Effective transport energy versus the energy of most probable jumps in disordered hopping systems

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An analytic expression for the effective transport energy in a positionally random and energetically disordered hopping system is obtained. It is shown that multiple carrier jumps within pairs of occasionally close localized states strongly affect the position of the effective transport level on the energy scale and lead to a noticeable difference between the effective transport energy and the energy of most probable jumps. In a hopping system with a Gaussian density-of-states energy distribution, the equilibrium carrier mobility is found to be an almost factorized function of temperature and concentration of localized states.

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I. INTRODUCTION

Charge carrier transport in positionally and energetically disordered hopping systems is notoriously difficult for exact analytic consideration. Among several approximate methods, suggested over the last decades,[1–4] the concept of effective transport energy[5,6] was especially efficient as far as the problems of energy relaxation and dispersive or equilibrium carrier mobility are concerned.[7,8] The use of this concept considerably simplifies the problem and essentially reduces it to trap-controlled transport with a broad energy distribution of localized states.[9,10]

The occurrence of an effective transport energy was first revealed in Monte Carlo simulation[5] and was later proved by analytic consideration[6] of charge carrier kinetics in disordered hopping systems. In such systems, the rate of carrier jumps from a given starting hopping site of energy E_s to a target site of energy E_t is determined by the interplay between the energy difference $E_t - E_s$ and the jump distance r. In general, the probability that the jump will be made to some site of the specific energy E_t depends upon the temperature T, the density-of-state (DOS) distribution $g(E)$, the localization radius $(1/\gamma)$, *and* the energy of the starting site. However, if the DOS function is sufficiently steep and if the starting site is sufficiently deep, the most probable value of the energy E_t does not depend upon E_s. In other words, practically all carriers, localized in a deep tail of the DOS distribution, will sooner or later jump to one of the shallower states whose energies are close to some universal value, which is traditionally referred to as the transport energy E_{tr}.

It was usually implied that after an energetically upward jump into a hopping site, which belongs to the transport level, a carrier will make several downward jumps to other states than the starting one. This assumption was also made and is certainly valid for the trap-controlled transport, but justification thereof for a more general case of carrier hopping in disordered systems needs special consideration. Carrier drift and diffusion in the trap-controlled transport mode occur via a band of extended states. Once a carrier was released from a trap to an extended state, lots of other localized states are available for trapping and the probability to be captured by the same trap is negligibly small. However, in a pure hopping system the target site at the transport level is still a localized state that normally has only a few hopping neighbors accessible for the next jump. The starting site is inevitably one of those states, and it is quite possible that, after an upward jump, a carrier will return to the initially occupied deeper site. Such a jump contributes to neither transport nor energy relaxation. Therefore, one must distinguish between the energy level onto which most carriers jump from deeper states, and the genuine transport level, jumps onto which will most probably draw the carrier away from the initially occupied state. That these two are different was already indicated by previous Monte Carlo simulations.[11]

In the present paper we develop an analytic model of charge carrier hopping in disordered hopping systems, taking into account possible correlations between energies and positions of localized states which may lead to ''multiple hopping'' of a carrier between occasionally close hopping neighbors. It is shown that accounting for such cases leads to a meaningful distinction between the energy level of most probable upward carrier jumps and the genuine transport energy. The latter is calculated for both exponential and Gaussian DOS distributions. The obtained results are applied to a calculation of the equilibrium charge carrier mobility in a random hopping system with a Gaussian DOS distribution. It is worth noting that our approach is based on the traditional approach to hopping in disordered systems. This approach disregards possible correlation between energies and positions of hopping sites although such correlations may play an important role as far as charge transport characteristics are concerned.[12,13]

