Diffusion-to-streaming transition of transport electrons in polar semiconductors

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A Monte Carlo simulation of the motion of transport electrons in a polar semiconductor is performed. The electrons are subjected to an electric field; they are in a parabolic band and undergo scattering with optical phonons. For small electric fields the electrons diffuse, while for strong electric fields they perform a streaming motion. A model is introduced which describes this diffusion to streaming transition. Although the model is simple, it leads to good agreement with the Monte Carlo results.

I. INTRODUCTION

Conduction electrons in polar semiconductors which are subjected to relatively high electric fields (e.g., typically $E \sim 50$ V/cm for InSb at $T=77$ K, $E \sim 100$ V/cm for AgBr, $E \sim 500$ V/cm for AgCl perform a streaming motion. This was first proposed by Shockley[1] who introduced a quasiclassical model in which the electron undergoes acceleration cycles which are interrupted by LO-phonon emission. This Shockley model results in an average velocity which equals half the critical velocity for emission of a longitudinal-optical phonon. The saturation of the electron velocity typical for this streaming motion is nicely illustrated by recent experiments[2] in the strongly polar crystals AgBr and AgCl and to a lesser extent in InSb.[3]

Subjected to sufficiently low electric fields, conduction electrons undergo *diffusive* motion which can be described by a quasi-isotropic electron-momentum distribution function.[4] *Streaming* motion on the contrary is characterized by an anisotropic electron-momentum distribution. This was first suggested by Bray and Pinson[5] and later elaborated by Vosilius and Levinson[6] who introduced a "needlelike" distribution in the electron momentum. A Monte Carlo simulation of the electron streaming motion which, at least in principle, is equivalent[7] to the solution of the Boltzmann equation was realized by Kurosawa[8] and confirmed the highly anisotropic character of the electron-distribution function.

In the present paper we consider the ideal situation in which the electrons are in a parabolic conduction band and scattering is with LO phonons only. Aas and Blotekjaer[9] studied this particular situation and used the Monte Carlo technique. They elaborated on (i) the transverse cooling of the electron distribution at the intermediate electric fields and (ii) the runaway of electrons at high electric fields. The pure streaming condition was investigated by Devreese and Evrard[10] who solve the Boltzmann equation quasianalytically at zero temperature using a so-called "two-circle" model approach. Thornber and Feynman[11] used the Feynman polaron model[12] to investigate the velocity (v)—electric-field (E) relation for aribitrary electron-phonon coupling strength. The theory of Ref. 11 was recently reviewed in Ref. 13 where it was shown that the electron-momentum distribution function corresponding to the work of Ref. 11 is a drifted Maxwellian. A comparison between the Monte Carlo results and the results based on the Thornber-Feynman theory is presented in Ref. 14.

The aim of the present paper is to propose a simple model which can account for the "diffusion-to-streaming" transition. This model, which is presented in Sec. II, is based on a distinction between two states for the electron motion: diffusion and streaming. It is assumed that a given electron has a well-defined probability to be found either in the diffusion state or into the streaming state. Simple intuitive arguments are used in the construction of our model. The correct qualitative features of the diffusion-to-streaming transition are obtained. In Sec. III the results of the present model are compared with the results of Monte Carlo simulations.

II. MODEL FOR THE DIFFUSION-TO-STREAMING TRANSITION

The essential physics of the diffusion-to-streaming transition is contained in a one-dimensional picture of the electron motion. A distinction will be made between two different electron states.

A. The *diffusive* state

This state is characterized by an electric-field independent mobility, i.e., the average electron velocity increases linearly with the electric field. The electron velocity is limited by quasielastic scattering processes which are described by a scattering rate $1/\tau_d$. The electron velocity distribution is chosen to be a displaced Maxwellian:

$$f_d(v) = \left[\frac{\beta m}{2\pi}\right]^{1/2} e^{-\beta(m/2)(v-v_d)^2} \tag{1}$$

which is centered around

$$v_d = \frac{e\tau_d}{m} E \tag{2}$$

with $\beta = 1/k_B T$ (k_B is Boltzmann's constant, T is the lattice temperature), m is the electron effective mass, and e is the electron charge.

