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J. Phys.: Condens. Matter **13** (2001) 6233–6246 PII: S0953-8984(01)21991-2

Applicability of the Fermi golden rule and the possibility of low-field runaway transport in nitrides

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Received 14 February 2001, in final form 16 May 2001
Published 29 June 2001
Online at stacks.iop.org/JPhysCM/13/6233

Abstract
We investigated electron transport characteristics of wide-band polar semiconductors with intermediate strength of the electron–phonon interaction. Electron energy loss to the lattice was calculated as a function of electron velocity for various materials in the frameworks of (a) a perturbative approach based on the calculation of scattering rates from Fermi's golden rule and (b) a non-perturbative approach based on the path-integral formalism of Thornber and Feynman. Our results suggest that the standard perturbative treatment can be applied to GaN and AlN despite the relatively strong electron–phonon coupling in this material system, with intercollision times of the order of the period of the phonon oscillation. Our findings also indicate the possibility for unique long-distance runaway transport in nitrides which may occur at the pre-threshold electric fields. The polaron ground-state energy and effective masses are calculated for GaN and AlN as well as for GaAs and Al_2O_3. An expression for the Fröhlich coupling constant for wurtzites is derived.

1. Introduction

One of the main factors determining electron transport characteristics in polar semiconductors is the scattering of the electrons by polar optical phonons. For relatively weak electron–phonon interactions, when scattering events can be considered as independent, use of Fermi's golden rule for the calculation of energy-dependent frequencies of electron transitions provides an adequate description of experimentally obtained velocity–field curves. Upon increase of the interaction, however, the polaronic effects induced by autolocalization of an electron by the inertial part of the crystal polarization become more prominent and they determine the character of the scattering. Intensification of the electron–phonon interaction leads eventually to a situation where the average intercollision time becomes less than the duration of a collision. Such a strong coupling, therefore, requires taking proper account of the quantum interference effects and makes the problem of electron drift essentially non-linear. This complicates

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dramatically the theoretical treatment of carrier scattering and field-dependent transport since, for the given case, the standard perturbation technique is not applicable.

To ensure energy conservation for the short-time perturbations, the inverse scattering rate τ must be large enough to satisfy the inequality $\tau \gg \hbar/\Delta\mathcal{E}$, where $\Delta\mathcal{E}$ is the electron transition energy. This criterion, however, does not allow one to conclude as to whether or not a wide class of materials in which the transition energy may become of the order of the linewidth can be described successfully in the framework of standard perturbation approaches. To such a class of materials belong, in particular, nitrides of Al and Ga. These semiconductors have been investigated recently quite intensively due to the fact that a number of their unique properties can be utilized in the current state-of-the-art semiconductor technology. However, most attempts to describe scattering processes in nitrides have been undertaken assuming the validity of the Fermi golden rule. Moreover, despite the possibility of growing the nitrides of group III in zinc-blende-like structures, their crystal structure at ambient conditions is wurtzite-like. For wurtzites, it is generally necessary to account for optical anisotropy when considering the carrier–optical phonon interactions. Since optical phonon spectra of wurtzites are far more complicated than those of cubic crystals, the majority of theoretical results have been obtained by ignoring the features of the phonons in optically anisotropic media. Recently, a formalism has been developed [1] for evaluation of the rates of scattering in bulk wurtzite-like semiconductors and heterostructures by taking into account peculiarities of the phonon spectra obtained in the framework of the macroscopic dielectric continuum model [2]. In view of the anisotropy-induced complexity of the problem, reference [1] took advantage of the perturbation theory. However, as indicated by the previously discussed considerations, the validity of such an approach requires independent confirmation.

The present paper examines the applicability of Fermi's golden rule for describing adequately the electron–longitudinal phonon interaction in materials with intermediate polaronic coupling by comparing the field–velocity dependences obtained in the frameworks of (a) the perturbation theory and (b) the non-perturbative path-integral approach of Thornber and Feynman [3] (TF). Moreover, the investigation discusses the possibility of unique long-distance, low-field runaway transport in such materials (particularly in the nitrides of Ga and Al). An experimental approach is proposed to verify the results obtained in this study.

2. Model

The most systematic and self-consistent approach for evaluating the long-range polaron ground-state energy G and polaron effective mass m_0 for both strong- and weak-coupling limits of electron–phonon interaction has been developed by Feynman [4]. In reference [3], the problem of electron drift in a parabolic band under steady-state conditions is considered quantum mechanically [5] assuming that all the energy losses are due to the interaction of electrons with polar optical modes. Taking advantage of Fröhlich's polaron model, the authors have used the path-integral approach developed in reference [4] to eliminate the lattice coordinates from the momentum balance equation and have obtained an expression for the magnitude of the electric field E that is required to maintain a particular magnitude of electron expectation, steady-state velocity V at arbitrary temperature and interaction strength characterized by the coupling constant

$$\alpha = \frac{e^2}{\hbar}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\left[\frac{m^*}{2\hbar\Omega}\right]^{1/2}. \tag{1}$$

Herein, e is the elementary charge. Evaluation of α requires four parameters: electron effective mass m^*; frequency of the longitudinal phonon Ω; static dielectric constant ϵ_0; and

high-frequency dielectric constant ϵ_∞. All these parameters can be measured experimentally and they are the only external parameters required for calculation of energy loss per unit distance eE versus V.