II. THEORY

Most models of carrier hopping in disordered materials, both numeric and analytic, are based on the Miller-Abrahams

expression[14] for the tunneling jump rate ν, which can be written in terms of the hopping parameter u as

$$\nu=\nu_0\exp(-u),\quad u=2\gamma r+\frac{E_t-E_s}{kT}\eta(E_t-E_s), \tag{1}$$

where ν_0 is the attempt-to-jump frequency, γ the inverse localization radius, k the Boltzmann constant, and η the unity-step function. If the starting site is fixed, every target site can be characterized by its hopping parameter u. In a positionally random system of localized states, the average number of target sites, $n(E_s,u)$, whose hopping parameters are not larger than u can be calculated as

$$\begin{aligned}n(E_s,u)&=4\pi\int_0^{u/2\gamma}dr\,r^2\int_{-\infty}^{E_s+kT(u-2\gamma r)}dE_t g(E_t)\\&=\frac{4\pi}{3}\left(\frac{u}{2\gamma}\right)^3\left[\int_{-\infty}^{E_s}dE_t g(E_t)+\int_{E_s}^{E_s+kTu}dE_t g(E_t)\right.\\&\left.\times\left(1-\frac{E_t-E_s}{kTu}\right)^3\right].\end{aligned} \tag{2}$$

The first term on the right-hand side of Eq. (2) gives the number of target states which are deeper than the starting site and the second one describes the number of shallower states. The former is important as far as downward carrier jumps are concerned, while the latter governs the rate of upward jumps. In the present paper we consider the effect of the ''round-trip hopping'' on the effective transport energy. This concept is relevant to upward carrier jumps and, concomitantly, in the following we concentrate on consideration of this hopping mode.

Carring out the replacement of variables,

$$E_j=E_s+kTu, \tag{3}$$

yields the following expression for the number of shallower hopping neighbors of a starting site of energy E_s:

$$n(E_s,E_j)=\frac{\pi}{6}(\gamma kT)^{-3}\int_{E_s}^{E_j}dE_t g(E_t)(E_j-E_t)^3. \tag{4}$$

An upward carrier jump from a starting site is possible if there is at least one such hopping neighbor, i.e., from $n(E_s,E_j)=1$ on. The use of this condition in Eq. (4) leads to the following transcendental equation for the energy of the most probable upward jumps:

$$\int_{E_s}^{E_j}dE_t g(E_t)(E_j-E_t)^3=\frac{6}{\pi}(\gamma kT)^3. \tag{5}$$

If the DOS distribution decreases with energy faster than $|E|^{-4}$, then (i) the value of the integral on the left-hand side of Eq. (5) is practically independent of the lower bound of integration for sufficiently deep starting sites and (ii) a major contribution to the integral comes from states with energies around E_j. Physically, it means that target sites for thermally assisted upward carrier jumps are located around the energy E_j independent of the energy of starting sites and, therefore, Eq. (5) reduces to

$$\int_{-\infty}^{E_j}dE_t g(E_t)(E_j-E_t)^3=\frac{6}{\pi}(\gamma kT)^3. \tag{6}$$

However, the result given by Eq. (6) is obtained disregarding the possibility of backward carrier jumps into starting sites. If a carrier jump is most probably followed by the return of the carrier back to initially occupied state, both these jumps do not contribute to hopping transport and relaxation. Therefore, although Eq. (6) does determine the energy level of most probable upward jumps, the energy E_j is not necessarily the genuine transport energy. In order to calculate the latter, one must account for the backward jumps. Now we embark on this calculation.

After an upward jump over the distance r, a carrier will, most probably, not return to the starting site if there is another hopping neighbor of the target site with a hopping parameter that is smaller than $2\gamma r$ *outside* the sphere of radius r centered at the starting site. The average number of such neighbors, $n_b(E_t,r)$, increases with increasing both E_t and r as

$$\begin{aligned}n_b(E_t,r)&=2\pi\int_0^r dr' r'^2\int_{\arccos(r'/2r)}^{\pi}d\vartheta\sin\vartheta\\&\times\int_{-\infty}^{E_t+2\gamma kT(r-r')}dE' g(E')\\&=\frac{\pi r^3}{12}\left\{11\int_{\infty}^{E_t}dE' g(E')\right.\\&+\int_{E_t}^{E_t+2kT\gamma r}dE' g(E')\left[8\left(1-\frac{E'-E_t}{2kT\gamma r}\right)\right.\\&\left.\left.+3\left(1-\frac{E'-E_t}{2kT\gamma r}\right)^4\right]\right\}.\end{aligned} \tag{7}$$