B. The *streaming* state

With increasing electric field an increasing number of electrons gain sufficient velocity to reach the threshold for emission of an optical phonon. Those electrons participate in the streaming motion and the time evolution of their velocity is a "sawtooth" function. For relatively small electric fields the average electron velocity (v_s) of electrons in the streaming state is independent of the electric field: $v_s = \frac{1}{2} v_{\rm LO}$, with $v_{\rm LO} = (2\hbar\omega_{\rm LO}/m)^{1/2}$ the threshold velocity to emit a LO phonon with energy $\hbar\omega_{\rm LO}$. With increasing electric field, the electron participating in the streaming motion will penetrate the region $v > v_{\rm LO}$ and will emit an LO phonon after it has reached some velocity $v_m > v_{\rm LO}$. The velocity of the electron after it has emitted an LO phonon is $\pm v'$ with $v'^2/2m = v_m^2/2m - \hbar\omega_{\rm LO}$. The probability for an electron to reach the velocity $\pm v'$ is

$$1 \Bigg/ \left[1 \mp \frac{v'(v'^2 + v_{\rm LO}^2)^{1/2}}{(v'^2 + v_{\rm LO}^2/2)}\right]$$

which for $v' \ll v_{\rm LO}$ is practically equal to 1. We will assume that on the average the electron is scattered to final states with zero velocity $v' = 0$ The average streaming velocity v_s is equal to $\frac{1}{2} v_m$. The velocity v_m is determined from the energy balance equation[15]

$$\langle evE \rangle = \int_{\hbar\omega_{\rm LO}}^{(m/2)v_m^2} d\epsilon \frac{1}{\tau_e[(2m\epsilon)^{1/2}]} , \tag{3}$$

where the left-hand side of Eq. (3) expresses the average energy gain of an electron due to the electric field and the right-hand side of Eq. (3) is the energy loss due to emission of LO phonons. The scattering rate for LO-phonon emission is[16]

$$\frac{1}{\tau_e(mv)} = \omega_{\rm LO} 2\alpha \frac{v_{\rm LO}}{v} (1+\bar{n}) \operatorname{arccosh}\left[\frac{v}{v_{\rm LO}}\right] \Theta(v - v_{\rm LO}) \tag{4}$$

with $\bar{n} = 1/(e^{\beta\hbar\omega_{\rm LO}} - 1)$ representing the LO-phonon occupation number. Inserting (4) into (3) and noting that $\langle v \rangle = \frac{1}{2} v_m$ one finds

$$E/E_0 = 4\alpha(1+\bar{n}) \left[\operatorname{arccosh}\left[\frac{v_m}{v_{\rm LO}}\right] - \left[1 - \frac{v_{\rm LO}^2}{v_m^2}\right]^{1/2}\right] \tag{5}$$

with $E_0 = \omega_{\rm LO}(2m\omega_{\rm LO})^{1/2}/e$. For small electric fields one readily finds for the penetration velocity

$$v_m = v_{\rm LO}\left[1 + \frac{1}{2}\left[\frac{3E/E_0}{4\alpha(\bar{n}+1)}\right]^{2/3}\right] . \tag{6}$$

This electric-field dependence of the penetration velocity is similar to the one found in Ref. 17. For InSb at $T = 77$ K, Eq. (6) becomes

$$v_m = v_{\rm LO}(1 + 6.8 \times 10^{-3} E^{2/3})$$

with E expressed in V/cm.

At a fixed value of the electric field n_s electrons will be in the streaming state with a streaming velocity $v_s = v_m/2$. The other electrons are in the diffusion state. We obtain for the average electron velocity

$$\langle v \rangle = \langle v \rangle_d + n_s v_s \tag{7}$$

with

$$\langle v \rangle_d = \int_{-v_s}^{v_s} dv\, v f_d(v) \tag{8a}$$

and

$$n_s = \int_{v_s}^{\infty} dv\, f_d(v) - \int_{-\infty}^{-v_s} dv\, f_d(v) . \tag{8b}$$

To derive Eqs. (8a) and (8b) we noticed that (i) $f_d(v)$ is the velocity distribution for the case of diffusive motion; (ii) electrons with a velocity $|v| > v_s$ do not diffuse, they are in the streaming state.