Thornber and Feynman [3] have calculated $eE(V)$ for three coupling constants (α = 3, 5, 7) over a wide range of reciprocal temperatures $\beta = \hbar\Omega/(k_B T)$, where k_B is the Boltzmann constant and T is the temperature of the lattice. The general result of these calculations can be summarized briefly as follows. For each particular α, $eE(V)$ has a maximum at some threshold value V_{th}. For $\beta > 1$, location of this maximum becomes independent of temperature. For $V < V_{th}$, eE is an increasing function of velocity. This interval of velocities corresponds to a stable situation when energy loss to the lattice due to the absorption and emission of optical phonons can be compensated by the energy gained by the electron from the applied field in such a way that at the given E, a small deviation ΔV of the velocity from its steady-state value V_s creates a force, $e[E(V_s) - E(V_s \pm \Delta V)]$, which stabilizes the velocity at V_s. When the external field approaches the value $E_{th} = E(V_{th})$, the dependence tends to saturate since the magnitude of the energy loss due to interaction with optical phonons is finite.

The case $E > E_{th}$ was excluded from consideration because no steady-state conditions can be reached for such fields and the electron would accelerate infinitely. The theory, however, predicts the existence of solutions for $V > V_{th}$. In this region, eE is a decreasing function of the velocity which leads to an unstable steady-state situation. For this case, any deviation of the velocity from V_s would lead to either deceleration of the electron to velocity $V < V_{th}$ which is stable at the given field, or a *gradually* increasing acceleration if ΔV leads to an increase in velocity. It is essential that for $V > V_{th}$ the dependence $eE(V)$ can also be interpreted as a time-dependent relation for the loss of momentum in time in the absence of the external field. This loss would coincide with the rate of electron momentum loss if the criterion

$$\mathrm{d}V/\mathrm{d}t \ll V/\tau^* \tag{2}$$

is satisfied, where, for the long-range interaction with polar optical phonons, τ^* can be estimated as the intercollision time in the weak-coupling limit and the 'collision' time in the strong-coupling limit. It is important for the effects considered in this paper to stress that this loss would also coincide with the rate of energy loss with distance if, in addition to fulfilment of the criterion of equation (2), there is appreciable persistence of the initial carrier momentum [3]. For $\beta > 1$, $eE(V > V_{th})$ becomes independent of temperature as well.

In order to simplify the comparison, and taking into account the fact that the strongest electron–polar optical phonon scattering is due to emission of the longitudinal optical (LO) phonons, we will consider the case where $\beta \approx 4$. In the nitrides, such a value of β would correspond to room temperature. For GaAs, which we take as a reference point in our investigation, $\beta = 4$ would correspond to lattice temperature of the order of 104 K. Since β_{GaAs} is slightly higher than 1 at room temperature, the result obtained for maximum energy loss per unit distance can be compared to the experimental *velocity–field* dependences (see, for example, reference [7] and citations therein). Indeed, at some threshold field E_{th}, the dependence $V(E)$ has a maximum caused by transitions of the carriers to an upper valley with a higher effective mass. In terms of the TF model, these transitions would start to occur when the energy supply from the external field exceeded the maximum loss to the lattice; i.e., at $E \gtrsim E_{th}$.

Thus, if the average kinetic energy of electrons obtained in the framework of the TF model at E_{th} does not exceed the energy of band separation and the effects of the increased effective mass due to non-parabolicity of the Γ band can be neglected, the value of the argument at the maximum of the $V(E)$ dependence has to coincide with the field which corresponds to the extremum of the $eE(V)$.

Under the assumptions made above, we use a simple model (SM) for the estimation of energy loss to the lattice in the framework of the perturbation theory. In this model, we calculate the dependence of the scattering rate $1/\tau$ due to the emission of LO phonons on a single-electron kinetic energy $\mathcal{E}$ using Fermi's golden rule. For an optically isotropic material, the scattering rate is [6]

$$\frac{1}{\tau} = \left(\frac{2m^*}{\mathcal{E}}\right)^{1/2} \frac{e^2\Omega(N_q+1)}{\hbar}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right) \ln\left[\sqrt{\frac{\mathcal{E}}{\hbar\Omega} - 1} + \sqrt{\frac{\mathcal{E}}{\hbar\Omega}}\right] \qquad (3)$$

where N_q is the phonon occupation number. Then, we assume that a carrier with velocity $V = \sqrt{2\mathcal{E}/m^*}$ loses the energy $\hbar\Omega$ to the lattice in a distance τV. We must note that such an estimation is always valid in the weak-coupling limit for $V \approx V_{th}$, where the stable steady-state situation is realized. Analysis of the momentum balance equation given by Thornber and Feynman, however, shows that for $V > V_{th}$, the approach used in the SM is valid only if the criterion of equation (2) and requirement of the carrier momentum persistence are satisfied. The latter requirement is automatically fulfilled in the SM.

Since we consider low temperatures ($k_B T < \hbar\Omega$), phonon absorptions are not taken into account due to the low phonon population. According to a general result from the TF model, such an approximation will not modify the $eE(V \geqslant V_{th})$.

3. Results and discussion

3.1. Limiting cases

The energy loss per unit distance versus the electron velocity calculated for GaAs at room temperature in the framework of the model which uses Fermi's golden rule is depicted in figure 1 by the thin solid line. As anticipated, the maximum of the dependence is in a good agreement with the experimental data which give the maximum of $V(E)$ at $E \approx 3.4$–$3.9\ \mathrm{kV\ cm^{-1}}$. One should note that since calculations are made in a one-electron approximation and for a single parabolic band, they overestimate the velocity obtained at the maximum. The experimentally measured values at the maximum of $V(E)$ [7] reflect the averaging of the velocities over bands with different effective masses as well as effects of non-parabolicity.

