High-field hopping transport in band tails of disordered semiconductors

B. Cleve
Fachbereich Physik und Zentrum für Materialwissenschaften der Phillipps Universität Marburg, D-35032 Marburg, Germany

B. Hartenstein and S. D. Baranovskii
Fachbereich Physikalische Chemie und Zentrum für Materialwissenschaften der Phillipps Universität Marburg, D-35032 Marburg, Germany

M. Scheidler and P. Thomas
Fachbereich Physik und Zentrum für Materialwissenschaften der Phillipps Universität Marburg, D-35032 Marburg, Germany

H. Baessler
Fachbereich Physikalische Chemie und Zentrum für Materialwissenschaften der Phillipps Universität Marburg, D-35032 Marburg, Germany

(Received 10 January 1995)

Interplay between temperature T and high electric field F concerning their influence on the hopping transport in disordered semiconductors is studied theoretically. A series of computer simulations of transient and steady-state conduction is carried out with emphasis on the verification of the concept of the so-called effective temperature. According to this heuristic concept the influence of T and F can be parametrized by a single quantity $T_{\rm eff}(T,F)$. We show that such functions $T_{\rm eff}(T,F)$ do exist for both transient and steady-state phenomena; however, they do not coincide with each other for these two cases, implying that there is no universal effective temperature for all transport phenomena. This conclusion is supported by a calculation of the conducting path of carriers under the influence of a high electric field. Theoretical results obtained provide rather a good understanding of experimental data available.

I. INTRODUCTION

Transport phenomena in amorphous semiconductors under the influence of high electric field has recently become the object of intensive experimental and theoretical study. This was implied by observations of strong nonlinearities in the field dependences of the dark conductivity,[1–3] of the photoconductivity,[4] and of the carrier drift mobility[5–11] at high electric fields.

We are not aware of any consistent theory which describes the nonlinear field dependences of the conductivity and drift mobility in *a*-Si:H. However, the corresponding theory of low-field transport has been developed for all regimes discussed, i.e., for the dark conductivity,[12] the drift mobility,[13] and the stationary photoconductivity.[14] In all these theoretical descriptions, hopping transitions of electrons between localized states in the exponential band tails play the decisive role and determine the temperature dependence of transport, provided the thermal energy kT is small comparing to the characteristic energy of the band tail ϵ_0. At higher temperatures, all these approaches converge to the conventional multiple-trapping model in which hopping between localized states is unimportant, the movement of carriers through extended states determining the current. The field nonlinearities of the transport are most pronounced at low enough temperatures,[1–11] when transport is determined by hopping, and below we will discuss the influence of electric field on the hopping of carriers in the band tails.

Studying the hopping transport in amorphous and doped crystalline semiconductors subjected to a strong electric field, Shklovskii[15] has shown that electric field plays a role similar to that of temperature. In order to obtain the field dependence of the conductivity $\sigma(F)$ at high fields, Shklovskii[15] replaced the temperature T in the well-known dependence $\sigma(T)$ for low fields by a function $T_{\rm eff}(F)$ of the form

$$T_{\rm eff}=eFa/2k\ , \tag{1}$$

where e is the elementary charge, k is the Boltzmann constant, and a is the localization length of electrons in the tail states.

A very similar result was obtained later by Gruenewald and Movaghar[16] in their study of the hopping energy relaxation of carriers through band tails at very low temperatures and high fields. It is easy to understand why the electric field plays a role similar to that of temperature. Indeed, in the presence of a field the number of sites available at $T=0$ is greatly enhanced in the field direction, and an electron can relax faster at higher fields. From the formulas of Gruenewald and Movaghar[16] one can easily infer that relation (1) should be valid for relaxation as well.

The same idea was used recently by Shklovskii *et al.*,[14] who suggested that, at $T=0$, one can calculate the field dependence of the steady-state photoconductivity in amorphous semiconductors by replacing the laboratory temperature T in formulas of the low-field finite-

temperature theory by an effective temperature $T_{\text{eff}}(F)$. At $T=0$, expression (1) was recovered.[14]

However, experiments are usually carried out not at $T=0$, but at finite temperatures, and the question arises how to describe the transport phenomena in the presence of both factors finite T and high enough F. Cleve *et al.*[17] suggested for the effective temperature T_{eff} the expression $kT_{\text{eff}}=kT+eF\langle R\rangle$, where $\langle R\rangle$ is the mean jump distance in the field direction. A similar expression $kT_{\text{eff}}=kT+eFa/2$ has been analyzed by Nebel[18] (mistakenly ascribing this formula to Ref. 14), and it was shown that experimental data for the dark conductivity and drift mobility cannot be accounted for by such an effective temperature. For higher T, when multiple trapping dominates the transport phenomena, the expression $T_{\text{eff}}=\max(T,eFa/k2)$ has been suggested by Esipov,[19] which, however, cannot be valid for the hopping regime. In a recent attempt[20] to develop an analytical theory for the hopping regime, the stochastic nature of the hopping transport process was obscured as a consequence of the averaging procedure.

Recently, Marianer and Shklovskii[21] solved numerically linear balance equations for electron transitions between localized states in the exponential tail under the condition of finite T and F. They found a Boltzmann distribution for electrons with an effective temperature $T_{\text{eff}}(T,F)$, which in the limit of $eFa \gg kT$ is close to $0.67eFa/k$. On the basis of the calculation, they found the heuristic formula for the effective temperature at finite T,

$$T_{\text{eff}}^2(F,T)=T^2+(\gamma eFa/k)^2 , \tag{2}$$

where the numerical factor γ has the value $\gamma\approx 0.67$. Calculating conductivity, Marianer and Shklovskii found that it is the effective temperature defined via Eq. (2) which determines the conductivity of the system and which accounts for the combined effects of the electric field F and the lattice temperature T. Baranovskii *et al.*[22] studied the distribution function of electrons over localized tail states by a Monte Carlo computer simulation. They also obtained a Boltzmann distribution function with an effective temperature described by Eq. (2) with $\gamma=0.69\pm 0.03$, in good agreement with the result of Marianer and Shklovskii. Transport phenomena, however, were not simulated by Baranovskii *et al.*[22]

The concept of the effective temperature appears to be useful for hopping in the quantum Hall regime,[23] and has also been suggested for the magnetic susceptibility of hopping electrons.[24] However, this hypothesis is far from being proven either experimentally or theoretically.

