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ROLE OF RECOMBINATION AND IMPACT IONIZATION IN INTERVALLEY REPOPULATION EFFECTS

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It is shown that electron recombination and impact ionization with donors give contribution to the intervalley scattering (IS) in many-valley semiconductors. The IS probability (ISP) due to recombination coincides with the phenomenological ISP which was previously introduced to explain experimental results. The electron concentration n increases monotonically, when the electric field E increases, and it is practically independent of the orientation of **E** relative to crystallographic axes in the range of $E < E_c$, where recombination gives the main contribution to the ISP. n strongly depends on the orientation of **E** for $E > E_c$ and the dependence of n on E may be even N-shape due to strong intervalley repopulation.

IN MANY-VALLEY SEMICONDUCTORS at low temperature T, interaction with forbidden low energy intervalley phonons gives an essential contribution to the intervalley scattering (IS) [1–4] in addition to the allowed high energy phonons [4, 5]. The IS probability (ISP) decreases exponentially as T decreases and is strongly dependent on the electric field strength E [1–4, 6, 7]. This accounts for the divergence between calculated and measured current-voltage characteristics which become very large for small E when the current **j** is parallel to [1 0 0] in n-Si for $T < 45$ K and **j** $\parallel$ [1 1 1] in n-Ge for $T < 20$ K, where the calculated intervalley repopulation steeply increases for infinitesimally small E [2, 3]. An additional E-independent ISP caused by ionized impurities, τ_0^{-1}, was introduced in the calculations of [6, 7] to avoid this divergence and to explain new experimental results on the multivalued electron distribution in n-Si. The τ_0^{-1} was varied in the range $10^7 \div 10^8\ \mathrm{s}^{-1}$ to obtain agreement between theory and experiment at 27 K. In paper [8] the probability W_e of the "elastic" process, in which an electron was scattered directly between valeys by the donor-ion field, was calculated. The W_e was in good agreement with experimental values [9] for As in Ge at 40–90 K, but for Sb in Ge it was small in comparison with experiment. For n-Si the τ_0^{-1} is also sufficiently larger than W_e for ionized impurity concentrations realized in the experiments [6, 7] ($N_D^+ \simeq N_A \simeq (5–9) \cdot 10^{12}\ \mathrm{cm}^{-3}$).

It is shown in this paper that recombination of the electrons with positively charged donors in Si gives the contribution to the IS because the electron recombined from one valley is thermally activated to any other valley with equal probability. Without any parameter, this new ISP coincides with τ_0^{-1} [6, 7], in order of magnitude. The impact ionization may also contribute to the IS.

The variation of carrier concentration with the electric field E due to recombination and impact ionization with the impurity were studied previously for many-valley Ge and Si [10–12]. The quantitative analysis was incomplete because the continuity equation for a one-valley semiconductor was used [10–12]. Here the many-valley semiconductors are studied and the continuity equation is applied for each valley separately [5, 10–12]:

$$\begin{aligned}\operatorname{div} \mathbf{j}_\alpha/e + \partial n_\alpha/\partial t &= -\sum_{\beta=1}^{\lambda} ({}^{n}\alpha/\tau_\alpha - {}^{n}\beta/\tau_\beta) \\ &- [B_{T,\alpha}(N_A + n)\, n_\alpha - A_T(N_D - N_A - n)/\lambda] \\ &+ \sum_{\beta=1}^{\lambda} A_{I,\beta}(N_D - N_A - n)\, n_\beta/\lambda - \\ &- \gamma[A_{I,\alpha}(N_D - N_A - n)\, n_\alpha - \\ &\sum_{\beta=1}^{\lambda} A_{I,\alpha}(N_D - N_A - n)\, n_\beta/\lambda], \quad \alpha = 1 \div \lambda, \end{aligned} \tag{1}$$

e is the electronic charge, j_α and n_α are the current density and the electron concentration in the α valley respectively, λ is the number of valleys. τ_α is the phonon assisted IS time from valley α to valley $\beta \neq \alpha$ [13]. The factors A_T, $B_{T,\alpha}$ and $A_{I,\alpha}$ denote the thermal ionization of the donor, the recombination of the electron from valley α with donors and impact ionization by the primary electron from valley α. N_D, N_A and n are

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concentration of the donors, acceptors and electrons:

$$n = \sum_{\alpha=1}^{\lambda} n_\alpha. \quad (2)$$

In equation (1) the Auger processes are not included, and n will in the following be neglected when compared with N_A and $N_D - N_A$, because only the low temperature and pre-breakdown case is analysed, where $n \ll N_A$, $N_D - N_A$. Thus the model can not describe the impact-ionization-induced negative differential conductivity S-shape (sigmoid) as it is treated, for instance, in paper [14].