The curve calculated in the SM at 104 K ($\beta = 4$) is given by the thick solid line. The $eE(V)$ dependence computed for $\beta = 4$ in the framework of the TF model (upper dashed line) exhibits a maximum located at significantly higher fields. This disagreement appears in addition to the well known fact that in the weak-coupling limit the low-field, low-temperature mobility calculated from standard Boltzmann treatment does not agree with the mobility which follows from the TF model [3]. The discrepancy can be attributed to the fact that the zero-order distribution for the electrons in the TF model reduces to a drifted quasi-Maxwellian in the weak-coupling limit. An essential requirement for such a distribution to be valid in the given case is the presence of a high electron concentration and strong electron–electron interactions, which provide randomization of the direction of electron momentum between the scattering events [8, 9]. The latter type of interaction is not included in the TF model. In the weak-coupling limit of electron–phonon interaction, this leads to a paradoxical result: the model predicts a distribution valid for the randomized, or three-dimensional carrier momenta whereas the actual motion of the carriers in the near-threshold fields is essentially one-dimensional.

Two factors contribute to this type of motion: the inversely proportional dependence of the emission probability on the square of the magnitude of the emitted phonon momentum which follows from the Coulombic nature of the interaction, and the orientational influence of the external field on the direction of carrier momentum. These factors lead eventually to

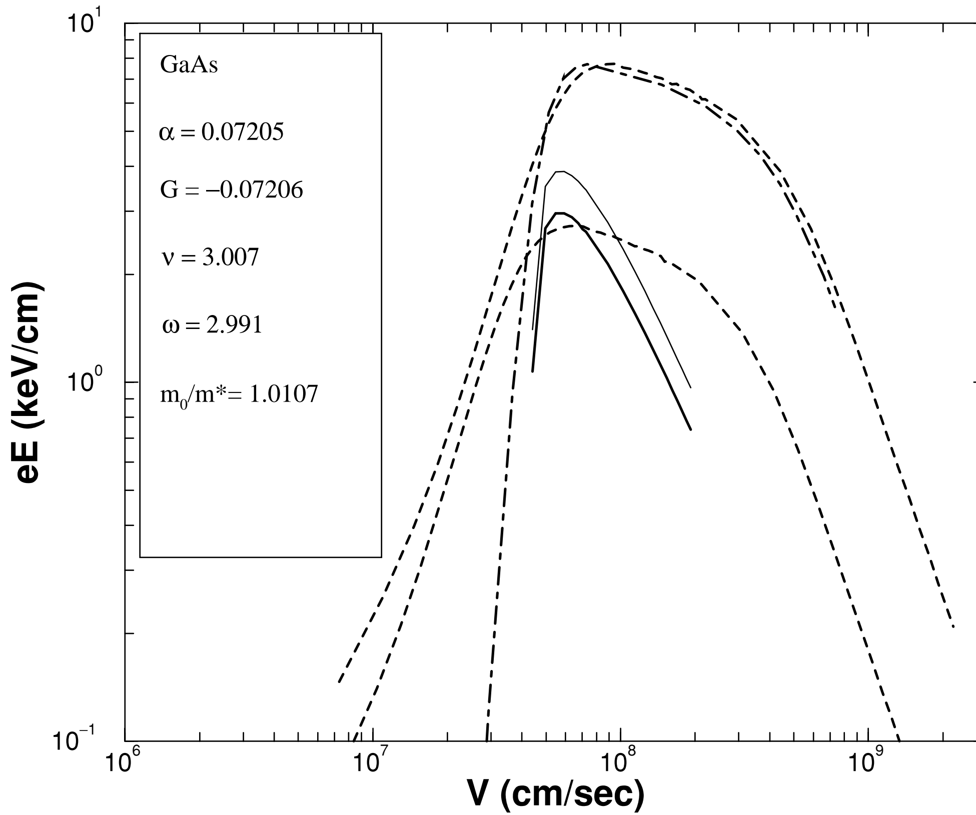

Figure 1. The energy loss per unit distance versus electron velocity in GaAs. Perturbative model: room temperature—thin solid line; $T = 104$ K—thick solid line. TF model: $T = 104$ K—upper dashed line; $T \approx 20$ K—dash-dotted line. Corrected TF model: $T = 104$ K—lower dashed line. Polaron parameters are given in the inset. G, ν, and ω are given in units introduced by Feynman: $\hbar = \Omega = m^* = 1$.

the focusing of carrier motion in the direction of the electric field when the intercollision time exceeds the duration of a single collision. The focusing effect has been considered in detail by Dumke [10] and has to be taken into account in order to avoid a large overestimation (by about an order of magnitude) of energy losses that can be introduced when using the Maxwellian distribution [9, 11].

The failure of the TF model to fit the low-field mobility, as well as the discrepancy detected in this paper, may be understood from the following consideration. In order to avoid extreme complexity in calculations and to eliminate the lattice coordinates from the path integral, Feynman used a harmonic potential instead of the Coulomb potential in the expression for the trial action [4]. In such an approach the polaron ground state and effective mass can be obtained quite precisely since, for these quantities, consideration of thermal electrons in a polar crystal can be utilized. In this case, no directional dependence for the carrier momentum is involved and the variational principle calculations of the influence functional [4] can be accomplished with high accuracy, introducing the fitting parameters in order to compensate for the potential replacement when minimizing the polaron energy. Since the same path-integral approach is the basis of the TF model, we suggest that in the weak-coupling limit the lack of exact accounting for the interaction potential leads to the observed discrepancy: the dependence of

the scattering probability on $1/q^2$ is virtually eliminated and, consequently, the focusing of the carrier movement in the direction of the external field is underestimated.