Experimental results for the dark conductivity[2] and for transient transport phenomena[6,25] under the influence of a high electric field were compared with Eq. (2), and no contradiction was established between this expression and experimental data. However, the accuracy of the experiments does not allow us to consider these experimental data as a confirmation of the concept of the effective temperature, i.e., to claim that the theoretical description of all transport phenomena in amorphous semiconductors can be parametrized by a single quantity $T_{\text{eff}}(T,F)$. Moreover, it has been claimed[5] that this hypothesis is not valid for such an important transport phenomenon as the dispersive transport in amorphous semiconductors. The dispersion parameter was claimed[5] to be dependent on temperature solely and not on the electric field strength F at $T>90$ K. Careful analysis of the experimental data in Refs. 2 and 6 also shows that the function $T_{\text{eff}}(T,F)$ describing the dark conductivity differs from that describing the dispersion parameter. The effective temperature approach was recently claimed to be valid for the photoconductivity in intrinsic hydrogenated amorphous silicon,[26] but the expression suggested for $T_{\text{eff}}(T,F)$ differs from Eq. (2).

In order to verify the concept of effective temperature, we have carried out a series of straightforward computer simulations of the transport phenomena determined by hopping of electrons in the band tails of amorphous semiconductors. In Sec. II, the algorithms and simulation results for transient dispersive transport are given, confirming relation (2) with $\gamma\approx 0.6$. The results of the simulation show that the non-Markovian, homogeneous dispersive transport theory is a rather good approximation for the description of the Markovian hopping transport in real inhomogeneous systems under study. In Sec. III, the simulation results for the steady-state hopping conductivity are presented. They allow parametrization with T_{eff} determined by Eq. (2), but with the value of $\gamma\approx 0.9$ different from that obtained for dispersive transport. This implies that there is no universal quantity T_{eff} for all transport phenomena. In order to analyze the concept of effective temperature more deeply, analytical theory is developed in Sec. IV for the transport path of electrons in the exponential band tail under the influence of the high electric field at $T=0$, and it is shown that this path differs from the well-known transport energy level at $F=0$ and finite T even if the quantity T_{eff} determined by Eq. (2) is kept constant assuming the value $\gamma=0.67$ corresponding to the equilibrium distribution function.[21,22] Computer simulation of the transport path confirms this result, thus also implying that there be no universal effective temperature describing the various transport phenomena. Nevertheless, the concept of an effective temperature can be used as a rough but useful approximation. Concluding remarks together with discussion are gathered in Sec. V.

II. COMPUTER SIMULATION OF TRANSIENT CURRENTS

Photocurrent transients at low electric fields measured under pulse illumination in a time-of-flight or charge-collection experiment at low temperatures are dispersive. The initial current decay (at $t<t_\tau$, where t_τ is the transient time) is well described by a power-law dependence[5,6]

$$I(t)\propto t^{-1+\alpha} , \tag{3}$$

where $I(t)$ is the current and $\alpha\in(0,1)$ is the dispersion parameter.

Pollak[27] has shown that this behavior can to some extent be treated by a non-Markovian, homogeneous transport theory. In this theory carriers are allowed to hop between sites of a lattice. A carrier on a site leaves this

site a time $t\pm\frac{1}{2}dt$ after arrival with the probability $\psi(t)dt$. The model is homogeneous in the sense that all the sites are assumed to have the same $\psi(t)$. To produce the current decay described by Eq. (3), the function $\psi(t)$ must have the form

$$\psi(t)\propto t^{-(1+\alpha)} , \tag{4}$$

which can be the consequence of multiple trapping of photocarriers from extended states into localized tail states with exponential energy distribution[27]

$$g(\epsilon)=\frac{N_0}{\epsilon_0}\exp\left[-\frac{\epsilon}{\epsilon_0}\right] . \tag{5}$$

Here the energy ϵ is measured positive from the mobility edge ($\epsilon=0$) toward the gap center, N_0 is the total concentration of tail states, and ϵ_0 is the tailing parameter. The dispersion parameter α has then the temperature dependence[27]

$$\alpha=\frac{kT}{\epsilon_0} . \tag{6}$$

This multiple-trapping approach with activation of trapped electrons to the mobility edge is valid in a-Si:H for $T>170$ K.[6,28] At lower temperatures, the mobility edge in the multiple-trapping description should be replaced by the energy level in the tail called the transport energy,[13] and hopping of electrons between localized tail states dominates the transient photocurrent. Silver, Schönherr, and Bässler[29] showed that, in this pure hopping regime, the transient photocurrent response is described by the same equations (3) and (6), thus demonstrating the equivalence of multiple trapping and hopping.

At high electric fields F and low temperatures $50<T<160$ K, the dispersive photocurrent response determined by Eq. (3) was also observed,[6] with the parameter α strongly depending on F. Below we describe our computer simulation of the dispersive photocurrent at various values of F and T, concentrating our efforts on the study of the parameter α in Eqs. (3) and (4).

