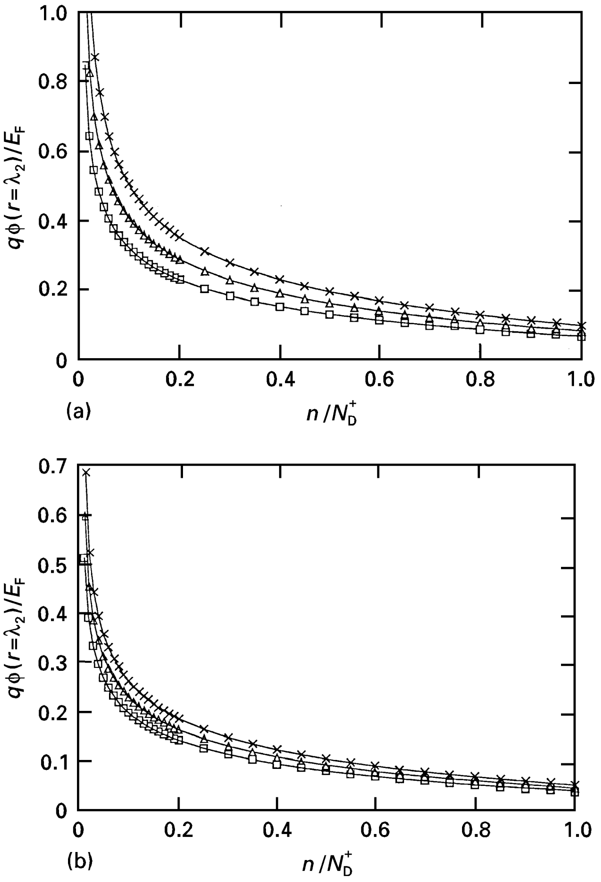

Figure 2 Variation of $q\phi(r = \lambda_2)/E_F$ versus n/N_D^+ for $Hg_{1-x}Cd_xTe$ at $T = 20$ K and (a) $n = 10^{21}$ m^{-3}, and a screening length of λ, and (b) $n = 10^{22}$ m^{-3} and a screening length of λ_2. (□) $x = 0.19$, (△) $x = 0.2$, (×) $x = 0.21$.

$q\phi(r = \lambda) \ll E_F$ and $\lambda < \lambda_2$ are verified, we must have

$$q\phi(r = \lambda_2) \ll E_F \tag{6}$$

Variations of $q\phi(r = \lambda_2)/E_F$ versus n/N_D^+ ($n = 10^{21}$ and 10^{22} m^{-3}) are shown in Fig. 2a and b for $T = 20$ K. There curves prove that, in heavily compensated $Hg_{1-x}Cd_xTe$ ($19 \leqslant x(\%) \leqslant 21$), the linearization of Poisson's equation in $q\phi/k_BT$ is meaningless and the calculation leading to λ (Equation 3) is no longer valid.

We have now to find a mobility model suited to a heavily compensated non-parabolic conduction band semiconductor. Falicov and Cuevas [15] proposed a modified version of existing theories [14, 19, 20] for ionized impurity scattering. This theory, valid in compensated semiconductors with parabolic bands, depends essentially on the pair correlation function between acceptors and donors. We thus modify the Szymanska–Dietl relaxation time using the scattering potential proposed by Falicov and Cuevas.

3. Modified theory

Because our theory is essentially an extension of that of Szymanska and Dietl [11], which can be applied to a compensated semiconductor, we follow their procedure but with an appropriate Fourier transform of the scattering potential, $\phi(r)$. The transition probability $W(\boldsymbol{k}, \boldsymbol{k}')$ from either the $j_z = 1/2$ or $j_z = -1/2$ state (j_z: electron spin projection on the z-axis) is given by the Equation 3.6 in [9], which can be written in the form

$$W = \frac{2\pi}{\hbar V^2}|q\phi(|\boldsymbol{k}-\boldsymbol{k}'|)|^2\delta[E(k') - E(k)] \times \left\{1 - 4a^2(1-a^2)\sin^4\frac{\theta}{2} + \left[2b^2\left(2c - \frac{b}{2^{1/2}}\right)^2 - 4(1-a^2)\right]\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}\right\} \tag{7}$$

where $|q\phi(|\boldsymbol{k}-\boldsymbol{k}'|)|^2$ denotes the square of the Fourier transform of the potential; a, b and c are the three coefficients appearing in the electron Bloch function of Kane's model, V is the volume, θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$. As the electron scattering is supposed to be elastic, the Dirac function $\delta[E(\mathbf{k}') - E(\mathbf{k})]$ is introduced.

