Current injection from a metal to a disordered hopping system. II. Comparison between analytic theory and simulation

V. I. Arkhipov,* U. Wolf, and H. Bässler

Institut für Physikalische Chemie, Makromolekulare Chemie und Kernchemie und Zentrum für Materialwissenschaften, Philipps Universität, Hans-Meerwein-Strasse, D-35032 Marburg, Germany

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Monte Carlo simulations of hopping injection from a metal into a random-organic dielectric, described in the previous paper (I), have been compared to results of analytic theory. Good agreement has been found for the field dependence of the yield of charge carriers as a function of the energy barrier at the interface. This is a crucial test for the validity of the assumptions required in order to render an analytical approach of hopping in a disordered system in the presence of a long-ranged Coulombic potential tractable. The most serious of these is the Onsager-like homogenous medium approach to treat the escape of a charge carrier from the Coulomb well once injected. The primary injection event into the dielectric has been treated in terms of hopping theory implying the concept of transport energy. [S0163-1829(99)08511-2]

I. INTRODUCTION

Dark charge-carrier injection from a metallic electrode into the bulk of an insulator is known to be restricted by a potential barrier, $U(x)$, that is formed by a superposition of an external electric field and the Coulomb field binding the carrier with its image twin on the electrode

$$U(x)=\Delta-\frac{e^2}{16\pi\varepsilon_0\varepsilon x}-eFx, \qquad (1)$$

where x is the distance away from the metal-insulator interface, located at $x=0$, Δ the barrier height in the absence of both the external field and the image charge effect, F the external field, e the elementary charge, ε the dielectric constant, and ε_0 the dielectric permittivity. To be injected from a metallic electrode into the bulk of an insulator a charge carrier must either acquire a thermal energy sufficient to cross the maximum of the potential distribution or tunnel through the potential barrier (see Fig. 1). At an electric field ranging from 10^5 to 10^6 V/cm in an insulator with dielectric constant $\varepsilon=3.5$ the maximum of the potential distribution is located between 3.2 and 0.8 nm away from the interface. Since, in disordered organic solids, charge-carrier transport occurs via hopping and the typical jump distance is around 0.6 nm, a carrier cannot cross the potential barrier by a single thermally assisted or tunneling jump. Monte Carlo simulations[1,2] of dark charge-carrier injection from a metallic electrode into a polymer, described as a random-hopping system, prove this to be a multijump process.

A model describing dark current injection into a noncrystalline organic dielectric must, therefore, be based on the concept of carrier random walk within a positionally and energetically disordered hopping system and within the potential distribution described by Eq. (1). This problem is too

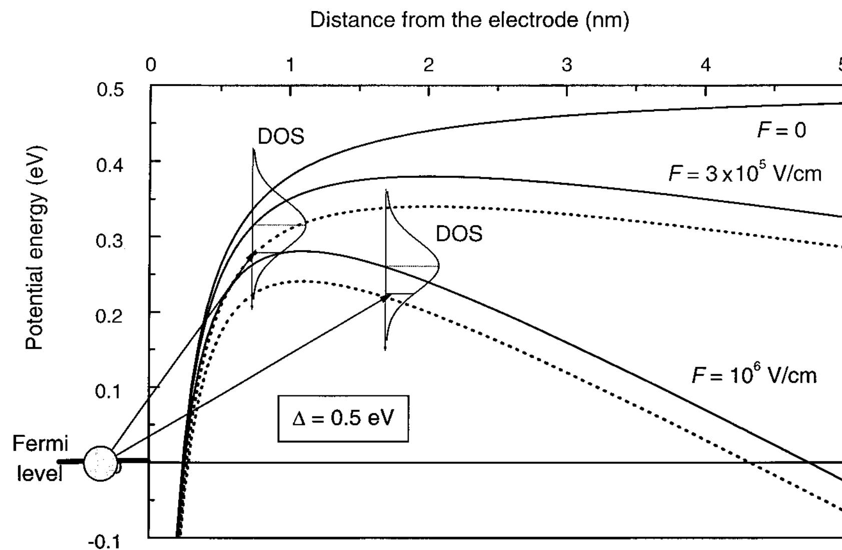

FIG. 1. Potential energy distribution and initial carrier jumps at the metal-polymer interface. Solid lines show the average electrostatic energy of a charge carrier in the Coulombic field of the image charge and in the external electric field. Dotted lines represent the energy of the transport level for the regime of upward carrier jumps.