Equation (7) gives a relation between the average electron velocity $\langle v \rangle$ and the electric field E. The latter is contained in $f_d(v)$ through $v_d = e\tau_d E/m$. In this paper, the only scattering mechanism which is considered is LO-phonon scattering. As was observed by several authors (see, e.g., Ref. 9) the absorption (and successive) emission of an LO phonon is a quasielastic process. Consequently the diffusion time τ_d is determined by the LO-phonon absorption scattering rate ($p = mv$):

$$\frac{1}{\tau_a(p)} = \omega_{\rm LO} 2\alpha\bar{n} \frac{v_{\rm LO}}{v} \operatorname{arcsinh}(v/v_{\rm LO}) \tag{9}$$

through

$$\frac{1}{\tau_d} = \left\langle \frac{1}{\tau_a(p)} \right\rangle = \sum_{\mathbf{p}} e^{-\beta p^2/2m} \frac{1}{\tau_a(p)} \Bigg/ \sum_{\mathbf{p}} e^{-\beta p^2/2m} \tag{10}$$

which gives

$$\omega_{\rm LO}\tau_d = \frac{1}{\alpha}\left[\frac{\pi}{\beta_0}\right]^{1/2} \frac{\sinh(\beta_0/2)}{K_0(\beta_0/2)} \tag{11}$$

with $\beta_0=\beta\hbar\omega_{\rm LO}$ and $K_0(x)$ is the modified Bessel function of the first kind. In the low-temperature limit, Eq. (11) becomes

$$\omega_{\rm LO}\tau_d=\frac{1}{2\alpha\bar{n}} \tag{12}$$

which [using Eq. (2)] gives the standard Fröhlich result for the polaron mobility.[18]

Using the model introduced above we can study the diffusion-to-streaming transition. The numerical results are shown in Fig. 1 for $\alpha=0.02$ (InSb). The v-E relation is practically linear when less than 10% (i.e., $n_s=0.1$) of the electrons are in the streaming state. When more than 90% of the electrons are in the streaming state (i.e., $n_s=0.9$) the electron average velocity is essentially saturated and we say that the system is in the streaming state. From Fig. 1 it is apparent that at low temperature the electric field range over which Ohmic behavior occurs is extremely small. One can see this also from Eq. (7) by making an expansion for $v_d/v_{\rm LO}\ll 1/(\beta_0)^{1/2}$ and $\beta_0\gg 1$ which leads to

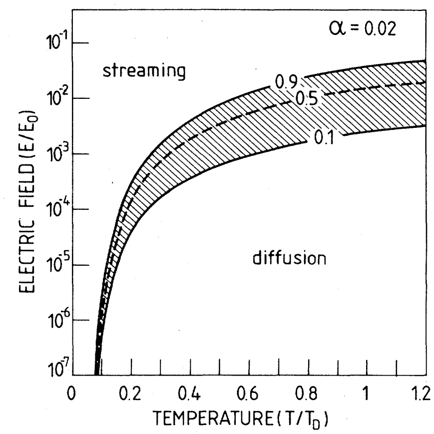

FIG. 1. Electric field [unit $E_0=\omega_{\rm LO}(2m\hbar\omega_{\rm LO})^{1/2}/e$]—temperature (unit $T_D=\hbar\omega_{\rm LO}/k$) diagram for the diffusion-to-streaming transition. The transition region (cross-hatched region) is bounded from above by the condition that 90% (i.e., $n_s=0.9$) of the electrons are streaming, and from below by the condition that 10% (i.e., $n_s=0.1$) of the electrons are streaming.

$$\langle v\rangle=v_d\left\{1+\left[\frac{\beta_0}{\pi}\right]^{1/2}e^{-\beta_0/4}\left[\left[\frac{3eE}{2\alpha}\right]^{2/3}-\frac{2}{\beta_0}+\cdots\right]\right.$$
$$\left.+\left[\frac{v_d}{v_{\rm LO}}\right]^2 e^{-\beta_0/4}\frac{\beta_0^{5/2}}{6\sqrt{\pi}}\left[\left[1-\frac{\sqrt{\pi}}{2}\right]+\left[\frac{3eE}{2\alpha}\right]^{2/3}+\cdots\right]+\cdots\right\}. \tag{13}$$