The probability $w(E_t,r)$ that the target site of energy E_t has at least one hopping neighbor of the hopping parameter smaller than $2\gamma r$ is determined by the Poisson distribution:

$$w(E_t,r)1-\exp[-n_b(E_t,r)]. \tag{8}$$

Since the round-trip carrier jumps do not contribute to transport and relaxation, only those hopping neighbors should be accounted for from which carrier jumps back to initially occupied starting sites are improbable. For upward jumps this condition leads to

$$\begin{aligned}n(E_s,u)&=4\pi\int_0^{u/2\gamma}dr\,r^2\int_{E_s}^{E_s+kT(u-2\gamma r)}dE_t g(E_t)\\&\times\{1-\exp[-n_b(E_t,r)]\}\\&=4\pi\int_{E_s}^{E_s+kTu}dE_t g(E_t)\int_0^{(1/2\gamma)[u-(E_t-E_s)/kT]}\\&\times dr\,r^2\{1-\exp[-n_b(E_t,r)]\}.\end{aligned} \tag{9}$$

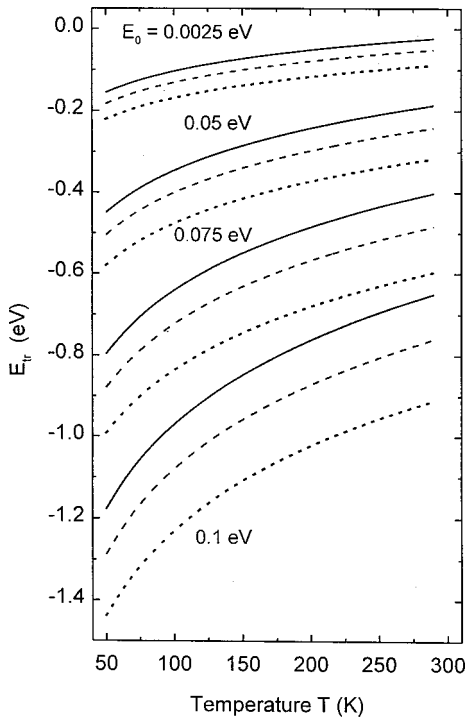

FIG. 1. Temperature dependence of the effective transport energy (solid lines) and the energy of most probable jumps (dashed and dotted lines) in a disordered hopping system with an exponential DOS distribution. The data shown by the solid, dashed and dotted lines are calculated from Eqs. (10), (6), and (12), respectively, for $\gamma = 1\ \mathrm{nm}^{-1}$ and $g_0 = 10^{23}\ \mathrm{cm}^{-3}\ \mathrm{eV}^{-1}$.

Making again the change of variables described by Eq. (3), with E_{tr} substituting for E_j, and using the condition $n(E_s, E_{\mathrm{tr}}) = 1$ yields the relationship

$$4\pi \int_{-\infty}^{E_{\mathrm{tr}}} dE_t g(E_t) \int_0^{(E_{\mathrm{tr}}-E_t)/2\gamma kT} dr\, r^2 \{1 - \exp[-n_b(E_t, r)]\} = 1 \tag{10}$$

where $n_b(E_t, r)$ is given by Eq. (7). Equations (7) and (10) thus determine the genuine transport energy which precludes the return of carriers into initially occupied states and, in a sense, is fully equivalent to a transport band edge.

III. E_{tr} AND E_j IN SYSTEMS WITH EXPONENTIAL AND GAUSSIAN DOS DISTRIBUTIONS

In order to comparatively illustrate the results given by Eqs. (6) and (10), we employ an exponential DOS function which is commonly used as a model of band-tail energy distributions in inorganic disordered semiconductors:

$$g(E) = g_0 \exp\left(-\frac{E}{E_0}\right). \tag{11}$$

Temperature dependences of the transport energy calculated from Eqs. (7), (10), and (11) are shown by solid lines in Fig. 1, parametric in the characteristic energy of the DOS distribution. For comparison, the dashed lines illustrate the temperature dependence of E_j calculated ignoring the possibility of backward carrier jumps. As one should expect, accounting for backward carrier jumps raises the transport level to a higher energy. The difference between values of E_{tr} and E_j increases with increasing E_0 and remains typically less than 0.1 eV for realistic values of the latter parameter. It is also remarkable that this difference is almost independent of the temperature, especially at smaller values of E_0. It is worth noting that the density of states described by Eq. (11) monotonically increases with increasing energy. This inevitably implies the occurrence of the mobility edge at some energy E_m. Therefore, the hopping mode of carrier transport can dominate only at lower temperatures at which the effective transport level is still below E_m.