It is necessary also to stress that the thermal ionization does not depend on electric field and upon final state valley, i.e. the electron goes with equal probability $A_T(N_D - N_A)/\lambda$ into any valley.

The calculation of the probability of impact ionization from neutral donors in many valley semiconductors has not previously been performed. This is why the parameter γ is introduced to combine in equation (1) two possible ionization processes.

1. $\gamma = 0$. The primary electron from valley β ionizes the secondary electron from a neutral donor with equal probability, $A_{I,\beta}(N_D - N_A)n_\beta/\lambda$, into any of the valleys. The primary electron stays in the same valley β after ionization.

2. $\gamma = 1$. For the secondary electron it is the same as 1, but the primary electron leaves the primary valley and after ionization it may be found with equal probability in any of the valleys. Variation of γ from 0 to 1 gives the opportunity to change the contribution of processes 1 and 2. This parameter is unknown, but we can say at least that there is no reason for $\gamma \equiv 0$ owing to strong energy and momentum exchange between the primary electron and the donor under ionization.

Summing over the α the equation (1) for all valleys gives the continuity equation for the total current

$$\mathbf{j} = \sum_{\alpha=1}^{\lambda} \mathbf{j}_\alpha.$$

In the steady and homogenous state

$$\operatorname{div} \mathbf{j} \equiv \operatorname{div} \mathbf{j}_\alpha \equiv \frac{\partial n}{\partial t} \equiv \frac{\partial n_\alpha}{\partial t} \equiv 0. \quad (3)$$

the continuity equations become simpler. The equation for the total current becomes the equation for the determination of the total concentration n (neglecting $n \ll N_A$, $N_D - N_A$)

$$A_T(N_D - N_D) - \sum_{\beta=1}^{\lambda} [B_{T,\beta} N_A - A_{I,\beta}(N_D - N_A]\; n_\beta = 0. \quad (4)$$

And for each valley α we divide equation (4) by λ and subtract from equation (1) which gives

$$\sum_{\beta=1}^{\lambda} (n_\alpha/\tau_\alpha^* - n_\beta/\tau_\beta^*) = 0, \qquad \alpha = 1 \div \lambda - 1, \quad (5)$$

where

$$1/\tau_\alpha^* = 1/\tau_\alpha + [B_{T,\alpha} N_A + \gamma A_{I,\alpha}(N_D - N_A)]/\lambda. \quad (6)$$

is an effective ISP (from valley α to another valley $\beta \neq \alpha$). The effective ISP is a sum of the phonon assisted ISP, the recombination and type 2 ionization probabilities. (Note that to obtain an out-scattering probability (OSP) from valley α it is necessary to multiply equation (6) by $\lambda - 1$, i.e. by the number of the valleys for IS).

Taking into account equation (2) it is easy to find from equation (6) an ordinary solution [4, 5] for the valley population:

$$n_\alpha = n\tau_\alpha^* / \sum_{\beta=1}^{\lambda} \tau_\beta^*. \quad (7)$$

Substituting (7) in (4) one obtains

$$n = A_T(N_D - N_A)/[B_T^* N_A - A_I^*(N_D - N_A)], \quad (8)$$

where

$$(A_I^*, B_T^*) = \sum_{\alpha=1}^{\lambda} (A_{I,\alpha}, B_{T,\alpha}) n_\alpha / n \equiv \sum_{\alpha=1}^{\lambda} \times (A_{I,\alpha}, B_{T,\alpha}) \tau_\alpha^* / \sum_{\alpha=1}^{\lambda} \tau_\alpha^*. \quad (9)$$

A_I^* and B_T^* depend on $A_{I,\alpha}$ and $B_{T,\alpha}$, respectively in each valley and on the intervalley redistribution (7, 9).