The simulation technique is similar to that used previously by Silver, Schönherr, and Bassler,[29] and is only briefly outlined here. A cubic lattice with $70\times70\times70$ sites and a lattice constant b has been used. We employ periodic boundary conditions, effectively making the dimensions infinite. In order to simulate the energy distribution of sites described by Eq. (5), the energy ϵ_i of a site has been chosen by a random number R_i between 0 and 1 such that

$$\epsilon_i=-\epsilon_0\ln(1-R_i) . \tag{7}$$

After the energies for all the 357 911 sites have been determined, a particle was sent across the system. The starting site is chosen at random. The hopping rate ν_{ij} from site i to site j is governed by

$$\nu_{ij}=\nu_0\exp\left[-\frac{2r_{ij}}{a}\right]\exp\left[-\frac{(\epsilon_j-\epsilon_i)-eF(x_j-x_i)}{kT}\right] \tag{8a}$$

for $\epsilon_j-\epsilon_i-eF(x_j-x_i)>0$, and

$$\nu_{ij}=\nu_0\exp\left[-\frac{2r_{ij}}{a}\right] \tag{8b}$$

for $\epsilon_j-\epsilon_i-eF(x_j-x_i)<0$, where r_{ij} is the distance between the sites involved, x_i and x_j being the coordinates of the sites along the field direction, and ν_0 is the attempt-to-escape frequency. The quantity ν_0^{-1} defines the time scale of the simulation only. We have used $\nu_0=10^{12}$ s^{-1}. The value $b=a$ was chosen in order to eliminate the influence of the lattice structure on the simulation results. The smaller b is, the easier the tunneling and the smaller the difference in the hopping rates between tunneling events to different lattice neighbors. However, it is unreasonable to choose b smaller than a because electron states are no longer localized on separate sites if $b<a$. Hence $b=a$ seems to be the most reasonable choice. This small value of b implies that the possibilities of hopping to many neighbors from each initial site must be taken into account. For the chosen parameters it was enough to consider the hopping possibilities to $15\times15\times15$ neighbors for each initial site. We have checked that the increase of this number to $19\times19\times19$ did not change our simulation results. The probability that a particle will jump to site j from site i is given by

$$P_{ij}=\frac{\nu_{ij}}{\sum_{k\neq i}\nu_{ik}} . \tag{9}$$

The mean time required for the hop is

$$t_i=\left[\sum_{k\neq i}\nu_{ik}\right]^{-1} . \tag{10}$$

Thus to simulate the motion of a particle by hopping through the described system, two random numbers $0<R<1$ are needed per hopping event. The first random number specifies to which site j a particle jumps from site i. The other random number specifies the time for the jump from i to j. After a particle has jumped, the calculation is repeated for the next jump from site j. The particle is followed until it reaches the plane $x=100$, the initial plane being denoted as $x=1$. At that time, the computation is terminated and another particle is started. The calculations were made for 300 particles at each set of F and T. Two quantities were studied, namely $\psi(t)$, averaged over all sites visited by particles, and $I(t)$. A typical curve for $I(t)$ is shown in Fig. 1 for parameters $\epsilon_0/k=500$ K, $F=510$ kV/cm, and $T=0$.

The power-law behavior described by Eqs. (3) and (4) was observed for all sets of $\epsilon_0>kT$, eFa studied. It is worth noting that the values of α in Eq. (3) coincide with those in Eq. (4) in all simulation runs, thus confirming that the homogeneous non-Markovian approach describing the current $I(t)$ in terms of the waiting-time distribution $\psi(t)$ is a rather good approximation.

We started our simulations at low-F values in the linear regime. For the sets of parameters $\epsilon_0/k=500$ K, $T=350$ K and $\epsilon_0/k=290$ K, $T=90$ K, dependences (3)

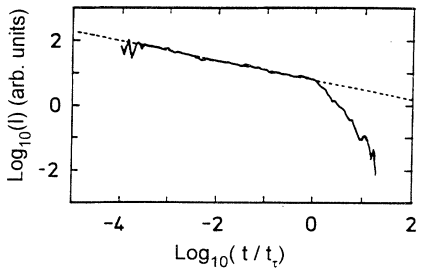

FIG. 1. Dispersive transient photocurrent at $T=0$ and high electric field (solid line) for the simulation parameters given in the text. Dashed line corresponds to Eq. (3) with $\alpha=0.7$.

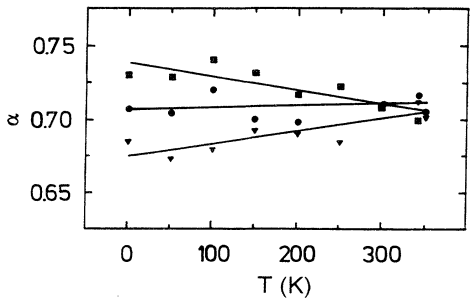

FIG. 3. Dependences of α on T at constant $T_{\text{eff}}=350$ K in Eq. (2) for $\gamma=0.6$ (■); 0.59 (●); 0.58 (▼). Solid straight lines show the minimal squared deviation fits for the simulated data.

and (4) were obtained with $\alpha=0.70$ and 0.31 correspondingly, confirming the validity of Eq. (6) for the hopping regime, in agreement with the previous simulations of linear dispersive hopping transport.[29] Then the simulations were carried out at $T=0$. The values of F were chosen such that T_{eff} determined by Eq. (2) with different γ values was equal to 350 and 90 K for $\epsilon_0/k=500$ and 290 K, respectively. Again, dependences (3) and (4) were recovered with values of α dependent on the choice of γ and hence on the choice of $F=kT/\gamma ea$. The values of $\alpha(\gamma)$ inferred from $I(t)$ [see Eq. (3)] and $\psi(t)$ [Eq. (4)], respectively, are plotted in Figs. 2(a) and 2(b). If the concept of effective temperature described by Eq. (2) is valid, then we must conclude from this figure that $\gamma\approx 0.59/0.60$, because only this value of γ provides consistency with the simulation results $\alpha=0.70$ and 0.31 for $\epsilon_0/k=500$ and 290 K, correspondingly, obtained for the linear regime, i.e., small F and finite T. It is worth noting that the value $\gamma\approx 0.6$ does not depend on the choice of the band-tail slope ϵ_0, hence being universal for different densities of states.