The energy of most probable jumps can also be calculated within the framework of the traditional Mott approach to the variable-range hopping with a nonuniform distribution of localized states.[15,16] The result reads

$$g(E_j)\left[\int_{-\infty}^{E_j} dE\, g(E)\right]^{-4/3} = \frac{1}{kT}\left(\frac{9\pi}{2\gamma^3}\right)^{1/3}. \tag{12}$$

For the exponential DOS function, Eq. (12) yields[6,15]

$$E_j = E_0 \ln\left[\frac{2\gamma^3}{9\pi E_0 g_0}\left(\frac{kT}{E_0}\right)^3\right]. \tag{13}$$

The temperature dependence of E_j calculated from Eq. (13) is shown by dotted lines in Fig. 1. Although Eq. (13) predicts a deeper level of most probable carrier jumps, its temperature dependence mimics that of both the transport level and the level of most probable jumps calculated from Eq. (6).

In disordered organic materials, the DOS distribution is commonly believed to be described by a Gaussian function of energy as

$$g(E) = \frac{N_t}{\sqrt{2\pi\sigma}} \exp\left(-\frac{E^2}{2\sigma^2}\right), \tag{14}$$

where N_t is the total density of hopping sites and σ the DOS variance. The density of hopping sites in these materials is normally not high enough to provide for the occurrence of extended states and, therefore, the charge transport will be due to carrier hopping independent of temperature. The temperature dependence of the effective transport energy is illustrated in Fig. 2 parametric in the Gaussian DOS width. Dashed and dotted lines in this figure show the temperature dependences of the most probable jump level calculated from Eqs. (6) and (12), respectively. At variance with the results obtained for an exponential DOS distribution, E_{tr} and E_j in a Gaussian hopping system reveal rather different temperature dependences, especially if E_j is calculated from Eq. (12).

A common feature of these results for the Gaussian DOS is that, at some temperature, every curve crosses the zero-energy level at which the DOS has a maximum. At first glance this seems to be an artifact. Even at very high temperatures, most carriers cannot jump to states far above $E = 0$ where the density of states is relatively low and steeply decreases with increasing energy. In order to resolve this

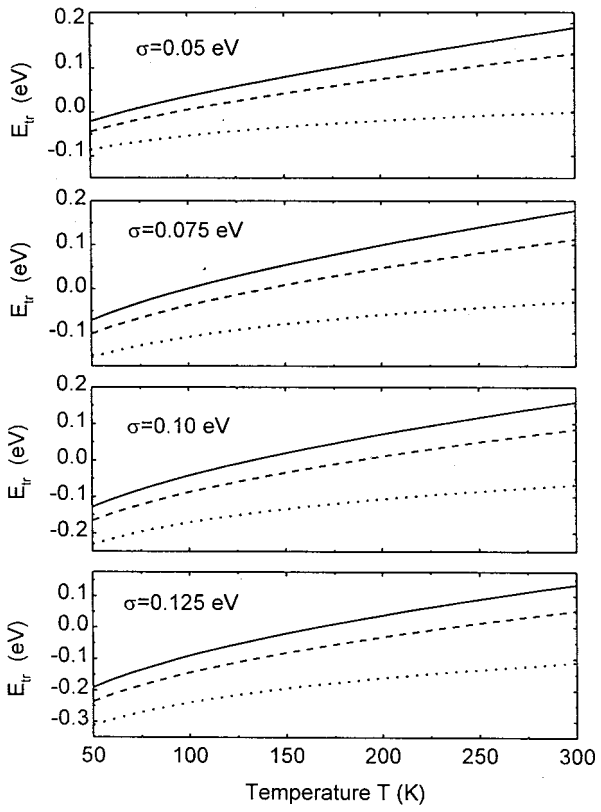

FIG. 2. Temperature dependence of the effective transport energy (solid lines) and the energy of most probable jumps (dashed and dotted lines) in a disordered hopping system with a Guassian DOS distribution. The data shown by the solid, dashed and dotted lines are calculated from Eqs. (10), (6), and (12), respectively, for $\gamma = 10\,\mathrm{nm}^{-1}$ and $N_t = 10^{22}\,\mathrm{cm}^{-3}$.