An ordinary Monte Carlo procedure [2, 3, 6, 7, 15] is used, and the ellipsoidal surface of constant energy in each valley α are transformed into spheres and as a consequence an effective electric field

$$E_\alpha = E(m_t/m_1)^{1/3}\,(1 + \sin^2 \phi_\alpha (m_1 - m_t)/m_t)^{1/2} \quad (10)$$

in valley α must be introduced [4, 7]. Here m_t and m_1 are the transverse and longitudinal effective masses, ϕ_α is the angle between electric field $\mathbf{E}$ and longitudinal axes of the valley α. Calculations are performed for n-Si (it means that in the following calculations $\lambda = 3$ i.e. we refer to two valleys on the same $\langle 1\,0\,0 \rangle$ axis as to one valley and we consider g-scattering as an intra valley one) at 27 K with the same scattering parameters as in [6, 7]. $B_{T,\alpha}$ and $A_{I,\alpha}$ are calculated in addition to [6, 7]:

$$B_{T,\alpha} = \sum_{\mathbf{p}} v\sigma_T f_{\mathbf{p},\alpha} / \sum_{\mathbf{p}} f_{\mathbf{p},\alpha}; A_{I,\alpha} = \sum_{\mathbf{p}}{}' v\sigma_I f_{\mathbf{p},\alpha} / \sum_{\mathbf{p}} f_{\mathbf{p},\alpha}. \quad (11)$$

Here $f_{\mathbf{p},\alpha}$ is the distribution function of the electrons in valley α, the prime denotes that summation is restricted to states $\mathbf{p}$ with an energy ϵ greater than ionization

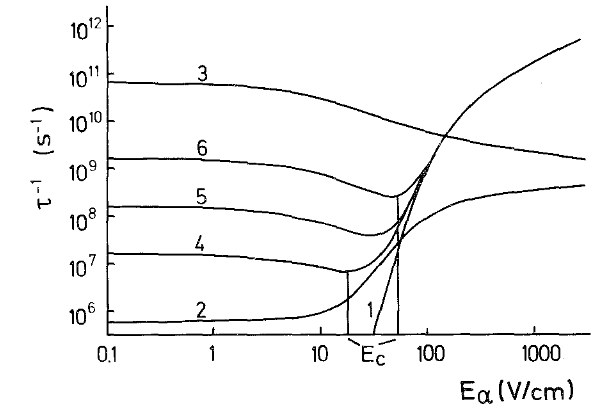

Fig. 1. Dependence of the probability of scattering from valley α due to emission of high energy phonons $1/\tau_1$ (1), emission and adsorbtion of low energy phonons $1/\tau_2$ (2), of the recombination $B_{T,\alpha} \cdot 10^{15}$ cm^{-3} (3) and the ionization $A_{I,\alpha} \cdot 5.5 \cdot 10^{18}$ cm^{-3} (1) probabilities and of the effective probability of out scattering from valley α, $2/\tau_\alpha^*$, for $N_A = 4 \cdot 10^{12}$ cm^{-3} (4), $4 \cdot 10^{13}$ cm^{-3} (5), $4 \cdot 10^{14}$ cm^{-3} (6) on the effective electric field E_α in valley α in n-Si at 27 K.

energy ϵ_I. An ordinary expression for $\sigma_T(\epsilon(\mathbf{p}))$ [16] and $\sigma_I(\epsilon(\mathbf{p}))$ [17] as in one valley isotropic semiconductors were used in each valley owing to the above mentioned transformation.

The calculated dependence of the OSP from valley α, $1/\tau_1$, on the effective electric field E_α is shown in Fig. 1 for high energy ($\hbar\omega_1 \simeq 545$ K) phonons (curve 1), and also for low energy ($\hbar\omega_2 \simeq 210$ K) phonons, $1/\tau_2$ (curve 2). $1/\tau_1$ sharply increases when E_α increases. The dependence of $B_{T,\alpha}$ on E_α is also shown in Fig. 1 (curve 3). It decreases one order of magnitude as E_α varies from 0 to 100 V cm^{-1} and by an additional factor of three as E_α varies from 100 to 1000 V cm^{-1}. It is accepted that for $E_\alpha \to 0$ $B_{T,\alpha} = 6 \cdot 10^{-6}$ cm^3 s^{-1} in accordance with [10, 16, 18].