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difficult for rigorous analytic treatment and some simplifications must be made to get an analytic solution. In the recent work of the authors[3] the injection has been considered as a two-step process. On the first step, carriers make initial jumps from the Fermi level of the metal contact into a localized state close to the metal-polymer interface. The rate of such a jump ν_{in} is determined by the initial jump distance x_0 and by the energy of a target state E. On the second step, the carrier random walk within the system of hopping sites is described as a continuous diffusive motion. Concomitantly, the probability to cross the potential barrier ω_{esc} for a carrier that has made an initial jump over the distance x_0, is calculated as the one-dimensional (1D) Onsager probability to avoid geminate recombination for a pair of a carrier and its image twin *independent* of the energy of a site into which the carrier have made the initial jump. The rate of carrier injection is then calculated by averaging the product $\nu_{in}(x_0,E)\omega_{esc}(x_0)$ over x_0 and E. In other words, two basic assumptions have been made to make an analytic solution possible: (i) the carrier random walk within the positionally and energetically disordered network of hopping sites has been approximated by continuous motion of carriers within a smooth potential landscape and (ii) the probability to cross the potential barrier has been assumed independent of the energy of the target localized state for the initial carrier jump.

An argument in favor of the former assumption is obvious: if the barrier thickness exceeds the typical intersite distance a finite distance of every individual jump cannot strongly affect the probability to cross the barrier.Justification of the latter assumption is the essence of the present paper. It will be shown that, for carrier injection through a high barrier, most of the initial carrier jumps are made to localized states that belong to the effective transport level and that the regime of upward carrier jumps is, therefore, established by initial carrier jumps. Since this regime is equivalent to trap-controlled transport[4,5] one can calculate the escape probability as a 1D Onsager quantum yield. Current injection under the regime of mostly downward jumps of carriers is also possible for lower barriers and broader energetic distributions of localized states. Under these conditions the rate-limiting step is carrier jumps between hopping sites close to the top of the potential barrier. The characteristic feature of this regime is shown to be a weak temperature dependence of the injection current. Predictions of the analytic model are shown to be in a good quantitative agreement with the results of Monte Carlo simulation, which is based on essentially the same microscopic picture of the injection process.

II. THEORETICAL CONSIDERATIONS ON ENERGY RELAXATION AND TRANSPORT OF CHARGE CARRIERS IN A DISORDERED HOPPING SYSTEM

Consider a carrier localized in a hopping site with the energy E. This site is surrounded by other hopping sites that are characterized by their energies E' and distances r from the currently occupied localized state. The rate of possible carrier jumps to a particular hopping site $\nu(E,E',r)$ is then described by the well-known Miller-Abrahams expression[6] as,

$$\nu(E,E',r)=\nu_0\exp(-2\gamma r)\mathrm{Bol}(E,E'), \tag{2a}$$

$$\mathrm{Bol}(E,E')=\begin{cases} 1 & : \quad E'>E \\ \exp\left(-\dfrac{E-E'}{kT}\right) & : \quad E'<E, \end{cases} \tag{2b}$$

where ν_0 is the attempt-to-jump frequency, γ the inverse localization radius, T the temperature, and k the Boltzmann constant. Note that the direction of the energy scale is chosen to assign higher energy values to deeper states. In a random hopping system the values r and $\Delta E=E-E'$ are also random. Amongst all neighboring sites there is one of them that is characterized by a minimum value of the hopping parameter u,

$$u=2\gamma r+\begin{cases} 0 & : \quad E'>E \\ \dfrac{E-E'}{kT} & : \quad E'<E. \end{cases} \tag{3}$$

That site will be referred to as the nearest-hopping neighbor. Since ν depends exponentially upon the hopping parameter the rate of carrier jumps to the second nearest-hopping neighbors in diluted hopping systems is normally much smaller than that for the nearest neighbor. This allows us to estimate the total jump rate from a given site as the rate of jumps into the nearest-hopping neighbor and to neglect the probability of jumps into other sites.