In the case of strong coupling, the TF model provides a good explanation for the experiment. In figure 2 we depict the energy losses calculated for Al_2O_3. The maximum of the dependence obtained in the TF model (dashed curve) is in excellent agreement with the experimentally obtained maximum losses in this material, 0.03 eV Å^{-1} [14]. We emphasize that for this case, the directional persistence of the carrier momentum disappears due to the strong electron–phonon interaction. Since for $\alpha > 1$ the intercollision time becomes less than the duration of the collision, the motion of carriers again becomes three-dimensional. The almost simultaneous carrier 'collisions' with many phonons eventually lead to the randomization of carrier momentum even in the presence of an external field.

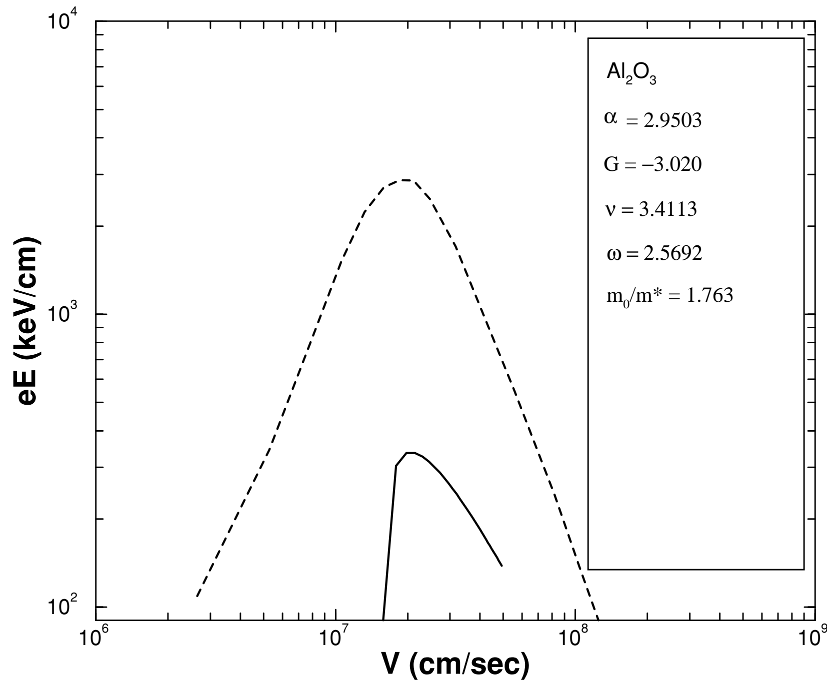

Figure 2. The energy loss per unit distance versus electron velocity in Al_2O_3 at room temperature. Perturbative model: solid line; TF model: dashed line. Polaron parameters are given in the inset. G, ν, and ω are given in units introduced by Feynman: $\hbar = \Omega = m^* = 1$

Unlike the TF model, the SM uses the Fröhlich interaction Hamiltonian derived on the basis of the Coulomb potential. Consequently, it explicitly takes the q^{-2}-dependence of the transition probability and, related to this dependence, field-induced focusing of the carrier momenta into account. Conservation of energy and momentum, valid in the weak-coupling limit, require the angle γ between the initial momentum of the carrier k_i and the momentum of the emitted phonon

$$q = k_i \cos(\gamma) \pm \sqrt{k_i^2 \cos^2(\gamma) - 2m^*\Omega/\hbar}$$

to be no more than $\arccos(\sqrt{\hbar\Omega/\mathcal{E}})$. Considering the equi-energy surfaces in momentum space, one can show that a carrier with energy of about $2\hbar\Omega$ (near the maximum in $eE(V)$) oriented initially in the direction of the external field will change the direction of movement

after emission of a phonon by no more than $\arctan[\sin(\gamma)/(2-\cos(\gamma))] \approx 20^\circ$. This small-angle scattering facilitates fast orientation of the momentum (in the direction of the external field) between the scattering events if these events are separated in time and space.

Although the large-angle scattering events, which lead to the appearance of carriers with negative final momentum, are included in equation (3), we have ignored their influence on the development of the focusing effect. These scattering events require significantly larger q, so the probability of these transitions is relatively small. Moreover, estimating the maximum deviation angle in the previous example we have assumed an isotropic carrier distribution in the momentum space. Focusing, however, will lead to a strongly anisotropic (streaming-like) distribution [9, 12] resulting in a decrease of the magnitude of allowed values of γ as well as a sharper separation between momenta magnitudes of phonons emitted to small and large angles. Finally, the validity of our assumptions is strongly supported by the good agreement between the extremum in $eE(V)$ and the values of the argument at maximum of $V(E)$ obtained by Monte Carlo calculations and experimental measurements [7]. At the extremum of the field, strong anisotropy of the distribution is achieved due to the strong field-related orientational effect.

Because the TF model cannot account for the strong anisotropy of the carrier transport, it overestimates the energy losses to the lattice in the weak-coupling limit. Two facts indicate this overestimation. First, the argument at the extremum of the $V(E)$ characteristics known for GaAs is located at a field which is almost four times below the value predicted by the TF model. It is important to stress that physically the experimental value of E_{th} straightforwardly shows the extremal value of the energy losses to the lattice, i.e., the maximum of $eE(V)$. Second, since the TF model takes into account phonon absorption, one can estimate the low-field mobility and compare it to the experimentally known values. Here again, the TF model gives a value of $\approx 5 \times 10^4$ cm^2 V^{-1} s^{-1} which is almost 2 times *smaller* than the experimentally observed values at $T \approx 100$ K [13].