For a spherical energy band with an arbitrary dispersion law having a minimum in $k = 0$, the effective mass entering the general transport theory is not defined as for parabolic bands. One has to consider the energy dependent effective mass given by [21]: $1/m^* = 1/(\hbar^2 k)\,\partial E/\partial k$. The inverse relaxation time can then be deduced from Equation 7 by (Equation 3.7 in [9])

$$\frac{1}{\tau(k)} = \frac{VN}{8\pi^3}\int W(\boldsymbol{k}, \boldsymbol{k}')\,(1 - \cos\theta)\,\mathrm{d}^3k' \tag{8}$$

where N is the number of charged ions in the volume, V.

Falicov and Cuevas [15] considered a compensated n-type semiconductor with a parabolic isotropic dispersion law. Following their treatment, and if a temperature independent exponential distribution is considered, one finds that the Fourier transform of the screened Coulomb potential of an ion is (where $\sigma = |\boldsymbol{k} - \boldsymbol{k}'|$)

$$|q\phi(\sigma)|^2 = \left(\frac{4\pi q^2}{\kappa}\right)^2\frac{(2u^2 + \sigma^2)}{\sigma^2(u^2 + \sigma^2)^2} \tag{9}$$

The static inverse correlation length, u, depending on N_A and N_D, is given by (Equation 2.11 in [15]) $u^3 = 8\pi(N_D - N_A)$.

We are now able to calculate the relaxation time for impurity scattering in compensated $Hg_{1-x}Cd_xTe$ ($19 \leqslant x(\%) \leqslant 21$) by using Equation 9 for $|q\phi(|\boldsymbol{k} - \boldsymbol{k}'|)|^2$.

In the spherical co-ordinate system the only nontrivial integration is over θ. Then, by making the same substitutions as Falicov and Cuevas (Equations 2.13–2.15 in [15]) and replacing Equations 9 and 7 in Equation 8 we obtain for the relaxation time

$$\frac{1}{\tau(k)} = \frac{2\pi e^4 N_I}{\hbar^3\kappa^2}\frac{m^*}{k^3}G_{\mathrm{imp}} \tag{10}$$

where $N_I = N/V$ is the concentration of charged ions.

G_{imp} is given by

$$G_{\mathrm{imp}} = \ln(1+\eta) + \frac{\eta}{1+\eta} + \left\{2b^2\left[2c - \frac{b}{(2)^{1/2}}\right]^2 - 4(b^2+c^2)\right\}\frac{\eta}{1+\eta} - \frac{1}{2}\left\{2b^2\left[2c - \frac{b}{(2)^{1/2}}\right]^2 - 4(b^2+c^2)^2\right\} \times \left[1 - \frac{2}{\eta^2}\ln(1+\eta) + \frac{2}{\eta(1+\eta)}\right] \qquad (11)$$

with $\eta = 4k^2u^{-2}$.

The first two terms in Equation 11 give the Falicov–Cuevas contribution [15] to G_{imp}. The other terms take into account the non-parabolicity of electron dispersion law following Kane's treatment [7]. Very close to the bottom of the band, i.e. for $E \ll E_g$, we have $a \sim 1$ and $b \sim c \sim 0$. Therefore conduction band wave functions contain only the s-component and G_{imp} reduces to the Falicov–Cuevas expression [15] obtained for the parabolic band.

Considering the energy dependent effective mass, electron mobility, μ, is obtained by using the general expression that can be applied to a non-parabolic band with a minimum in $k = 0$ and spherical energy surfaces [22, 23]

$$\mu = \frac{4e}{3h^2 n}\int_0^{\infty} \tau k^2 \left(\frac{\partial E}{\partial k}\right)\left(-\frac{\partial f}{\partial E}\right)\mathrm{d}E \qquad (12)$$

where f is the Fermi–Dirac function.

