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Influence of the scattering anisotropy in the interaction with the acoustic-phonon deformation potential on the transport phenomena in *n*-type Si in heating electric fields

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The Monte Carlo method is used to allow for the influence of the scattering anisotropy in the interaction with the acoustic-phonon deformation potential on the electron distribution function, the drift velocities of electrons, and the populations of the valleys in *n*-type silicon subjected to heating electric fields. The dependences of the probability of the scattering by longitudinal and transverse acoustic phonons on their energy and on the angle between the momentum and the axis of a heavy-mass valley are given. The influence of this anisotropy on the effects associated with electron transfer between the valleys is demonstrated.

1. The scattering of carriers in the interaction with the the acoustic-phonon deformation potential is one of the more important energy relaxation mechanisms. However, in an analysis of the transport phenomena in n-type silicon, which is a strongly anisotropic semiconductor, it is quite usual to ignore the distinction between the intravalley scattering by longitudinal and transverse acoustic phonons and replace both by an artifically selected "isotropic" mechanism; the probability of such scattering includes fitting parameters.[1-4] It is shown in Ref. 5 that such simplifications are justified if the distribution function is nearly isotropic and $N_q \gg 1$. However, these conditions are frequently not satisfied,[2] which may give rise to an incorrect approach to the problem.

We shall use the Monte Carlo method to study the influence of the scattering anisotropy and the interaction with the deformation potential of acoustic phonons on the transport phenomena and the negative differential conductivity due to intervalley transfer in n-type Si. We shall compare the results obtained with those of simplified calculations.[1-4]

2. In calculations of the transport properties by the Monte Carlo method it is necessary to know the probabilities of the loss of electrons from a given state to another state as a result of the interaction with one particular phonon. Silicon (like other semiconductors with a cubic symmetry) is characterized by different scattering of carriers in the interaction with longitudinal (LA) and transverse (TA) acoustic phonons. Since the centers of the valleys are located along the ⟨100⟩ axis in the Brillouin zone, it follows from the symmetry considerations that we can express the matrix elements in terms of two independent constants Ξ_u and Ξ_d (Refs. 6 and 7). Knowing the matrix elements,[7] we can write down the probabilities of the loss of an electron from a given state with a wave vector **k** to any other state **k'** accompanied by the absorption of W^+ phonons or the emission of W^- phonons with the wave vector q because of the interaction with the longitudinal $W_L^{\mp}$ and two transverse $W_T^{\mp}$ branches:

$$W_{L,T}^{\mp}=\frac{\Xi_u^2}{8\pi^2\rho u_{L,T}}\int d\mathbf{q}\, q F_{L,T}^2\left(N_q^{L,T}\pm\frac{1}{2}+\frac{1}{2}\right)\delta\left(\varepsilon_{\mathbf{k}\mp\mathbf{q}}-\varepsilon_{\mathbf{k}}\pm u_{L,T}q\hbar\right), \tag{1}$$

where $F_T = \cos\theta \sin\theta$; $F_L=(\Xi_d/\Xi_u)+\cos^2\theta$, ρ is the density; $u_{L,T}$ are the velocities of longitudinal and transverse sound; θ is the angle between q and the axis of the heavy-mass valley.

Integration with respect to q is most conveniently carried out in a spherical system of coordinates. If these coordinates are adopted, then after integration with respect to q there remain integrals with respect to the polar angle θ and the azimuthal angle φ:

$$W_{L,T}^{\mp}=A_{L,T}\int d\cos\theta\int d\varphi\, a_{L,T}^2 F_{L,T}^2 \times\left[N(a_{L,T})\pm\frac{1}{2}+\frac{1}{2}\right](1-B\cos^2\theta)^{-1}, \tag{2}$$

where

$$A_{L,T}=\Xi_u^2(k_0T)^2 m_\perp/(2\pi)^2\rho u_{L,T}^3\hbar^4,$$

$$\varepsilon_{L,T}^*=\varepsilon/2m_\perp u_{L,T}^2,\quad B=1-m_\perp/m_\parallel,$$

$$a_{L,T}=\frac{2m_\perp u_{L,T}^2}{k_0T}\left[\frac{2\sqrt{\varepsilon_{L,T}^*}\left(\frac{m_\perp}{m_\parallel}\cos\alpha\cos\theta+\sin\alpha\sin\theta\cos\varphi\right)}{\sqrt{1-B\cos^2\alpha}}-1\right]\times(1-B\cos^2\theta)^{-1},$$

α is the angle between P and the axis corresponding to the heavy-mass valley.