The nearest-neighbor jump rate from a site with the energy E is subject to the condition that the hopping parameter is a minimum,

$$u=2\gamma r=\min \ : \ E'\geqslant E, \tag{4a}$$

$$u=2\gamma r+\frac{E-E'}{kT}=\min \ : \ E'<E, \tag{4b}$$

provided that the probability to find at least one neighboring site with energy $E''>E'$ within the sphere of radius r approaches unity, i.e.,

$$\frac{4\pi r^3}{3}\int_{E'}^{\infty}dE''g(E'')=1. \tag{5}$$

Here, $g(E)$ is the density-of-states (DOS) distribution. Equation (5) leads to the following expression for the jump distance to sites with energies $E''>E'$

$$r=\left[\frac{4\pi}{3}\int_{E'}^{\infty}dE''g(E'')\right]^{-1/3}. \tag{6}$$

Substituting Eq. (6) into Eq. (4b) yields,

$$2\gamma\left[\frac{4\pi}{3}\int_{E'}^{\infty}dE''g(E'')\right]^{-1/3}+\frac{E-E'}{kT}=\min, \tag{7}$$

or, equivalently,

$$g(E')\left[\int_{E'}^{\infty}dE''g(E'')\right]^{-4/3}=\frac{1}{kT}\left(\frac{9\pi}{2\gamma^3}\right)^{1/3}. \tag{8}$$

Solving Eq. (8) may yield either $E'<E$ or $E'\geqslant E$. The former inequality is in agreement with the condition restricting the applicability of Eq. (4b) while the latter implies that

downward carrier jumps dominate for such sites and that Eq. (4a) rather than Eq. (4b) should be addressed under these conditions. Equation (4a) requires the jump distance to be minimized. Equivalently, the value of the integral in Eq. (5) under the condition $E'>E$ has to be maximized. Substituting E instead of E' as the lower bound of integration in Eq. (6) than yields the following expression for the radius of downward jumps $r_{\downarrow}$

$$r_{\downarrow}=\left[\frac{4\pi}{3}\int_{E}^{\infty}dE''g(E'')\right]^{-1/3}. \tag{9}$$

An interesting and important feature of Eq. (8) is that it does not depend upon the energy of starting site E.[4] It means that, for upward jumps, the energy of a target site does not depend upon the energy of starting site. In other words, all carriers making upward jumps reach target sites with similar energy. This is reminiscent of trap-controlled carrier transport in inorganic disordered semiconductors with the sites of energies around E' playing a role of transport states and the energy E' being equivalent to the mobility edge. In the following, we shall refer to this energy as to the transport energy E_{tr}. At a given temperature, the energy E_{tr} separates localized states which involve mostly downward jumps and upward jumps, respectively.

Although general results obtained in the present work are applicable to practically all realistic DOS distributions we illustrate the general results given by Eqs. (8) and (9) employing a Gaussian DOS function that is typical for organic disordered systems[7]

$$g(E)=\frac{N_t}{\sqrt{2\pi}\sigma}\exp\left(-\frac{E^2}{2\sigma^2}\right), \tag{10}$$

where N_t is the total density of localized states and σ the width of the distribution. Substituting Eq. (10) into Eqs. (8) and (9) yields the radius of downward jumps and the transport energy for upward jumps, which can be written as

$$r_{\downarrow}=\left(\frac{3}{2\pi N_t}\right)^{1/3}\left[\operatorname{erfc}\left(\frac{E}{\sqrt{2}\sigma}\right)\right]^{-1/3}, \tag{11}$$