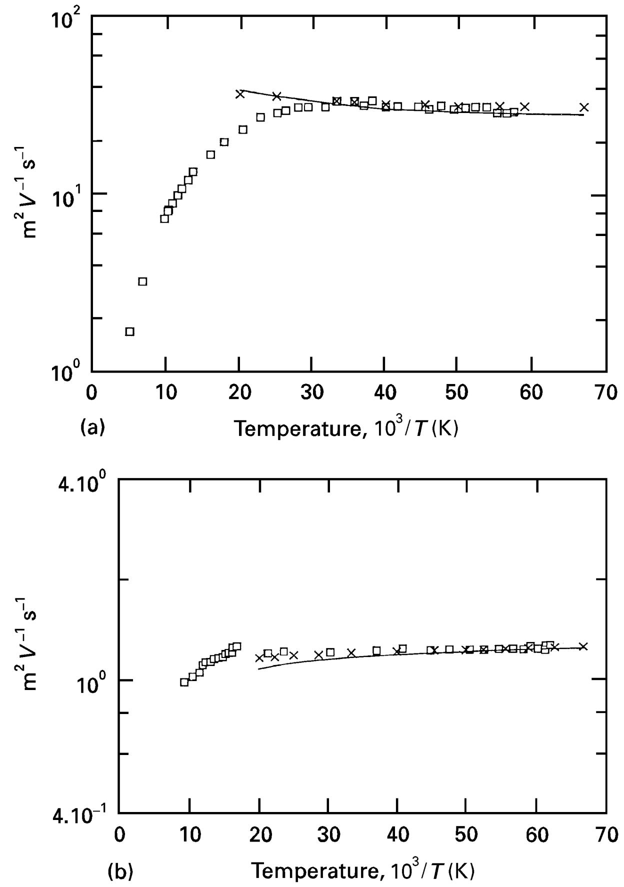

Figure 3 Hall mobility for (a) sample 1, and (b) sample 2. Experimental and theoretical curves (characteristics are given in Table II). (□) experiment, (——) our expression, (×) the Szymanska–Dietl model.

4. Discussion

To show the inadequacy of the approximation of linear screening, we compare both theories with experimental results. Data are for $Hg_{1-x}Cd_xTe$ with $x \sim 19.5\%$ (grown by Travelling Heather Method at S.A.T.: Société Anonyme de Telecommunication). Two samples are considered (values at $T = 20$ K)

sample 1: $n \sim 10^{21}\ \mathrm{m^{-3}}$ and $\mu_n \sim 30\ \mathrm{m^2\,V^{-1}\,s^{-1}}$

sample 2: $n \sim 2\times10^{22}\ \mathrm{m^{-3}}$ and $\mu_n \sim 1\ \mathrm{m^2\,V^{-1}\,s^{-1}}$

Characterization is made by simultaneously solving neutrality and mobility equations over the 20–50 K temperature range where the effects of phonons are weak and carriers are scattered by the electric field of ionized impurities. Both the relaxation times established by Szymanska and Dietl [11] and our modified expression are considered. Fig. 3a and b shows experimental and theoretical curves obtained using the Szymanska–Dietl model and our modified theory. Table II summarizes the N_A and N_D values. We see that it is always possible to find acceptor and donor concentrations to fit the data. But use of the Szymanska–Dietl expression yields $n/N_D^+ \sim 0.38$ and 6.2×10^{-2} for samples 1 and 2, respectively. From Fig. 2a and b we see that the statistical approach leading to λ is dubious for sample 1 and not applicable at all for sample 2 as we must have $q\phi(r=\lambda_2) \ll E_F$ $[q\phi(r=\lambda) \ll E_F$ and $\lambda_2 > \lambda]$. If for lightly doped materials (sample 1), the N_A and N_D concentrations are in the same range, then for heavily doped materials (sample 2) these values differ greatly. Consequently, although the Szymanska–Dietl theory leads to a good fit, the N_A and N_D concentrations obtained are meaningless and unrealistic.

TABLE II Characteristics of the two samples using the Szymanska and Dietl expression or the modified expression. The origin of energy is taken at E_C: bottom of the conduction band

	Szymanska–Dietl expression	Modified expression
Sample 1		
N_A, $\mathrm{m^{-3}}$	1.5×10^{21}	1.2×10^{21}
N_D, $\mathrm{m^{-3}}$	2.4×10^{21}	2.13×10^{21}
n/N_D^+	~ 0.38	~ 0.43
$e\phi(r=\lambda_2)/E_F$	~ 0.25	
λ_2/λ	~ 0.5	
Sample 2		
N_A, $\mathrm{m^{-3}}$	3.0×10^{23}	1.55×10^{24}
N_D, $\mathrm{m^{-3}}$	5.2×10^{23}	2.53×10^{24}
$E_D - E_C$, meV	37.8	37.9
n/N_D^+	$\sim 6.2\times10^{-2}$	1.3×10^{-2}
$e\phi(r=\lambda_2)/E_F$	~ 0.3	
λ_2/λ	~ 0.25	

These two examples demonstrate how correlation between charges has to be necessarily taken into account for a heavily compensated material in the study of electrical behaviour of extended defects in $Hg_{1-x}Cd_xTe$ [24, 25].

5. Conclusions

We have shown that the relaxation time for electron scattering by charged impurities calculated using the Brooks–Herring treatment is not appropriate for compensated (or not) $Hg_{1-x}Cd_xTe$ (MCT) ($0.19 \leqslant x \leqslant 0.21$). A relaxation time expression for impurity scattering in heavily compensated MCT is developed. The calculations are based on the Kane model of band structure, including explicit mixing of p-like components into the total wave function of the conduction band. Following the Falicov–Cuevas treatment, pair correlation function between acceptors and donors is assumed. The relaxation time expression is established considering the temperature independent exponential pair correlation function between acceptors and donors introduced by Falicov and Cuevas. At least we show how experimental results can be misinterpreted.

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