So far we have considered only the extreme cases $T=0$ and finite F, or finite T and very small F. Now we turn to the case that the contributions of T and F to T_{eff} in Eq. (2) are comparable. We have simulated current transients for the parameters set $\epsilon_0/k=500$ K and $T_{\text{eff}}=350$ K. First the value of γ was fixed and the values of T and F were varied such that T_{eff} given by Eq. (2) was always equal to 350 K. Then the γ value was changed and the whole procedure was repeated again. The corresponding temperature dependences of α are shown in Fig. 3 for three different values of γ. If the concept of effective temperature described by Eq. (2) is valid, α must be equal to 0.70, as in the linear regime, and must be temperature independent when $T_{\text{eff}}=350$ K is kept constant by adjusting the electric field F. We see in Fig. 3 that this is the case for $\gamma\approx 0.59$. Moreover, this figure allows us to evaluate the accuracy with which γ is determined, namely $\gamma=0.59\pm 0.1$. Hence we can conclude that the concept of an effective temperature described by Eq. (2) with this γ value is valid for dispersive transient hopping transport in a system with exponential band tails.

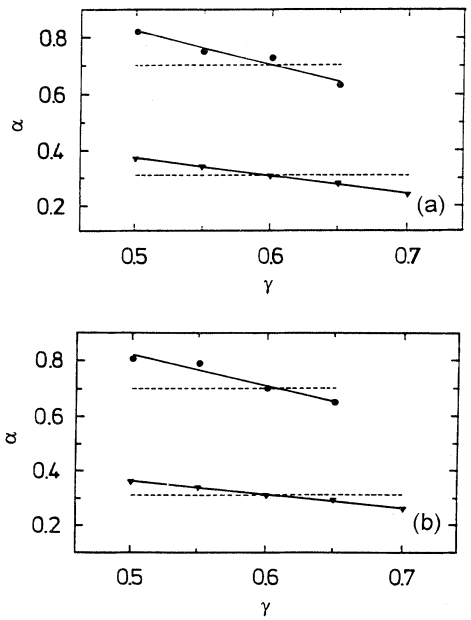

FIG. 2. Dispersion parameter α at $T=0$ inferred from simulation results for $I(t)$ (a) and $\psi(t)$ (b) at different values of γ in Eq. (2) with constant T_{eff}. Solid straight lines show the minimal squared deviation fits for the simulated data. Dashed line shows the corresponding α values in the linear regime.

III. COMPUTER SIMULATION OF A STEADY-STATE TRANSPORT

In order to simulate the steady-state transport, a slight modification of the algorithm described above has been used. Each particular hopping event was treated in the same way as described in Sec. II; however, many electrons were treated simultaneously, thus taking into account the occupation of tail states by electrons. The simulation algorithm was similar to that used previously for studying the energy distribution of electrons in the equilibrium[22] except that one subroutine calculating the conductivity (or mobility) of electrons was added. This subroutine calculates the spatial displacement of a moving particle due to the external field and divides it by the field strength F and the time required for the displacement. The result was averaged over all moving particles.

The simulation parameters $N_0=1.25\times 10^{20}$ cm^{-3}, $\epsilon_0=0.025$ eV, $\nu_0=10^{12}$ s^{-1}, and $a=10^{-7}$ cm were used

similar to those in Ref. 21. A density of $n=10^{17}$-cm^{-3} carriers in a real system then requires a simultaneous consideration of typically 200 carriers in the simulated array of $64\times64\times64$ sites.[22] The routine starts by first determining the time of the hop for each carrier, in accordance with Eq. (10). The carrier with the shortest waiting time executes its hop. The site to which it hops and the hopping time are determined as described in Sec. II. After the hop occurs, the hopping rates of all carriers are updated and the loop starts from the beginning. The loop is repeated typically 10^6 times, consuming a CPU time of about 10 min on a CRAY-Y-MP. Special attention has been given to avoid oscillations between sites close both in space and energy.

This algorithm was first used to study the energy distribution of carriers over the tail states.[22] It was shown that the distribution is well described by a Boltzmann function with an effective temperature $T_{\rm eff}$ determined by Eq. (2) with $\gamma=0.69\pm0.03$, in good agreement with the result of Marianer and Shklovskii,[21] who suggested $\gamma\approx0.67$.

The question arises whether or not the same expression for the $T_{\rm eff}$ determines the conductivity of the system. In Fig. 4, the dependence of the mobility on the electric field strength F is shown, the $T_{\rm eff}$ from Eq. (2) with $\gamma=0.67$ being kept constant and equal to 90 K. The values of the mobility clearly depend on F, thus unambiguously showing that equilibrium transport cannot be described in terms of the same $T_{\rm eff}$ that characterizes the energy distribution of electrons.[21–22]

Our simulation does, however, show that one can parametrize the results for the conductivity at different F and T by a single quantity $T_{\rm eff}$ described by Eq. (2), albeit with $\gamma\approx0.89\pm0.02$. In Fig. 5, the results are shown for the field and temperature dependences of the carrier mobility in the thermal equilibrium obtained by the algorithm described above. It is seen that field dependences of the mobility at different temperatures, and its temperature dependences at different fields can be well parametrized by the universal dependence of the equilibrium mobility on the effective temperature as shown in Fig. 5(c). Expression (2) was used here for the effective temperature $T_{\rm eff}$ with $\gamma=0.89$.

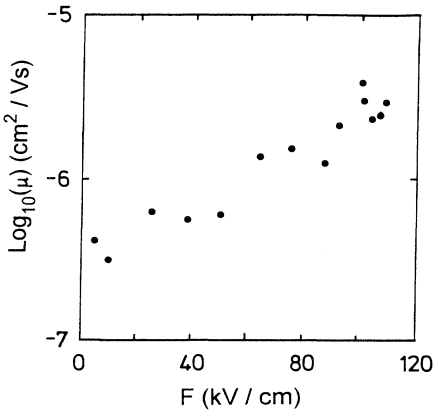

FIG. 4. Dependence of the mobility on the electric field at constant $T_{\rm eff}=90$ K for $\gamma=0.67$ in Eq. (2).