The integration of Eq. (2) with respect to φ and $\cos\theta$ is carried out within the limits set by the conditions $\mp a_{L,T}>0$. As before, the upper sign represents the emission of phonons and the lower the absorption of phonons.

We can see that in contrast to the isotropic approximation, the quantities $W_{L,T}^{\pm}$ now depend not only on the energy but also on the orientation of the vector P relative to the axis corresponding to the heavy mass. Quite reliable velocities of sound $u_L = 9\cdot10^5$ cm/sec and $u_T = 5.3\cdot10^5$ cm/sec are given in the literature, but there is a wide scatter of the reported values of Ξ_u and Ξ_d (Ref. 8). Calculations carried out for several sets suggest selection of $\Xi_u=9.1$, $\Xi_d=2$ eV. These and not other published values were selected by us because of the agreement between the low-field mobility deduced allowing for the scattering anisotropy using these values of Ξ_u and Ξ_d, and the mobility found in Refs. 1 and 2 in the isotropic approximation. This selection (for fully identical remaining param-

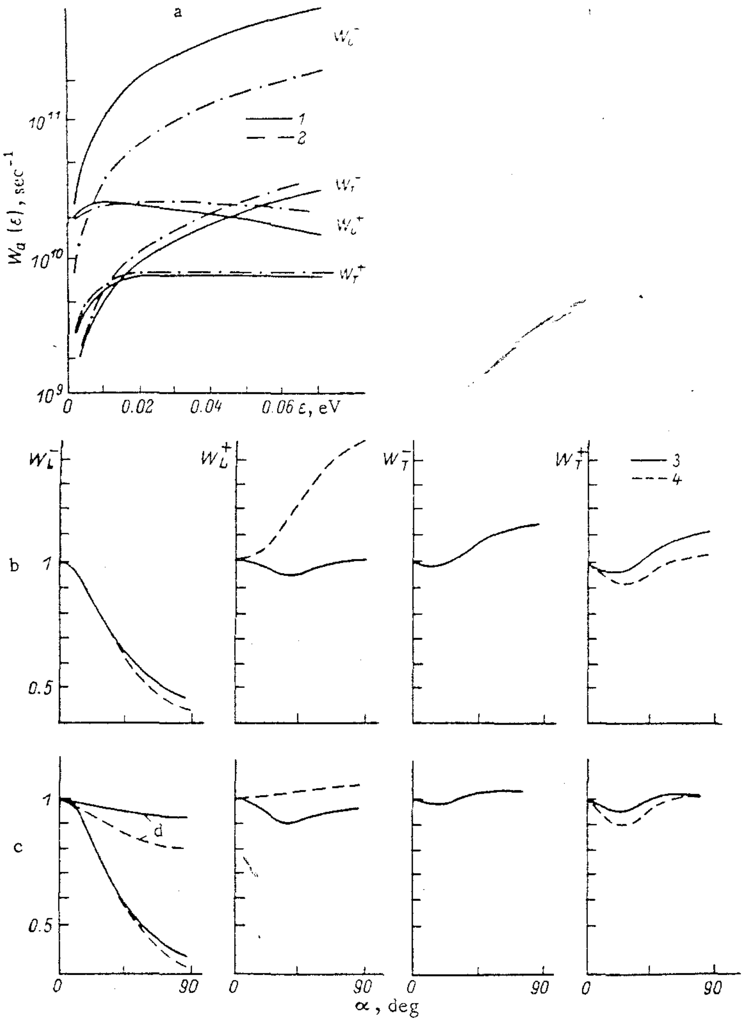

FIG. 1. Dependences of the scattering probabilities on the energy (a) and angle (b)-(d). Angle α(°): 1) 0; 2) 90. Energy ε (eV): 3) 0.01; 4) 0.1. Ξ_u(eV): a, b) 9.2; c) 8.6; d) 0. Ξ_d (eV): a, b) 2.0; c) − 0.65; d) 9.1.