A linear v-E relation is observed if

$$\frac{v_d}{v_{\rm LO}}\ll\frac{e^{\beta_0/8}}{\beta_0^{5/4}}\left[\frac{6\sqrt{\pi}}{1-(\sqrt{\pi}/2)}\right]^{1/2}.$$

Inserting Eqs. (2) and (12) results in

$$E/E_0\ll 2\alpha\frac{e^{-7\beta_0/8}}{\beta_0^{5/4}}\left[\frac{6\sqrt{\pi}}{1-(\sqrt{\pi}/2)}\right]^{1/2}. \tag{14}$$

For InSb, Eq. (11) shows that for $T=10$ K, respectively, 20 K, the Ohmic regime is limited (for LO-phonon scattering only) to the unrealistical small electric fields $E\ll 2.2\times10^{-9}$ V/cm and $E\ll 1.3$ mV/cm. A recent study[19] of the polaron Boltzmann equation confirms this conclusion.

III. COMPARISON BETWEEN THE MONTE CARLO RESULTS AND THE RESULTS OBTAINED WITH THE PRESENT MODEL

Applying the Monte Carlo simulation technique[7] we have calculated the electron-momentum distribution function at $T=77$ K for different values of the electric field (see Fig. 2). In Fig. 2 we used $\alpha=0.02$ which is the electron-phonon coupling constant for InSb. The electric field was directed along the z axis. Because of cylinder symmetry around the z axis, the electron-distribution function $f(p_\perp,p_z)$ is plotted in Fig. 2 which is defined as

$$f(p_\perp,p_z)=2\int dp_x\int dp_y f_{\rm 3D}(\mathbf{p})\delta(p_\perp^2-(p_x^2+p_y^2))$$

with $f_{\rm 3D}(\mathbf{p})$ the three-dimensional electron-momentum distribution function. The function $f(p_\perp,p_z)$ was scaled to $f(0,0)$. With increasing electric field, the distribution function evolves gradually from a quasi Maxwellian shape at $E=5$ V/cm to a more elongated needlelike shape which is characteristic for streaming motion of the electrons. The penetration of the electron momentum in the $|v|>v_{\rm LO}$ region increases with increasing electric field.

In Fig. 3 the average electron velocity is plotted as a function of the electric field for $\alpha=0.02$ and different values of the temperature. The Monte Carlo results are compared with the results for the present model. For InSb we have $v_{\rm LO}=7.8\times10^7$ cm/s, $E_0=2.28\times10^4$ V/cm, and $T_D=284$ K. The temperatures $T/T_D=0$, 0.176, 0.271, 0.5 correspond, respectively, with $T=0$, 50, 77, 142 K in the case of InSb. In Fig. 4 we plotted the relative density of streaming electrons, n_s, and the contribution of the diffusing electrons to the average velocity $\langle v\rangle_d$ versus the electric field for the same values