puzzle, one may consider the asymptotic behavior of E_{tr} and E_j at higher temperatures and/or low concentration of localized states. The latter condition corresponds to diluted hopping systems. Solving Eq. (6) at $T \to \infty$ and/or $N_t \to 0$ yields

$$E_j = kT\left(\frac{6\gamma^3}{\pi N_t}\right)^{1/3}. \tag{15}$$

This result is still puzzling: the energy level of most probable jumps linearly increases with temperature *above* the maximum of the DOS distribution. Substituting this formula into Eq. (3) leads to the following high-temperature and low-concentration asymptotic expression for the hopping parameter:

$$u = \left(\frac{6\gamma^3}{\pi N_t}\right)^{1/3} - \frac{E_s}{kT}, \tag{16}$$

which clarifies the situation. Equation (16) proves that, on the one hand, carriers do jump to states around $E=0$ through barriers whose thickness is around $(4\pi N_t/3)^{-1/3}$ and, on the other hand, E_j can be interpreted as a genuine level of most probable jumps only while this energy is still below the DOS maximum. The same is, of course, true for the transport energy defined by Eq. (10). Evaluating the high-temperature asymptote of E_{tr} from Eqs. (7) and (10) yields

$$E_{\mathrm{tr}} = \left(\frac{32}{11}\right)^{1/6} kT\left(\frac{6\gamma^3}{\pi N_t}\right)^{1/3} \cong 1.2kT\left(\frac{6\gamma^3}{\pi N_t}\right)^{1/3}, \tag{17}$$

indicating that the backward carrier jumps cause a genuine transport energy 20% higher than the energy of most probable jumps.

It may be noted that Eq. (12) predicts a different solution for E_j at high temperatures and/or low concentrations of hopping sites. The approximate solution reads

$$E_j = \sqrt{2}\sigma \ln\left[\left(\frac{2\gamma^3}{9\pi N_t}\right)^{1/3} \frac{kT}{\sqrt{2\pi}\sigma}\right]. \tag{18}$$

Being substituted into Eq. (3), this expression for E_j leads at $T \to \infty$ and/or $N_t \to 0$ to a hopping parameter which does not depend upon the concentration of hopping sites: $u = E_s/kT$. The energy given by Eq. (18) can hardly be considered as a genuine level of most probable jumps as well. At sufficiently high temperatures, this energy becomes positive, which can only be explained by inherent contributions from tunneling. Therefore, although Eq. (12), obtained on the basis of the Mott approach, qualitatively complies with the concept of transport energy, attempts[7] to apply this equation or its equivalent to a calculation of transport or relaxation characteristics will inevitably lead to wrong results for carrier transport in a disordered hopping system with a Gaussian DOS distribution.

IV. EQUILIBRIUM MOBILITY IN A GAUSSIAN RANDOM HOPPING SYSTEM

In order to illustrate the efficiency of the transport energy concept, we apply it to the calculation of the equilibrium carrier mobility μ_{eq} in a positionally random hopping system with a Gaussian DOS distribution at weak external electric fields. Estimating the equilibrium diffusivity D_{eq} as a squared typical jump distance multiplied by the average jump frequency and using the Einstein relation yields

$$\begin{aligned}\mu_{\mathrm{eq}} = \frac{e\nu_0}{kT}&\left[\int_{-\infty}^{\infty} dE\, g(E)\exp\left(-\frac{E}{kT}\right)\right]^{-1} \\ &\times\left[\int_{-\infty}^{E_{\mathrm{tr}}} dE\, g(E)\right]^{-2/3}\int_{-\infty}^{E_{\mathrm{tr}}} dE\, g(E)\exp\left(-\frac{E}{kT}\right) \\ &\times\exp\left(-\frac{E_{\mathrm{tr}}-E}{kT}\right) \\ = \frac{e\nu_0}{kT}&\left[\int_{-\infty}^{\infty} dE\, g(E)\exp\left(-\frac{E}{kT}\right)\right]^{-1} \\ &\times\left[\int_{-\infty}^{E_{\mathrm{tr}}} dE\, g(E)\right]^{1/3}\exp\left(-\frac{E_{\mathrm{tr}}}{kT}\right).\end{aligned} \tag{19}$$