Let us discuss the dependence of $A_{I,\alpha}$ on E_α. It is well known that for $\epsilon_I/k_BT \gg 1$ A_I depends mainly on ϵ_I/k_BT and $\mathbf{E}$, but not on the detailed dependence of σ_I on ϵ [17]. This was checked in our calculation in the following manner. The ionization energy ϵ_I of shallow donors in Si is close to the energy $\hbar\omega_1 = 545$ K of the high energy intervalley phonon [19], we took $\epsilon_I = \hbar\omega_1$ and performed calculations for

$$\sigma_I = \sigma_0(\epsilon/\epsilon_I - 1)/(\epsilon/\epsilon_i)^{1.25}$$

(from [17]) and for

$$\sigma_I = \sigma_0(2/\pi^{0.5}) \cdot (\epsilon/\epsilon_i - 1)^{0.5},$$

when the energy dependence of the integrand for $A_{I,\alpha}$ (10) is the same as for the emission of $\hbar\omega_1$ phonons. (Note that the normalization factor $2/\pi^{0.5}$ is introduced in order to have the same $A_{I,\alpha}$ for both cases as $E \to 0$).

In both cases the dependences of $A_{I,\alpha}$ on E_α are the same. The probability of the impact ionization varies as $N_D - N_A$ varies and the dependence of this probability on E_α coincides exactly with that of $1/\tau_1$ on E_α for $N_D - N_A = 5.5 \cdot 10^{18}$ cm^{-3} (we chose $\sigma_0 = 9.645 \cdot 10^{-14}$ cm^2 in accordance with [17]). This means that the dependence of $A_{I,\alpha} \cdot 5.5 \cdot 10^{18}$ cm^3 on E_α is defined by curve 1 (Fig. 1) of the dependence of $1/\tau_1$ on E_α. For the Si samples used in [6, 7] ($N_D - N_A \sim 5 \cdot 10^{13}$ $cm^{-3} - 5 \cdot 10^{14}$ cm^{-3}) the contribution of impact ionization to the effective ISP (6) is small, but in Ge, where ϵ_I is up to three times less [19] than the energy of the high energy intervalley phonons ($\hbar\omega \simeq 320$ K), this new mechanism may give larger contribution to $1/\tau_\alpha^*$ (6) than the emission of high energy phonons.

Curves 4–6 in Fig. 1 show the dependence of the effective OSP, $2/\tau_\alpha^*$, on E for three different concentrations of the ionized donors ($N_D^+ = N_A$): $4 \cdot 10^{12}$ cm^{-3}, $4 \cdot 10^{13}$ cm^{-3} and $4 \cdot 10^{14}$ cm^{-3}. Up to $E_\alpha = E_c$ ($E_c \simeq 20$ V cm^{-1} for $N_A = 4 \cdot 10^{12}$ cm^{-3} and $E_c \simeq 50$ V cm^{-1} for $N_A = 4 \cdot 10^{14}$ cm^{-3}) recombination is the main contribution to the effective OSP (6).

We have discussed dependences of $B_{T,\alpha}$, $A_{I,\alpha}$ and τ_α^* on E_α in the valley α. Equation (10) then gives the dependence of E_α on the value and the orientation of the electric field $\mathbf{E}$ with respect to the crystallographic axes. This means that for any given $\mathbf{E}$, we may find the effective field E_α and consequently $B_{T,\alpha}$, $A_{I,\alpha}$, τ_α^* etc. in each valley α. There are some common features which do not depend on the orientation of $\mathbf{E}$ in crystal.

If we chose an electric field E such that in each valley $E_\alpha < E_c$, equation (6) gives $1/\tau_\alpha^* = B_{T,\alpha}N/\lambda$. The products $B_{T,\alpha} \cdot \tau_\alpha^* = \lambda/N_A$ do not depend on α in the numerator of equation (9). This means that all valleys give an equal contribution to B_T^* for any orientation of $\mathbf{E}$. (It is the same with A_I^* for the opposite case when $E_\alpha > E_c$ and $1/\tau_\alpha^* = 1/\tau_\alpha = A_{I,\alpha} \cdot$ const.) If $N_D - N_A$ exceeds N_A by no more than factor of about 10, the contribution of the impact ionization in equation (8) may be neglected at least up to 600 V cm^{-1}. (This is easily seen in Fig. 1 from the dependences of $B_{T,\alpha}$ and $A_{I,\alpha}$ on E_α, because intersection of the curve A_I^* $(N_D - N_A)$ on E with the curve $B_T^* N_A$ on E determines the impact ionization threshold field). In this case $B_T^*(E)$ determines the dependence of n (8) on E, which is given in Fig. 2 (for $N_A = 4 \cdot 10^{12}$ cm^{-3}, $4 \cdot 10^{13}$ cm^{-3} and $4 \cdot 10^{14}$ cm^{-3} and for three directions of the current: $\mathbf{j} \parallel [111]$, $[100]$ and $[110]$). The E_α, $1/\tau_\alpha^*$ and valley population n_α are the same in all three valleys for $\mathbf{j} \parallel$