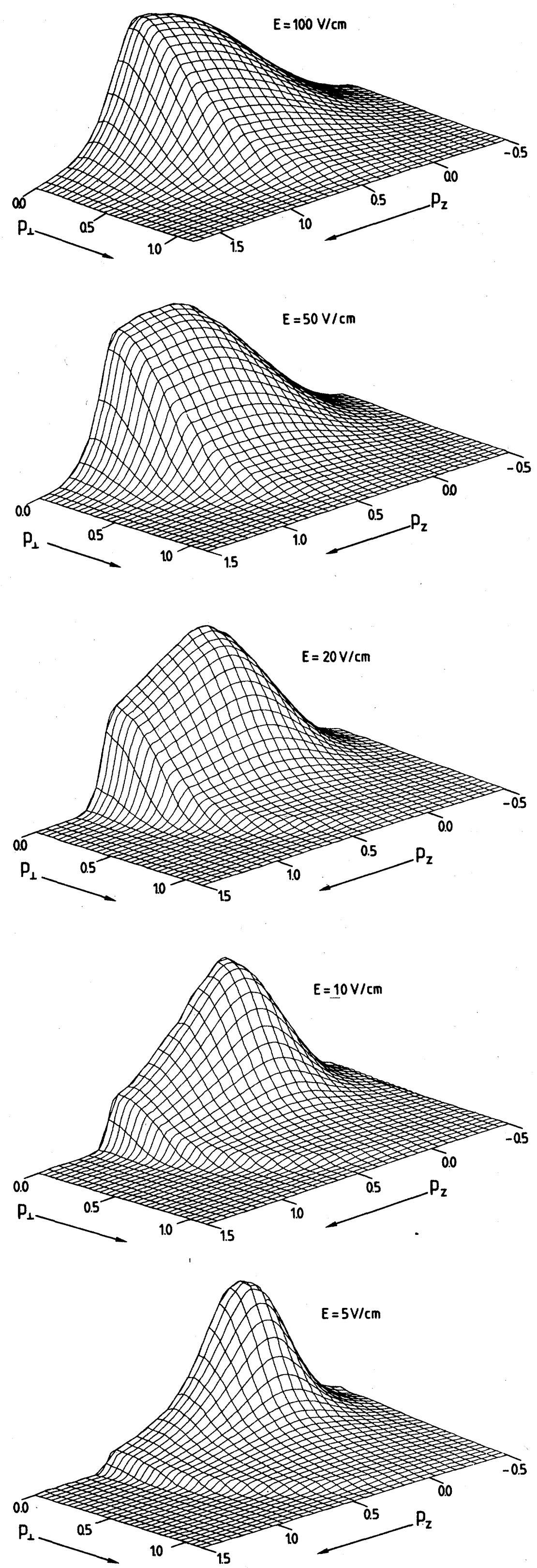

FIG. 2. Electron-momentum distribution function for $\alpha=0.02$, $T=77$ K, and different values of the electric field. The electron momentum is in units of $p_{\rm LO}=(2m\hbar\omega_{\rm LO})^{1/2}$.

of the temperature as in Fig. 1. For $T=0$ we have for all electric field values $n_s=1$ and $\langle v\rangle_d=0$.

As is apparent from Fig. 3, the model exhibits the following three regimes: (1) a linear regime, i.e., $\langle v\rangle \sim E$, for sufficiently small electric fields, (2) a saturation regime, i.e., $\langle v\rangle \simeq v_{\rm LO}/2$, for intermediate electric field values, and (3) a regime characterized by penetration of the streaming electrons in the momentum region dominated by LO-phonon emission. In the third regime the average velocity is $\langle v\rangle \gtrsim v_{\rm LO}/2$ which increases very slowly with the electric field. The above three regimes agree qualitatively with the Monte Carlo results.

Quantitatively, the results for $\langle v\rangle$ obtained with the model calculation differ at most with a factor of 2 from the Monte Carlo results. The model introduced here leads to a smaller transition region because (i) the linear region extends to slightly higher electric fields and (ii) the saturation of the average velocity sets in slightly faster as compared with the Monte Carlo results.

This can be understood as due to the one-dimensional nature of our model. In the actual three-dimensional situation the electron-momentum distribution will also be extended in the direction perpendicular to the electric field which as a consequence results in a more gradual diffusion-to-streaming transition. Remark also that the Monte Carlo results give a higher penetration of the electron momentum in the $v>v_{\rm LO}$ region in the high field limit than the results of the model. The reason is that at high electric fields the scattered state $+v'$, after emission of an LO phonon, has a higher probability, i.e.,

$$1\Bigg/\left[1-\frac{v'(v'^2+v_{\rm LO}^2)^{1/2}}{(v'^2+v_{\rm LO}^2/2)}\right]$$

than the state $-v'$ which has a probability

$$1\Bigg/\left[1+\frac{v'(v'^2+v_{\rm LO}^2)^{1/2}}{(v'^2+v_{\rm LO}^2/2)}\right].$$