Equation (19) is remarkably similar to the expression for the trap-controlled equilibrium carrier mobility.[17] The only two differences are the occurrence of a temperature-dependent transport energy instead of a fixed mobility edge and a weakly temperature-dependent mean jump distance instead

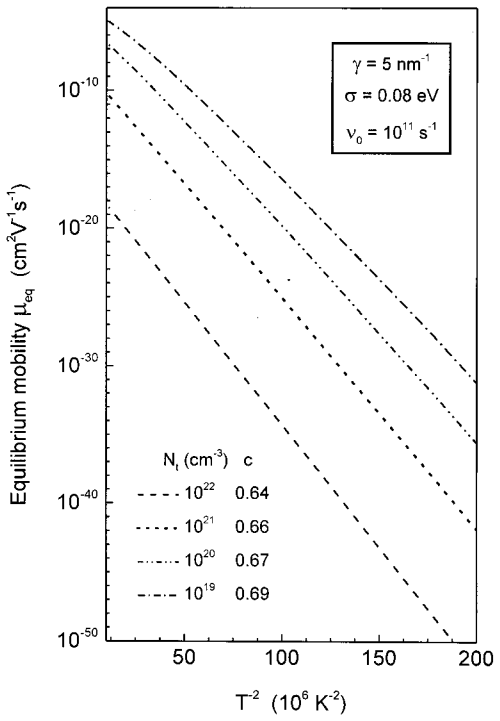

FIG. 3. Temperature dependence of the equilibrium carrier mobility in a random hopping system with a Gaussian DOS distribution.

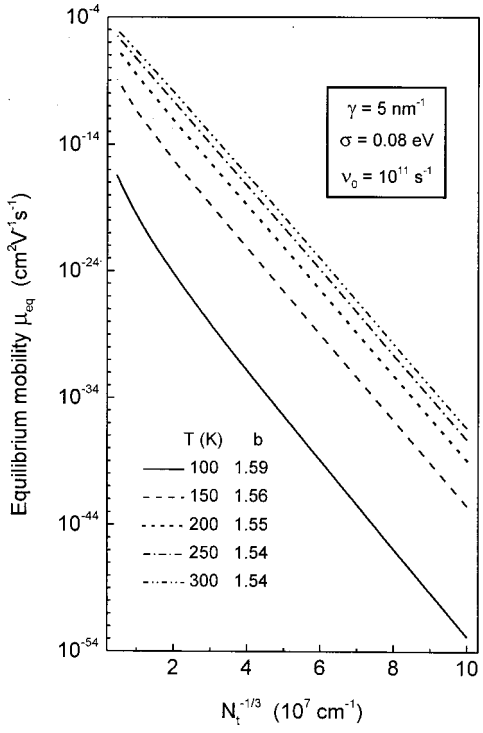

FIG. 4. Dependence of the equilibrium carrier mobility upon the concentration of hopping sites in a random hopping system with a Gaussian DOS distribution.

of a fixed mean free path of delocalized carriers. For a Gaussian DOS function, Eq. (19) reduces to

$$\mu_{\mathrm{eq}}=\frac{e\nu_0}{\sqrt[3]{2}kTN_t^{2/3}}\exp\left[-\frac{\sigma^2}{2(kT)^2}\right]\left[1+\mathrm{Erf}\left(\frac{E_{\mathrm{tr}}}{\sqrt{2}\sigma}\right)\right]^{1/3}\times\exp\left(-\frac{E_{\mathrm{tr}}}{kT}\right), \tag{20}$$

where Erf is the error function. Further simplication of this equation is possible at high T and/or low N_t. Substituting the high-temperature and low-concentration expression for E_{tr} from Eq. (17) into Eq. (20) yields

$$\mu_{\mathrm{eq}}=\frac{e\nu_0}{kTN_t^{2/3}}\exp\left[-1.2\left(\frac{6\gamma^3}{\pi N_t}\right)^{1/3}\right]\exp\left[-\frac{\sigma^2}{2(kT)^2}\right]. \tag{21}$$