In order to resolve this discrepancy, one can suggest—in analogy to the classical case—that at the same electron temperature, the reduction of the dimension would correspond to a reduction in the average carrier energy. Since the deviation of the direction of scattered electron momentum relative to the direction of the electric field is small but finite, for the weak-coupling limit we have reduced the energy scale in the TF model by a factor of two in order to match the maxima. This corresponds to decreasing the velocity and energy losses by factors of $2^{1/2}$ and $2^{3/2}$, respectively. The corrected curve $eE(V)$ is shown by the lower dashed line in figure 1. It is important to note that this rescaling in energy not only fits the maxima, but also provides consistency with the experimental value of the low-field mobility, $\approx 8 \times 10^4$ cm^2 V^{-1} s^{-1}.

The differences between the shapes of the curves obtained in the SM and the TF model for GaAs occur for the following reasons. The former model considers only the emission mechanism, whereas the latter model also takes into account absorption. As shown in figure 1 by the dash–dotted line calculated for the uncorrected case of the TF model for $\beta \approx 21$, elimination of phonon absorption by reducing the lattice temperature yields the same slope of $eE(V < V_{th})$ as in the simple model. As expected, for this temperature interval, the temperature decrease does not affect the shape of the curve at and beyond the maximum. This fact clearly indicates that for $\beta > 1$, phonon absorption does not influence $eE(V)$ for $V \geqslant V_{th}$. For $V > V_{th}$, the discrepancy in $eE(V)$ between the models appears to be due to the relatively high value of $\mathrm{d}V/\mathrm{d}t$ in the unstable region. In the framework of the TF model, one can estimate this value by eE/m_0, where m_0 can be obtained as $m_0 \approx m^* \nu^2/\omega^2$; ν and ω are the parameters of the TF model. We have computed these parameters from minimization of the free energy at zero temperature [4]. Our estimates show that the value of the derivative

would be much less than V/τ^* only for $V \sim 10^9$ cm s^{-1}. Thus, the simple model loses its validity for GaAs when $V > V_{th}$. Nevertheless, as follows from the previous discussion, the position of the maximum of $eE(V)$ can be used as a reference point in our comparison.

3.2. Intermediate case: nitrides

Due to the optical anisotropy inherent to wurtzites, the coupling parameter of polaron theory α becomes dependent on the angle θ between the phonon wavevector and the optical axis. Assuming that $\epsilon_z^\infty = \epsilon_t^\infty$, we have derived this dependence in the framework of the dielectric continuum model [1] as

$$\alpha(\theta) = \frac{e^2}{\epsilon^\infty \Omega}\sqrt{\frac{m^*}{2(\hbar\Omega)^3}}\left[\frac{\omega_{Lz}^2 - \omega_z^2}{\left(\Omega^2 - \omega_z^2\right)^2}\cos^2\theta + \frac{\omega_{Lt}^2 - \omega_t^2}{\left(\Omega^2 - \omega_t^2\right)^2}\sin^2\theta\right]^{-1} \tag{4}$$

where $\omega_{Lz}, \omega_z, \omega_{Lt}$, and ω_t are the characteristic frequencies of the A1(LO), A1(TO), E1(LO), and E1(TO) modes, respectively. The phonon frequency as a function of θ can be obtained from the dispersion relation for the extraordinary bulk phonons in a uniaxial crystal [2]. The dependence $\alpha(\theta)$ calculated for GaN is shown in figure 3. One can see that the dependence is not very strong and all the available values of α are in the interval [0.44–0.49]. Due to this, we assume that even for the wurtzite-phase nitrides the estimates can be made taking a single value of the coupling constant from this interval.

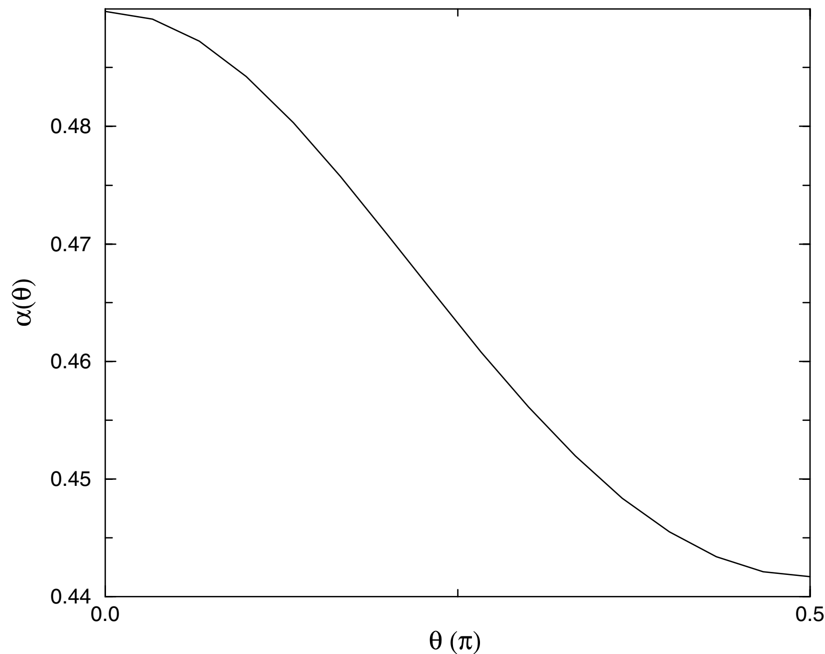

Figure 3. The dependence of the polaron coupling parameter α on the angle between the phonon wavevector and the optical axis in GaN.