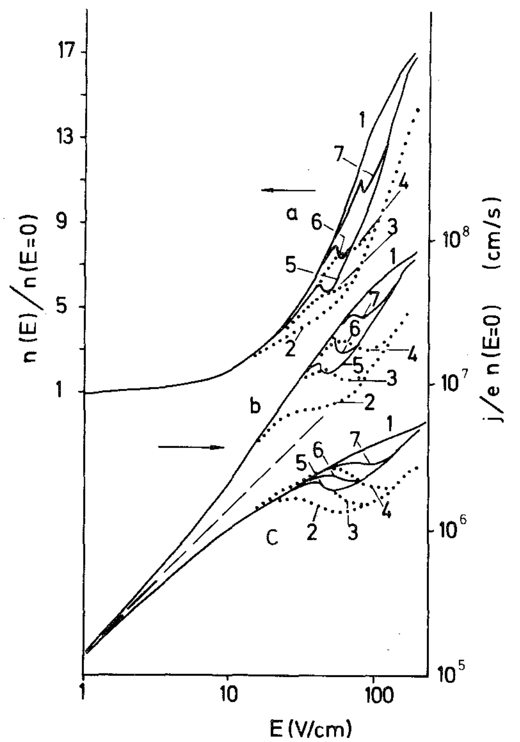

Fig. 2. Dependence of the concentration n on E, (a), and the dependence of the current on E, (b and c), in (b) the E dependence of n was taken into account while in (c) it was neglected: $J \parallel$ [1 1 1] (1), [1 0 0] (2, 3, 4), [1 1 0] (5, 6, 7) and different N_A : $N_A = 4 \cdot 10^{12}$ cm^{-3} (2, 5), $4 \cdot 10^{13}$ (3, 6), $4 \cdot 10^{14}$ cm^{-3} (4, 7). Dashed curve demonstrates Ohmic behaviour. n-Si, $T = 27$ K.

[1 1 1] for reasons of symmetry.†) The electron concentration n increases monotonically, as E increases. In the case $j \parallel$ [1 0 0] an effective field E_1 (10) in one valley ($\phi = 0$) is smaller than $E_2 = E_3$ in the other two ($\phi = \pi/2$), i.e. there are one cold valley and two hot valleys. Strong repopulation of electrons from the two hot valleys in the cold one is realized owing to the pronounced dependence of $1/\tau_\alpha^*$ on E_α (see Fig. 1). when $E_{2,3}$ reaches E_c with increasing E. The rate of increase of n with E (Fig. 2) is essentially slower in comparison with the case j $\parallel$ [1 1 1], because $B_{T,\alpha}$ in the cold valley is larger than in the hot one (Fig. 1). The N-shape dependence of n on E is found for $j \parallel$ [1 1 0] (curves 5, 6, 7 in Fig. 2), where the intervalley repopulation varies more sharply with E than for j $\parallel$ [1 0 0] [4, 6, 7].

Intervalley repopulation to the cold valley causes N-type negative differential conductivity (N-*ndc*), which has been studied previously [2, 4, 6, 7]. The E dependence of n was not taken into account in theoretical discussion, i.e. the current-voltage characteristics were taken as shown in Fig. 2c. The dependence of j on E changes from sub-Ohmic (Fig. 2c) to super-Ohmic when recombination is taken into account. The N-*ndc* is more pronounced for j $\parallel$ [1 1 0], where the dependence of n on E has also N-shape. On the contrary N-*ndc* decrease and may even disappear for j $\parallel$ [1 0 0] because the monotonically increase of n with E.

The proposed "anomalous" Sasaki effect [20] must occur when **E** is such that $E_\alpha < E_c$. That is, a transverse electric field in the opposite direction, as compared with the normally studied case (i.e. $1/\tau_\alpha^*$ increasing with E_α), arises if the current does not coincide with the crystallographic axes. It is caused by the predominant population of the hot valley in the range of E_α values where $1/\tau_\alpha^*$ decreases with E_α.

† We did not discuss here the "loop" solutions which are possible (for detail discussion see in papers [4, 7], in addition to the equal population of the valleys treated here.

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