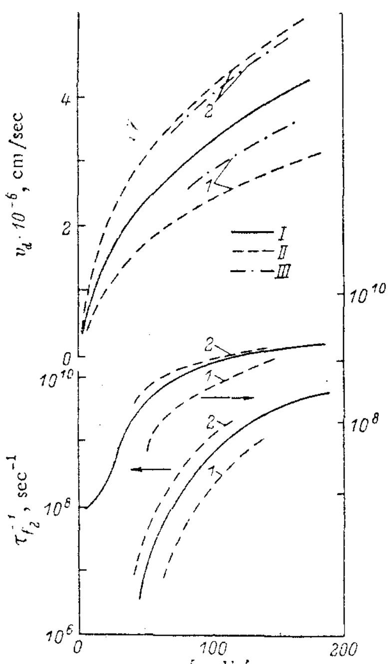

FIG. 2. Dependences of the drift velocity v_d and of the reciprocal intervalley transition time τ_f^{-1} on the effective electric field in a valley allowing for the anisotropy of the acoustic scattering for different angles ψ (°): 1) 0, 2) 90. I) Isotropic approximation. Ξ_u(eV): II) 9.2; III) 0. Ξ_d (eV): II) 2.0; III) 9.1.

eters – electric) allows us to estimate the influence of the scattering anisotropy on the parameters calculated in Refs. 1-4.

Figure 1a shows the dependences of the scattering probability $W^{\mp}_{L,T}(\varepsilon)$ for the angles $\alpha = 0$ and 90°, whereas Figs. 1b and 1c give the dependences $W^{\mp}_{L,T}(\alpha)$ for some fixed values of the energy and several sets of Ξ_u and Ξ_d, found by numerical integration of Eq. (2). We can see that the probability of the scattering by transverse phonons $W^{\mp}_T$ and the probability of absorption of longitudinal phonons W^+_L depend on the angle α much less than the probability of phonon emission W^-_L. Moreover, throughout most of the investigated range of energies, the dominant probability among these four is W^-_L. Therefore, in our calculations we shall consider only $W^-_L(\alpha)$.

3. In Refs. 2-4 the calculations were carried out in a deformed coordinate system

$$p'_k = a_k p_k, \quad v'_k = a_k^{-1} v_k, \quad E'_k = a_k E_k, \quad k = 1, 2, 3, \tag{3}$$

where $a_1 = a_2 = a_\perp = \sqrt{m/m_\perp}$; $a_3 = a_\parallel = \sqrt{m/m_\parallel}$; $m = (m_\perp^2 m_\parallel)^{1/3}$; $m_\parallel$ and $m_\perp$ are the longitudinal (heavy) and transverse (light) effective masses. We can see that the axis 3 coincides with the axis corresponding to the heavy-mass valley. In this approximation both the distribution functions and all the calculated values for a valley γ depend only on the effective heating field E_γ. In the case under investigation when the scattering is anisotropic be-

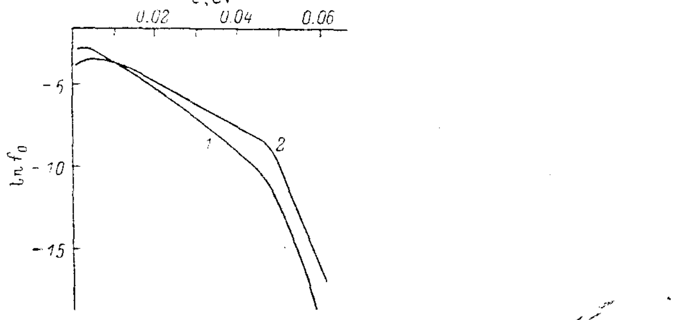

FIG. 3. Dependence of the distribution function on the energy. The effective electric field is E_γ = 90 V/cm. Angle ψ (°): 1) 0; 2) 90.

cause of the dependence of the scattering probability on the angle α, the calculated quantities depend on the electric field direction relative to the axis 3.