To obtain the $eE(V)$ dependence in the TF model we have taken $\alpha = 0.46$. This value is close to the average value of $\alpha(\theta)$ and corresponds to the energy of the LO phonon calculated for GaN in the cubic phase [15]. The energy of the LO phonon in cubic AlN is taken to be 113 meV which is—as for the GaN case—between the energies of the A1 and E1 LO modes in

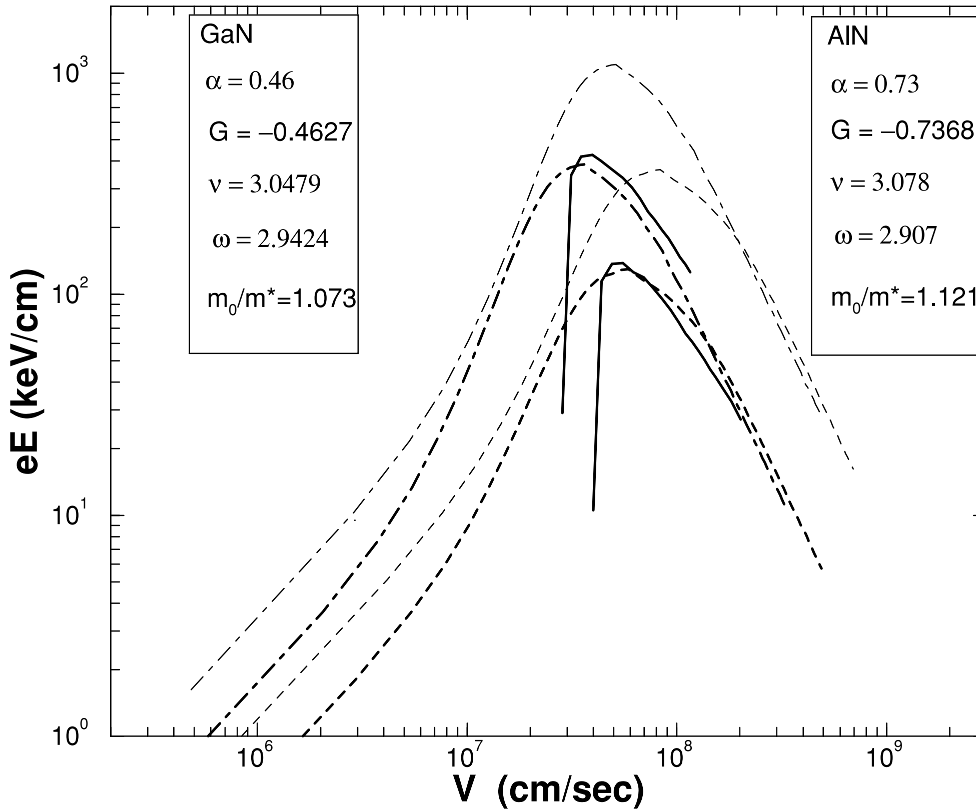

Figure 4. The energy loss per unit distance versus electron velocity in GaN and AlN calculated at room temperature. Perturbative model: AlN—upper solid line, GaN—lower solid line; TF model: AlN—dash-dotted lines, GaN—dashed lines. Thin and thick broken curves show the uncorrected and corrected dependencies, respectively. Polaron parameters are given in the insets. G, ν, and ω are given in units introduced by Feynman: $\hbar = \Omega = m^* = 1$.

the wurtzite phase [2]. The scattering rates are calculated according to the formalism developed in reference [1]. A comparison of the dependences obtained for the nitrides is given in figure 4. Again, the maxima obtained in the SM correlate very well with the threshold electric fields of the $V(E)$ dependences computed using the Monte Carlo technique [16] for a three-valley model of the conduction band: 140 kV cm^{-1} for GaN and 450 kV cm^{-1} for AlN. In order to match the maxima one needs to use *the same* reduction of the energy scale when calculating the energy losses in the TF model as for the case of GaAs. This fact indicates that the focusing effects are of similar nature and magnitude in all three materials. Additionally, one can see that the shapes of the dependences for $V > V_{th}$ are almost the same. This agreement between the simple and the TF models is due to the extremely short intercollision times, $\tau \sim 10^{-14}$ s [1]. The increase of the polaron effective mass cannot compensate for the increase in the energy loss near the threshold value and, therefore, cannot reduce $\mathrm{d}V/\mathrm{d}t$. Nevertheless, due to frequent collisions, the criterion $\mathrm{d}V/\mathrm{d}t \ll V/\tau^*$ is satisfied for the nitrides even at $V \to V_{th}^{+}$. Since appreciable persistence of electron momentum is inherent to the SM, the agreement discussed here provides additional support for our assumptions.

The low-field mobilities estimated from the corrected TF curves are also in excellent agreement with mobilities known for the materials considered, whereas uncorrected curves

of the TF model give the values *reduced* by a factor of 2. As follows from figure 4, the corrected TF model predicts a low-field mobility of about 1800 cm^2 V^{-1} s^{-1} in GaN and 600 cm^2 V^{-1} s^{-1} in AlN. Recent calculations of mobility restricted by carrier scattering with polar LO phonons in GaN give the value of $\approx$2000 cm^2 V^{-1} s^{-1} (see, for example, reference [17] and citations therein). For AlN, variational principle calculations [18] give for this mobility the value 600 cm^2 V^{-1} s^{-1} (see figure 8 of reference [18]).

Finally, to demonstrate that the agreement between the SM and corrected TF model is not accidental but follows from the carrier focusing effect, we have presented in figure 2 the losses calculated in the perturbative model for Al_2O_3 (solid line). One can see that no energy scale reduction can fit the dependences. Since for this case of $\alpha > 1$ the perturbation theory cannot be applied, the maximum loss obtained in this model is about an order of magnitude below the true value.

The comparison made here has allowed us to conclude that for materials for which $\tau\Omega \gtrsim 1$, the application of the Fermi golden rule to explain transport phenomena is almost as good as for materials traditionally handled with perturbation theory, i.e., for the materials for which a much stronger criterion, $\tau\Omega \gg 1$, is satisfied: almost the same energy rescaling of the TF model is required for GaAs, GaN, and AlN. The error introduced by the application of perturbation theory for nitrides is small and can be neglected in most estimations at least for $\beta > 1$.