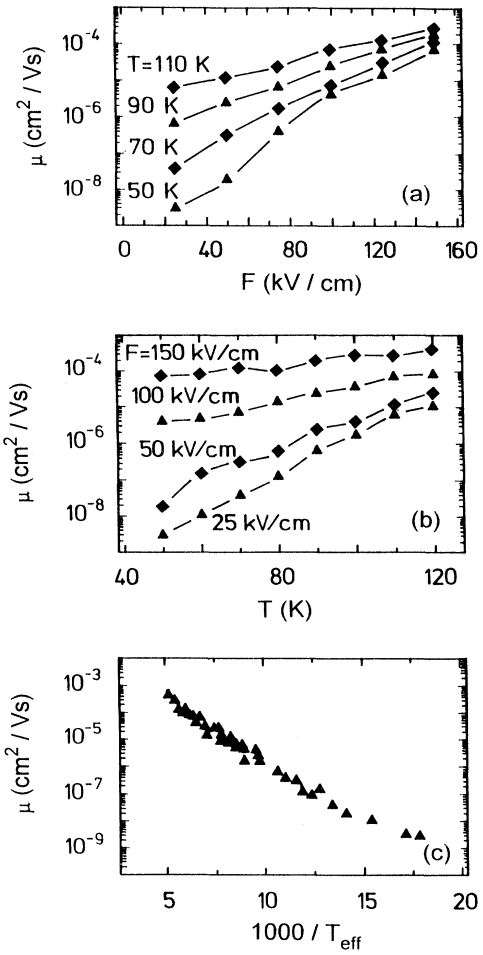

FIG. 5. (a) Field dependences of the mobility at different temperatures. (b) Temperature dependences of the mobility at different fields. (c) The same data as in (a) and (b) represented as a function of a single quantity $T_{\rm eff}$ described by Eq. (2) with $\gamma=0.89$.

We can conclude, therefore, that the equilibrium carrier conductivity depends on the single quantity $T_{\rm eff}(T,F)$ determined by Eq. (2) with $\gamma\approx0.9$. It differs from the value $\gamma\approx0.6$ obtained in Sec. II for the dispersion parameter. This difference between γ values for different transport phenomena implies the necessity of more detailed investigation of the interplay between T and F concerning their influence on the hopping transport. In Sec. IV, we try to analyze this interplay studying the transport path of carriers in the exponential band tail.

IV. TRANSPORT ENERGY FOR HOPPING IN A HIGH ELECTRIC FIELD

It is well known that at low electric fields a particular energy level in the band tail, called transport energy, plays a crucial role in the hopping transport under both equilibrium and nonequilibrium conditions and for both steady-state and transient phenomena.[12–14] In order to better understand the interplay between the high electric

field F and the temperature T concerning their influence on the hopping transport, we try below to extend the transport energy approach to the hopping of carriers at high electric fields. Assuming a density of tail states described by Eq. (5) and hopping rates described by Eq. (8), we consider the behavior of a single electron in two cases: (i) $F=0$, finite T; (ii) $T=0$, finite F.

(i) Let us consider an electron in a tail state at energy ϵ_i. The typical rate of a downward hop of such an electron to a neighboring (in space) localized state with some energy $\epsilon_j \geq \epsilon_i$ is

$$\nu_{\downarrow}(\epsilon_i)=\nu_0 \exp\left[-\frac{2R(\epsilon_i)}{a}\right], \tag{11}$$

where

$$R(\epsilon_i)\simeq\left\{(4\pi/3)\int_{\epsilon_i}^{\infty} g(x)dx\right\}^{-1/3}. \tag{12}$$

The typical rate of an upward hop of such an electron to a neighboring localized state with energy $\epsilon_j \leq \epsilon_i$ is

$$\nu_{\uparrow}(\epsilon_i,\delta_t)=\nu_0 \exp\left[-\frac{2R(\epsilon_i-\delta_t)}{a}-\frac{\delta_t}{kT}\right], \tag{13}$$

where $\delta_t=\epsilon_i-\epsilon_j\geq 0$.

We will analyze these hopping rates for a given temperature T and try to find the energy difference δ_t, which provides the fastest typical hopping rate for an electron placed initially at energy ϵ_i. The corresponding energy difference δ_t is determined by the condition

$$\frac{\partial \nu_{\uparrow}(\epsilon_i,\delta_t)}{\partial \delta_t}=0. \tag{14}$$

Using Eqs. (5), (12), and (13), we obtain that the hopping rate in Eq. (13) has its maximum at

$$\delta_t=\epsilon_i-3\epsilon_0 \ln\frac{3\epsilon_0(4\pi N_0/3)^{1/3}a}{2kT}. \tag{15}$$

The second term in the right-hand side of Eq. (15) is called the transport energy ϵ_t (after Monroe[13]),

$$\epsilon_t\equiv 3\epsilon_0 \ln\frac{3\epsilon_0(4\pi N_0/3)^{1/3}a}{2kT}. \tag{16}$$

We see that the fastest hop occurs to the state in the vicinity of the transport energy ϵ_t, independent of the initial energy ϵ_i, provided ϵ_i is deeper in the tail than ϵ_t, i.e., if $\delta_t\geq 0$. The width of this maximum determined as the energy range near ϵ_t, where the hopping rate $\nu_{\uparrow}(\epsilon_i,\delta_t)$ differs by less than a factor of e from the value $\nu_{\uparrow}(\epsilon_i,\epsilon_i-\epsilon_t)$, is[14]

$$W=(6\epsilon_0 kT)^{1/2}. \tag{17}$$

For states with $\epsilon_i\leq\epsilon_t$, the fastest hop is typically a downward hop to a nearest neighbor at some energy $\epsilon\geq\epsilon_i$ with the rate described by Eqs. (11) and (12). This means that electrons in shallow states with $\epsilon_i<\epsilon_t$ hop normally into deeper states with $\epsilon>\epsilon_i$, whereas electrons in the states with $\epsilon_i>\epsilon_t$ usually hop to states near ϵ_t in the energy interval W determined by Eq. (17) independent of the initial energy ϵ_i.