Figure 2 shows the dependences of the drift velocity of electrons v_d in a valley and of the reciprocal of the time constant of the intervalley scattering τ_f^{-1} by optical f phonons on the effective field E_γ in a valley γ calculated by the Monte Carlo method for two limiting orientations of the electric field relative to the axis 3 (ψ = 0 and ψ = 90°, where ψ is the angle between the axis 3 and E_γ). This figure gives the dependences on the effective field so as to facilitate a comparison with the isotropic case.[2] Since the scattering probability of α = 0° exceeds the probability for α = 90° and in heating electric fields the distribution function is elongated along the electric field,[2] it is clear that the heating of electrons when ψ = 0° is less (in the same electric field) and for ψ = 90°. This accounts for the difference between the two cases. Moreover, we can see from Fig. 2 that the influence of the anisotropy on τ_f is much stronger than on v_d, which shows that it is essential to allow for the scattering anisotropy in the calculations dealing with the effects due to high-energy electrons. This is demonstrated clearly in Fig. 3, which gives the dependences of the distribution function on the energy for the effective electric field E_γ = 90 V/cm when ψ = 0 and 90°. It should be pointed out that the influence of the scattering anisotropy is manifested only because of the anisotropy of the electron distribution function. In the range of electric fields 40–200 V/cm under consideration here the average energies range from about 3.5 kT to 8 kT, and the anisotropy of the distribution function at these energies reaches ~4. Clearly, in the case when the distribution function is isotropic there should be no effect.

It should be pointed out that the substitution in Eq. (1) of $\Xi_d \to \Xi$, $\Xi_u \to 0$, as is done – for example – in Ref. 9, does not result in isotropic scattering, since Eq. (1) contains the δ function which after integration gives the dependence of the scattering probability on α [see Eq. (2)]. Figure 1d gives the dependences $W_L^{\mp}(\alpha)$, whereas Fig. 2 gives the values of v_d calculated for this case when Ξ = 9.1 eV.

4. The dependences $v_d(E_\gamma)$ and $\tau_f^{-1}(E_\gamma)$ were used by us to calculate, by analogy with Ref. 2, the current-voltage characteristics averaged per one electron, i.e., $\tilde{v}_d(E)$ (Fig. 4a) and the populations of the valleys $n_\gamma(E)/n_\Sigma$ (Fig. 4b) for the j ∥ [100] orientation. For comparision, we shall also quote the data obtained in the isotropic ap-

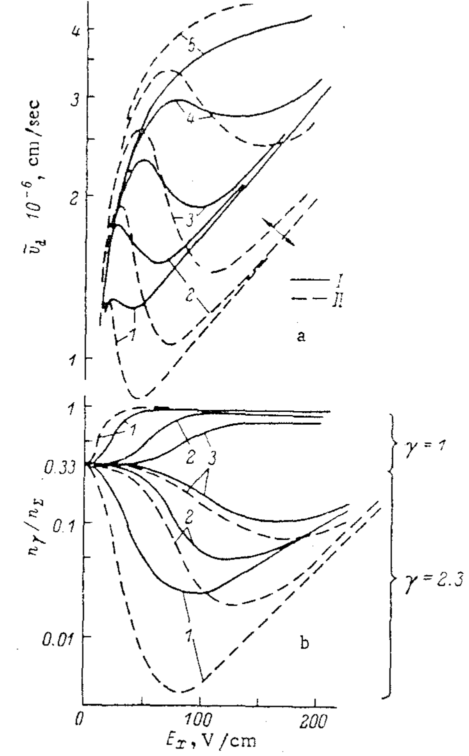

FIG. 4. Dependences of the drift velocity (a) and of the valley population (b) for j ∥ [100] and various values of τ_0^{-1} (sec^{-1}): 1) 10^6; 2) 10^7; 3) 10^8; 4) 10^9; 5) 10^{10}. I) Results of a calculation in the isotropic approximation; II) Ξ_u = 9.1 eV, Ξ_d = 2 eV.

proximation in Ref. 4. We can see that for any value of τ_0 (where τ_0 is the intervalley transfer time governed by the scattering on impurities – see Ref. 4) we have the following results: firstly, the lower field of the onset of a negative differential conductivity region shifts somewhat toward lower values of E and this is due to the fact that the main contribution to the drift velocity comes from the valleys 2 and 3 (ψ = 90°) and the populations of these valleys differ little from that in the isotropic case (Fig. 4b); secondly, there is a considerable widening and deepening of the N-type negative differential resistivity region, which is a consequence of a fuller depopulation of the valley 1 since the hot valley is hotter than in the isotropic case, whereas the cold valley is colder.

It should be pointed out that for any value of τ_0 a variation of Ξ_u and Ξ_d in the calculations should result in a parallel shift of the part of the current-voltage characteristic corresponding to the strongest transfer between the valleys. The directions of shift are shown by arrows in Fig. 4. This can probably be used to determine more accurately the values of Ξ_u and Ξ_d.

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