3.3. Low-field runaway transport

As follows from the previous discussion, the application of the TF model for the calculation of energy losses per unit distance requires correction for the essential anisotropy of carrier motions in the weak-to-moderate-coupling limit. In our treatment, this correction was made by simple energy rescaling. Remarkably, using just this correction allowed us to describe adequately the low-field mobilities, threshold fields, and energy losses by high-velocity carriers for all three materials considered herein. Since the modified TF model provides reasonable values for all of these quantities, we would like to emphasize another important result which follows from the application of the rescaled TF model to the explanation of dissipative transport in the nitrides. Figure 5 represents the dependencies of the energy losses on the electron kinetic energy obtained in the framework of the corrected TF model at room temperature for the three materials considered: GaAs, GaN, and AlN. In the figure, the vertical arrows indicate the energy of the closest upper valley in the corresponding conduction band. The picture shows clearly the possibility of achieving unique pre-threshold-field runaway transport in the nitrides. Indeed, let us consider a GaN sample in an external electric field of 100 kV cm^{-1}. As shown in the figure, the two steady-state solutions for the electron energy would correspond to such a situation. One of the solutions lies in the region $V < V_{th}$ and, consequently, it reflects a stable solution with respect to the electron energy fluctuations. Another one falls into the unstable area, $V > V_{th}$.

Suppose an electron is injected into the sample with an energy somewhere in between the energy which corresponds to the second, unstable, solution and the threshold energy. In this case, since the energy losses to the lattice would exceed the energy gain from the external field, the electron would decelerate until the stable solution at the given field was reached. If, however, the energy of the injected electron just slightly exceeds the value of the high-energy steady-state solution, the electron would accelerate, moving downwards on the unstable branch of the dependence, until it gained enough energy, $\mathcal{E}^*$, to appear in the nearest upper valley of the conduction band. The magnitude of the acceleration would gradually increase due to the increasing difference between the force caused by the external field, $F = 100$ keV cm^{-1},

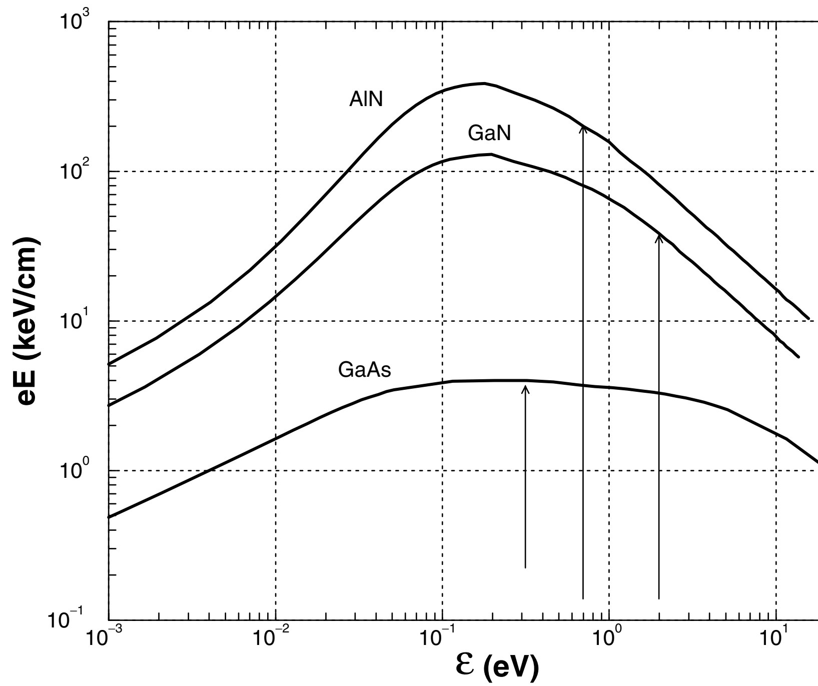

Figure 5. The energy loss per unit distance versus electron kinetic energy. Vertical arrows indicate the energy of the closest upper valley in the corresponding conduction band. $T = 300$ K.

and the force caused by energy losses to the lattice represented by the $eE(\mathcal{E})$ dependence. In order to estimate the minimum runaway length L_r, we have assumed that the energy of the injected electron is 0.7 eV and that the maximum force, $F - eE(\mathcal{E}^*)$, is constantly applied to the carrier. Under this assumption, we obtained $L_r^{\mathrm{GaN}} > 220$ nm.

It is easy to see that because the intervalley separation in AlN is smaller, the effect in this material is expected to be not as strong as in the previous case. Assuming an injection energy of 0.31 eV and applying a field of 300 kV cm^{-1}, we get $L_r^{\mathrm{AlN}} > 39$ nm. Our results also show that the previously discussed runaway transport cannot be achieved in GaAs due to the small intervalley gap and broad peak in the $eE(\mathcal{E})$ dependence.

The results presented in this paper were obtained ignoring non-parabolicity effects. These effects, however, would not change our main findings qualitatively. Indeed, investigating the applicability of the Fermi golden rule for theoretical treatment of wide-band semiconductors with $\alpha \lesssim 1$, we have extracted the 'pure' effect by comparing two models which use a single parabolic band. On the other hand, the predicted low-field runaway effect can occur at electron energies of the order of the LO phonon energy and higher. At these energies (about 0.1 eV for both materials), the non-parabolicity of the conduction band is expected to be negligible in AlN (energy gap 6.2 eV) and very small in GaN (energy gap 3.5 eV). Additionally, the impact of non-parabolicity on the possibility of realizing low-field runaway transport is not completely clear. It is believed that relatively strong non-parabolicity would, in general, tend to suppress the runaway effect. We would nevertheless like to point out that the TF model predicts that upon increasing the carrier effective mass, proper account for the polaronic coupling would lead to (a) a shift of the maximum of $eE(V)$ to smaller velocities and (b) a faster decrease of $eE(V)$ in the unstable region—both factors are favourable to the occurrence of low-field runaway.