(ii) Let us now consider the case of a strong electric field F and $T=0$. An electron in a deep state at energy ϵ_i will typically hop against the field direction due to the huge increase of the density of states (see Fig. 6); i.e., the nearest in space localized state with energy not higher than ϵ_i will be usually situated in the direction against the field, provided the distance of the hop x, parallel to the field, fulfills the inequality[14]

$$eFx>\epsilon_0. \tag{18}$$

Making such a hop against the field direction, an electron can increase its energy relative to the mobility edge by an amount

$$\delta_f=eFx. \tag{19}$$

This quantity δ_f is analogous to the energy difference δ_t from (i). However, its calculation must be carried out in a somewhat different way as compared to the calculation of δ_t. The quantities ϵ_i and δ_f are related by equation

$$\delta_f\approx eFR(\epsilon_i-eFR(\epsilon_i-\delta_f))-\epsilon_0, \tag{20}$$

where the term ϵ_0 takes into account that a typical transition occurs not horizontally in energy as shown in Fig. 6, but to some localized state deeper by amount ϵ_0 in the tail than the initial state.

At deep energies ϵ_i, when δ_f obtained by solving Eq. (20) is much greater than ϵ_0, the term ϵ_0 can be omitted and the relation between ϵ_i and δ_f becomes

$$\delta_f\approx eFR(\epsilon_i-\delta_f). \tag{21}$$

Solving this equation numerically, we come to the conclusion that, starting from a rather deep state at ϵ_i, an electron hops upward in energy, making successive hops so that each next hop is on average shorter in space than the previous one and corresponds to a smaller energy difference between two states involved. This inverse energy relaxation is illustrated in Fig. 7. The quantities δ_f involved in successive hops become smaller and the movement of an electron upward in energy stops at an energy ϵ_f when δ_f becomes comparable to ϵ_0. Hence one can evaluate ϵ_f, which is analogous to the transport energy ϵ_t

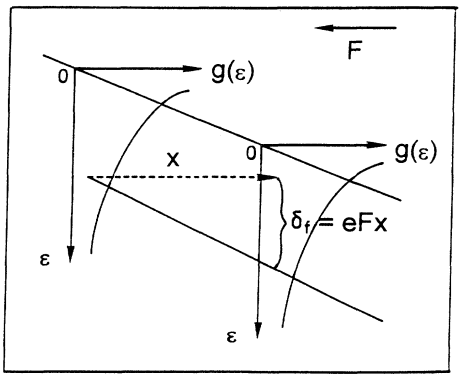

FIG. 6. Electron hop against an electric field over distance x.

of case (i), from the condition

$$eFR(\epsilon_f) \approx \epsilon_0 . \tag{22}$$

We see that the physical ideas which determine ϵ_f differ somewhat from those which were used to determine ϵ_t.

Let us now compare the positions of these two levels ϵ_t and ϵ_f for actual parameters of amorphous silicon under the premise that the values of T [from (i)] and F [from (ii)] correspond to the same effective temperature T_{eff}. In a-Si:H, for which $\epsilon_0 = 0.025$ eV, $a = 10^{-7}$ cm, $N_0 = 1.25 \times 10^{20}$ cm^{-3}, and the transport energy ϵ_t plays the most important role for transport phenomena at low electric field in the temperature range near 100 K.[14,28] Hence we choose the value $T_{\text{eff}} = 90$ K for the comparison between ϵ_f and ϵ_t. In case (i), $T = T_{\text{eff}} = 90$ K and Eq. (16) gives $\epsilon_t \approx 0.10$ eV. Since ϵ_t is only a statistically defined quantity featuring a width W [see Eq. (17)], the effective transport energy is shifted by an amount $W \approx 0.034$ eV relative to ϵ_t defined by Eq. (16) for the parameters given above. In case (ii), we first have to choose the value of γ in order to find the value of F corresponding to $T_{\text{eff}} = 90$ K. The following calculation is based upon $\gamma = 0.67$. This value corresponds to the equilibrium energy distribution of electrons in the band tail, as has been established by different techniques,[21,22] and it seems reasonable to use it, at least under the equilibrium conditions. The value $F = 116$ kV/cm then transfers into $T_{\text{eff}} = 90$ K. Solving Eqs. (22) and (12), we obtain $\epsilon_f \approx 0.05$ eV, i.e., our analytical consideration shows that the level ϵ_f is shifted to the shallower region of the band tail with respect to ϵ_t for the same T_{eff}. Moreover, the character of hopping in case (ii) is somewhat different to that in case (i), i.e., an electron initially situated at some deep level moves in energy to the level ϵ_f by a series of successive hops, as shown in Fig. 7, whereas, in case (i), an electron comes to the vicinity of ϵ_t by a single hop from any deep state. A numerical solution of Eq. (21) confirms this conclusion, yielding $\epsilon_f \approx 0.05$ eV as that energy level at which $\delta_f \approx 0$, consistent with the solution of the more simplified Eq. (22).