Equation (21) proves that the temperature and concentration dependences of the mobility are factorized at high temperatures and/or in diluted hopping systems. This result does suggest that these dependences will also be almost factorized at lower temperatures and in systems with higher concentrations of hopping sites as well. The algebraic $(1/T)$ factor in Eq. (21) will also affect the $\mu_{\mathrm{eq}}\propto\exp[-\sigma^2/2(kT)^2]$ temperature dependence of the mobility; this can be part of the reason for the difference between the numeric factor of 1/2 in Eq. (21) and the 4/9 obtained in Monte Carlo simulations.[18]

Figures 3 and 4 illustrate the dependences of the equilibrium mobility upon the temperature and concentration of hopping sites, respectively. The analysis of these data indeed leads to a factorized equation for the mobility of the form

$$\mu_{\mathrm{eq}}=\mu_0\exp\left(-\frac{b\gamma}{N_t^{1/3}}\right)\exp\left[-\left(\frac{c\sigma}{kT}\right)^2\right], \tag{22}$$

with constants b and c, which reveal only very weak dependences upon the temperature and concentration, respectively. The constant b changes from 1.59 at $T=100\,\mathrm{K}$ to 1.54 at $T=300\,\mathrm{K}$, while c ranges from 0.69 at $N_t=10^{19}\,\mathrm{cm}^{-3}$ to 0.64 at $N_t=10^{22}\,\mathrm{cm}^{-3}$.

Both the form of Eq. (22) and the value of the numeric parameters are in good agreement with the results of both Monte Carlo simulations[18] and the effective medium model,[2,3] which predicted $c=2/3\approx0.67$. Modeling the positional disorder is a notoriously difficult problem for Monte Carlo simulations. In order to avoid this difficulty Bässler and co-workers[18] performed simulations on a cubic lattice and introduced a Gaussian distribution of the localization radius $(1/\gamma)$. The underlying idea was that the jump rate depends only upon the product of the tunneling distance and the inverse localization radius and, therefore, a distribution of localization radii is to some extent equivalent to a random spatial distribution of hopping sites. An almost factorized dependence of the mobility upon the temperature and concentration of hopping sites also suggests the possibility of a simpler, although rougher, approach to hopping in disordered systems, based on configurational averaging.[19,20] Although this kind of averaging does lead to the omission of the concentration dependence, it yields the same functional dependence of the mobility upon the temperature with the numeric factor $c=0.5$.

V. CONCLUSIONS

The effect of multiple carrier jumps between localized states which are occasionally close neighbors in the energy-coordinate configurational space strongly affects the effective transport energy in a random hopping system. Therefore, one should distinguish between the energy level of most probable upward carrier jumps and the genuine transport level. At variance with the trap-controlled transport, the transport level and the level of most probable jumps do not represent the real energy of states via which the transport occurs. The difference is caused by the contribution of the tunneling exponent to the total carrier jump rate. This effect was not adequately accounted for in earlier evaluations of the effective transport energy based on the Mott averaging of hopping rates. Concomitantly, the use of the previously obtained expressions for E_{tr} in calculations of the carrier transport parameters would lead to incorrect results for the concentration dependences of these parameters.

The newly derived expression for the effective transport energy was applied for the calculation of the equilibrium carrier mobility as a function of the temperature and concentration of localized sites. It is shown that, in good quantitative agreement with both Monte Carlo simulations and experimental data, the temperature and concentration dependences of the mobility can be represented as a product of two functions. The first one depends almost solely upon the temperature and reveals only a weak concentration dependence, while the second one mainly governs the concentration dependence of the mobility and is almost independent of the temperature. These results support the predictions of the simpler models based on the effective medium approximation and configurational averaging.

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