Since the simple perturbative model used here ignores not only phonon absorption but also backscattering, one can expect that taking these two effects into account would lead to some increase in energy losses and a shift of E_{th} toward the uncorrected values of the TF model. However, the good agreement between the maxima obtained in our simple model and the fields at maxima of $V(E)$ calculated using the Monte Carlo technique for all three materials (experimentally measured for GaAs and GaN [19]) strongly indicates that for the semiconductors and temperatures considered these effects are not crucially important and, consequently, they cannot lead to an increase of E_{th} which would be strong enough to suppress the expected low-field runaway. The possible magnitude of such a shift can be estimated from the comparison of the threshold field obtained from the SM ($\approx$140 kV cm^{-1}) and that measured experimentally in reference [19] ($\approx$190 kV cm^{-1}). It is obvious that this shift is much smaller than that predicted by the unscaled TF model (threshold field: $\approx$400 kV cm^{-1}).

In order to improve the accuracy of the expected quantities, further investigation is required. We believe, however, that the best confirmation of the conclusions made in this paper can come only from experiment. Our analyses provide guidelines for experimentalists and indicate the possibility of observing this effect in wide-band polar semiconductors.

The abstract possibility of low-field runaway transport was mentioned initially by Thornber and Feynman [3]. Our results suggest that nitrides of Ga and Al promise to be materials where such transport may actually be realized. Detection of this effect in nitrides would prove straightforwardly the applicability of perturbative treatment for these materials. It follows from the fact that the two models, the SM and the modified TF model, provide nearly the same values for $eE(V \geqslant V_{th})$. On the other hand, the low-field runaway cannot be expected from the predictions of the non-modified TF model where, in order to realize this effect, the energy of the injected carrier would have to exceed the energy of the intervalley separation.

4. Summary

In present paper, we have compared the energy losses to the lattice calculated for different polar semiconductors within the frameworks of both the perturbative and the non-perturbative approaches of Thornber and Feynman. The results of this comparison are analysed taking into account available experimental data. We have revealed that—in the weak-coupling limit of the electron–phonon interaction—the TF model not only fails to explain the low-field, low-temperature mobilities observed experimentally and predicted by the perturbation theory, but also strongly overestimates the maximum values of the energy losses to the lattice. Taking into account the universal character of the approach used by Thornber and Feynman, we have assumed that the only source of this discrepancy is in the replacement of the Coulomb potential by a modified harmonic potential which results in a drifted quasi-Maxwellian distribution of carriers in the weak-coupling limit and, consequently, essentially underestimates the field-induced focusing of the carrier momenta inherent to the case where a finite intercollision time can be introduced. In order to eliminate the discrepancy, we have introduced into the TF model an estimated reduction of the energy scale to account for the actual quasi-one-dimensional carrier movement. We have found that at the same reciprocal lattice temperature, the same energy scale reduction provides good agreement between the TF model, perturbative model, and the experiments that we know of for GaAs and GaN (variational principle and Monte Carlo calculations for AlN). We have shown that in the strong-coupling limit, no energy rescaling can lead to an agreement between the models, since for this case the original TF model is correct and the perturbative model is not valid. This result suggests that at least at temperatures $T < \hbar\Omega/k_B$, application of the Fermi golden rule for calculation of the scattering

rates in nitrides, where $\tau\Omega \approx 1.5$, is as appropriate as application of this standard perturbative treatment for the materials where the well known criterion $\tau\Omega \gg 1$ is satisfied.

Experimental confirmation of this finding would dramatically simplify the analysis of transport phenomena in the wide-band polar semiconductors with intermediate magnitude of the polaron coupling factor, $\alpha \lesssim 1$. On the basis of the results of this paper, we have proposed such an experiment. The estimates of the field-dependent electron energy dissipation made within the frameworks of both the modified TF model and the SM for AlN, GaN, and GaAs show that the pre-threshold low-field runaway electron transport can be realized in the nitrides only if the perturbative treatment is adequate for the modelling of the electron transport in these materials. The conditions for the realization of such transport can be formulated as follows:

(a) the energy of the injected carrier should exceed the energy which corresponds to the solution of the momentum balance equation located on the unstable branch of $eE(V)$; and
(b) the separation between the energy of the injected carrier and the energy of the bottom of an upper valley must be high enough to provide a finite value of the runaway length—it must be at least a few times higher than the energy of the polar optical phonon; this effect cannot be expected from predictions of the non-modified TF model since, for this case, the energy of the injected carrier has to exceed the intervalley separation.

The accurate quantitative description of low-field runaway transport requires simultaneous incorporation of conduction band-structure details and polaronic effects as well as proper accounting for other scattering mechanisms. Solution of this problem is an extremely complicated theoretical task. The effect predicted in this paper may, however, be observed experimentally in a short sample with length $L < L_r$. Experimental detection of this effect in nitrides would prove the applicability of the perturbative treatment for adequate explanation of electron transport in these materials.

Polaron ground-state energies and effective masses are calculated for GaN and AlN as well as for GaAs and Al_2O_3. An expression for the Fröhlich coupling constant in wurtzites is derived.

Acknowledgments

This study was supported, in part, by the Office of Naval Research and by the US Army Research Office.

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