In order to verify these rather intuitive arguments, we have studied the energy distribution function of the states visited by electrons in course of their equilibrium movement via hopping in the band tail by a computer simulation described in Sec. III. For this purpose, a counter was introduced into the simulation algorithm whose purpose is to check how many times each particular energy range has been visited by electrons. The corresponding distribution functions are shown in Fig. 8 for cases (i) and (ii) at $T_{\text{eff}} = 90$ K. Since the initial stage of thermalization was excluded from the averaging procedure, the curves in Fig. 8 correspond to the equilibrium state of the system. We see that the maximum of the distribution in case (ii) is situated at somewhat higher energy than that in case (i). The positions of the maxima agree well with the values $\epsilon_f \approx 0.05$ eV and $\epsilon_t \approx (0.1 + 0.034)$ eV predicted by the analytical theory above. This picture confirms that, for the value $\gamma = 0.67$, which yields the same energy distributions of electrons in the cases (i) and (ii), the transport properties of carriers are nevertheless different. Electrons in case (ii) contribute more to the conductivity as compared to case (i), although the energy distributions are the same. The reason is that transport proceeds via energetically higher-lying states in the tail. This explains why the electric field affects equilibrium transport more strongly than the energy distribution of electrons, providing a higher value of $\gamma \approx 0.9$ in Eq. (2) for the conductivity as compared to the value $\gamma \approx 0.67$ for the energy distribution.

So far we considered the role of the energy levels ϵ_t and ϵ_f concerning the steady-state conductivity. It is known, however, that the same energy level ϵ_t also determines the transient relaxation of electrons in case (i).[13] The question arises then whether or not it is possible to find some analog of the level ϵ_f for such transient relaxation in case (ii) as well. In order to answer this question, we have studied the statistics of energy levels visited by a

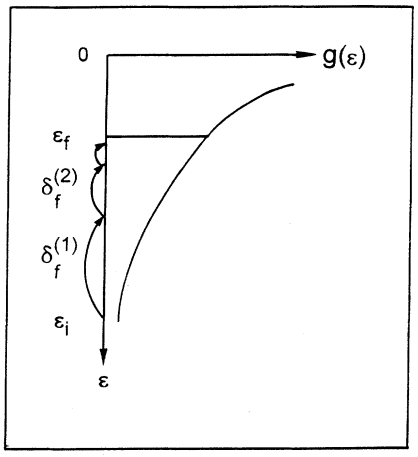

FIG. 7. Successive hops of an electron against the field direction increase its energy with respect to the local mobility edge ($\epsilon = 0$) by amounts $\delta_f^{(1)}$, $\delta_f^{(2)}$, etc.

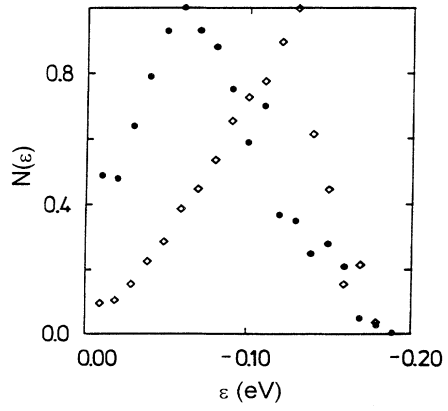

FIG. 8. Statistics of states visited by electrons in equilibrium conditions at $T_{\text{eff}} = 90$ K in the cases (i) (◇) and (ii) (●). Each state was counted as many times as it was visited by carriers. Curves are normalized to have maxima equal to unity.

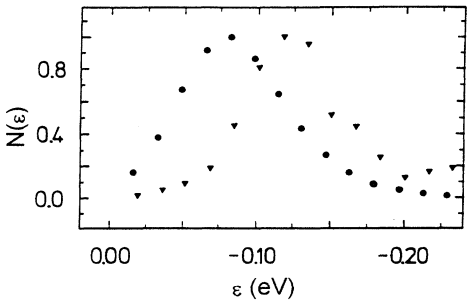

FIG. 9. Statistics of states visited by electrons in their nonequilibrium relaxation at $T_{\text{eff}}=90$ K in the cases (i) (▼) and (ii) (●). Curves are normalized to have maxima equal to unity.

carrier while relaxing through tail states within the algorithm described in Sec. II. This has been done by introducing a counter similar to that in the steady-state simulation into the algorithm of Sec. II. In Fig. 9, the energy distributions of states visited by a carrier during its energy relaxation are shown for cases (i) and (ii) with the same choice of $T=90$ K (i) and $F=116$ kV/cm (ii), as in the steady-state simulation described above. We see that the maximum of the distribution in case (ii) is again located at higher energy than the maximum in case (i). Moreover, the energy positions of these maxima are very close to those in Fig. 8. This is not surprising at all for case (i), for which it is known that the same energy ϵ_t determines both the steady-state and transient transport properties.[12–13] For case (ii) the result is interesting. It shows that at high electric field F and low T, a transport level ϵ_f exists as well, and determines both the steady-state conductivity and the transient relaxation of carriers.

V. DISCUSSION AND CONCLUDING REMARKS

We have studied the interplay between temperature T and high electric field F concerning their influence on the hopping transport in band tails of amorphous semiconductors employing a straightforward computer simulation. Both transient dispersive transport and steady-state conduction were simulated. It is shown that for each of these phenomena the influence of T and F can be parametrized by a single quantity $T_{\text{eff}}(T,F)$, defined via Eq. (2).