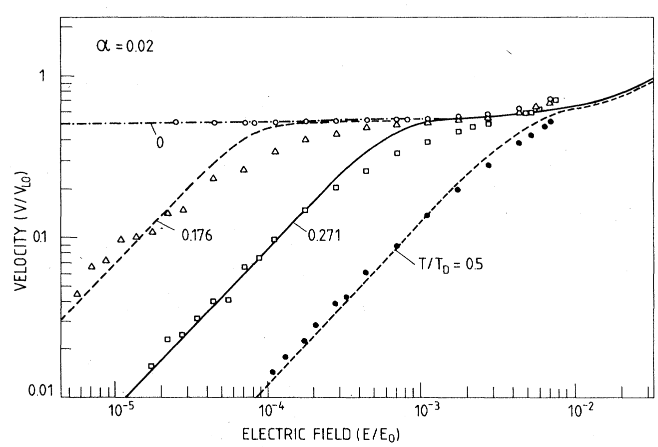

FIG. 3. Electron average velocity [unit $v_{\rm LO}=(2\hbar\omega_{\rm LO}/m)^{1/2}$] as a function of the electric field [unit $E_0=\omega_{\rm LO}(2m\hbar\omega_{\rm LO})^{1/2}/e$] for $\alpha=0.02$ and different values of the temperature (unit $T_D=\hbar\omega_{\rm LO}/k$). The curves are the results of the present model. The Monte Carlo results are represented by the different symbols.

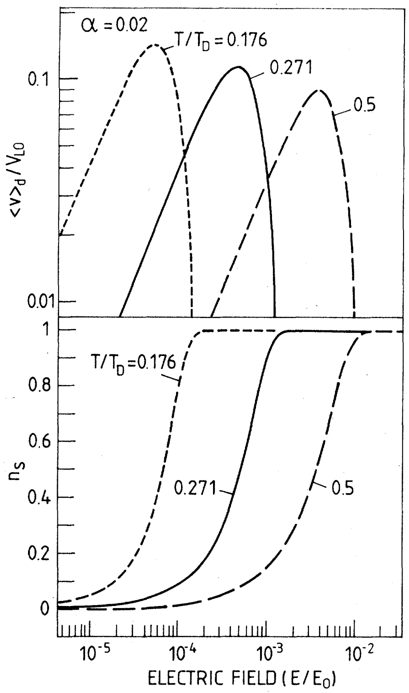

FIG. 4. Contribution of the diffusing electrons to the average electron velocity (i.e., $\langle v \rangle_d / v_{LO}$) and the relative number of streaming electrons (i.e., n_s) as a function of the electric field for the same parameters as in Fig. 3.

This implies that on the average, the electron is *not* scattered to a state $\langle v' \rangle = 0$, as assumed in our model, but $\langle v' \rangle$ will be positive. This leads to an average streaming velocity which is larger than $v_m/2$.

The absence of runaway in our model in the electric-field region $E/E_0 \sim 10^{-2}$ is understood in the following way. In the model we assumed that the emission of a LO phonon occurs at a fixed threshold velocity $v_m \geq v_{LO}$. In reality there are fluctuations in the momentum "penetration depth." Some of the electrons will penetrate deeply enough to enter the region where the scattering rate decreases with increasing velocity. Such electrons have a nonzero probability to gain more energy from the electric field per unit time than they lose by emitting LO phonons. Therefore their energy on the average increases with time. This runaway is apparent in the Monte Carlo results (see Fig. 3) for $E/E_0 > 0.6 \times 10^{-2}$.

In conclusion we have presented a simple model which can account for the diffusion-to-streaming transition of electrons in polar semiconductors. Fair quantitative agreement (within a factor of 2) was found with results obtained from a Monte Carlo calculation. The present model may be useful to obtain, with a relatively simple calculation, a qualitative idea of the behavior of electrons in polar semiconductors when they are subjected to an electric field. The extension of the present model to incorporate (i) the effects of quasielastic scattering processes as, e.g., impurities, acoustical phonons, etc., and (ii) of a magnetic field (crossed electric and magnetic fields) is postponed to further work.

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