Unfortunately, we do not have a satisfactory physical interpretation of Eq. (2). However, it is easy to understand why the effective temperature T_{eff} cannot be a simple sum

$$T_{\text{eff}}(T,F)=T+\gamma eFa/k \ . \tag{23}$$

Suppose the conductivity σ is dependent on T_{eff} solely. Then

$$\frac{d\sigma}{dF}=\frac{d\sigma}{dT_{\text{eff}}}\frac{dT_{\text{eff}}}{dF} \ . \tag{24}$$

In the Ohmic transport regime at $F \ll kT/ea$, the conductivity σ must be field independent, implying that

$$\frac{dT_{\text{eff}}}{dF}\rightarrow 0 \ \text{ as } F\rightarrow 0 \ . \tag{25}$$

The function described by Eq. (23) obviously does not fulfill this condition. However, any function of the form

$$T_{\text{eff}}(T,F)=\left[T^{\beta}+\left[\frac{\gamma eFa}{k}\right]^{\beta}\right]^{1/\beta} , \tag{26}$$

with $\beta>1$ is in accord with the Eq. (25) along with the necessary conditions $T_{\text{eff}}=T$ at $F=0$ and $T_{\text{eff}}\propto F$ at $T=0$. Our simulation results for hopping transport show that $\beta=2$, in agreement with the previous simulation data for the equilibrium energy distribution of carriers within localized tail states.[21,22]

However, the coefficient $\gamma_\alpha\approx 0.6$ determined from the T and F dependences of the dispersion parameter $\alpha(T,F)$ differs from the value of this coefficient $\gamma_\mu\approx 0.9$ determined from the mobility $\mu(T,F)$. This results agrees well with recent experimental data of Nebel *et al.*[6] The authors of Ref. 6 searched for a universal quantity T_{eff} which parametrizes their experimental data for the dispersion parameter α and the mobility μ at different values of T and F. They tried Eq. (2) with the fixed value of γ and found that one can parametrize the experimental data by choosing different values of the localization length a for describing the dispersion parameter α and the mobility μ. If a is kept constant, then one can fit the data in Fig. 16 of Ref. 6 by assuming that $\gamma_\alpha/\gamma_\mu\approx 6/9$. This agrees very well with our simulation results.

The difference between γ_α and γ_μ shows that the heuristic idea of the effective temperature[14,21] does not provide a universal description of different transport phenomena, though being a good first-order approximation.

ACKNOWLEDGMENTS

S.D.B. is thankful to B. I. Shklovskii for stimulating discussions. The financial support of the Deutsche Forschungsgemeinschaft, in particular through the Sonderforschungsbereich 383, and the help of the Computing Center Julich are highly appreciated.

[1] R. A. Street, Philos. Mag. B **60**, 213 (1989).
[2] C. E. Nebel, R. A. Street, N. M. Johnson, and C. C. Tsai, Phys. Rev. B **46**, 6803 (1992).
[3] A. Nagy, M. Hundhausen, L. Ley, G. Brunst, and E. Holzenkämpfer, J. Non-Cryst. Solids **164-166**, 529 (1993).
[4] R. Stahchowitz, W. Fuhs, and K. Jahn, Philos. Mag. B **62**, 5 (1990).
[5] H. Antoniadis and E. A. Schiff, Phys. Rev. B **43**, 13 957 (1991).
[6] C. E. Nebel, R. A. Street, N. M. Johnson, and J. Kocka, Phys. Rev. B **46**, 6789 (1992).

[7]G. Juska, G. Jukonis, and J. Kocka, J. Non-Cryst. Solids **114**, 354 (1989).
[8]R. I. Devlen, J. Tauc, and E. A. Schiff, J. Non-Cryst. Solids **114**, 567 (1989).
[9]G. Juska, K. Arlauskas, O. Klima, and J. Kocka, J. Non-Cryst. Solids **137&138**, 401 (1991).
[10]S. Imao, S. Nakajama, J.-I. Nakata, R. Hattori, J. Shirafuji, and Y. Inuishi, Jpn. J. Appl. Phys. Lett. **30**, L1227 (1991).
[11]K. Murayama, H. Oheda, H. Yamasaki, and A. Matsuda, Solid State Commun. **81**, 887 (1992).
[12]M. Gruenewald and P. Thomas, Phys. Status Solidi B **94**, 125 (1979).
[13]D. Monroe, Phys. Rev. Lett. **54**, 146 (1985).
[14]B. I. Shklovskii, E. I. Levin, H. Fritzsche, and S. D. Baranovskii, in *Advances in Disordered Semiconductors,* edited by H. Fritzsche (World Scientific, Singapore, 1990), Vol. 3, p. 161.
[15]B. I. Shklovskii, Fiz. Tekh. Poluprovodn. **6**, 2335 (1972) [Sov. Phys. Semicond. **6**, 1964 (1973)].
[16]M. Gruenewald and B. Movaghar, J. Phys. Condens. Matter **1**, 2521 (1989).
[17]B. Cleve, B. Movaghar, R. Schumacher, and P. Thomas, J. Non-Cryst. Solids **137&138**, 415 (1991).
[18]C. E. Nebel, J. Non-Cryst. Solids **137&138**, 395 (1991).
[19]S. Esipov, Phys. Rev. B **44**, 7930 (1991).
[20]V. I. Arkhipov and H. Bässler, in *Hopping and Related Phenomena 5,* edited by C. J. Adkins, A. R. Long, and J. A. McInnes (World Scientific, Singapore, 1994), p. 334; Philos. Mag. B **68**, 425 (1993); Philos. Mag. Lett. **69**, 241 (1994).
[21]S. Marianer and B. I. Shklovskii, Phys. Rev. B **46**, 13 100 (1992).
[22]S. D. Baranovskii, B. Cleve, R. Hess, and P. Thomas, J. Non-Cryst. Solids **164-166**, 437 (1993).
[23]D. G. Polyakov and B. I. Shklovskii, Phys. Rev. Lett. **70**, 3796 (1993).
[24]P. Phillips, Phys. Rev. B **49**, 4303 (1994).
[25]R. I. Devlen, H. Antoniadis, E. A. Schiff, and J. Tauc, Philos. Mag. B **68**, 341 (1993).
[26]C. Palsule, S. Yi, S. Gangopadhyay, U. Schmidt, and B. Schroeder, Phys. Rev. Lett. **73**, 3145 (1994).
[27]M. Pollak, Philos. Mag. **36**, 1157 (1977).
[28]S. D. Baranovskii, P. Thomas, and G. J. Adriaenssens, J. Non-Cryst. Solids (to be published).
[29]M. Silver, G. Schönherr, and H. Bässler, Phys. Rev. Lett. **48**, 352 (1982).