and

$$\exp\left(\frac{3E_{tr}^2}{8\sigma^2}\right)\operatorname{erfc}\left(\frac{E_{tr}}{\sqrt{2}\sigma}\right)=\left(\frac{8\sqrt{2}}{9\pi^2\sqrt{\pi}}\right)^{1/4}\left(\frac{kT}{\sigma}\right)^{3/4}\left(\frac{\gamma^3}{N_t}\right)^{1/4}, \tag{12}$$

where $\operatorname{erfc}(z)$ is the complementary error function. Since carrier jumps within the deep tail of the DOS distribution, $E\gg\sigma$, are the most important ones one can use the asymptotic expansion of the complementary function, $\operatorname{erfc}(z)\cong\pi^{-1/2}z^{-1}\exp(-z^2)$, $z\to\infty$, in Eqs. (11) and (12) yielding

$$r_{\downarrow}=\left(\frac{9}{8\pi}\right)^{1/6}\left(\frac{E}{\sigma N_t}\right)^{1/3}\exp\left(\frac{E^2}{6\sigma^2}\right), \tag{13}$$

and

$$E_{tr}\cong\sigma\sqrt{2\ln\left[\frac{9\sqrt{\pi}}{2\sqrt{2}}\left(\frac{\sigma N_t^{1/3}}{kT\gamma}\right)^3\right]}. \tag{14}$$

A carrier occupying a hopping site of the energy E below E_{tr} will, most probably, make the next jump upwards in energy into a state whose energy is around E_{tr}. The upward jump is normally followed by a series of either downward jumps or upward jumps with smaller energy difference between starting and target sites. The first upward jump is a rate limiting step for this sequence of jumps made by the same carrier until it is localized in a state of energy below E. Therefore, under the so-called ''regime of upward jumps'' a number of downward jumps occur. However, these are upward jumps which represent rate-limiting step and, thus, prescribe the kinetics of carrier thermalization and transport. In this sense, the regime of upward carrier jumps is similar to the trap-controlled carrier transport in materials having a broad energy distribution of DOS with the energy E_{tr} playing the role of the mobility edge. Eventually an equilibrium concerning the energy distribution of carriers will be established. For longer times the average energy of localized carriers remains constant and a constant value of average carrier mobility is achieved. The normalized equilibrium energy distribution of carriers $f(E)$ is determined by the interplay of the Boltzmann thermal exponent and the DOS function as

$$f(E)=\left[\int_{-\infty}^{\infty}dE\,g(E)\exp\left(\frac{E}{kT}\right)\right]^{-1}g(E)\exp\left(\frac{E}{kT}\right). \tag{15}$$

For a Gaussian DOS function Eq. (15) yields a Gaussian distribution as well,

$$f(E)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(E-E_0)^2}{2\sigma^2}\right], \tag{16}$$

shifted to deeper states by the energy E_0,

$$E_0=\frac{\sigma^2}{kT}, \tag{17}$$

which also represents the mean energy of localized carriers. In the following section we apply the above general results to analysis of charge injection from a metallic contact into a disordered hopping system.

III. CHARGE-CARRIER INJECTION THROUGH A METAL-POLYMER INTERFACE

Similar to hopping transport current injection can occur when the dominant mode of transport is either upward or downward jumps of carriers. A general theory of charge-carrier injection from a metal contact to a disordered hopping system must involve both these regimes as it is done in Monte Carlo simulations. However, such a theory can hardly provide an analytical equation describing field and temperature dependencies of the injection current as well as its dependencies upon the material parameters. Therefore, in the present paper we consider these two regimes of carrier injection separately and formulate the pertinent analytical models that specifically account for their essential characteristic features.

A. Current injection under the regime of upward carrier jumps

A carrier injected from a contact into a polymer finds itself within the potential well described by Eq. (1). Due to finite size of hopping sites in real materials, the distance from the contact to the nearest localized state in the bulk of a polymer cannot be shorter than the shortest intermolecular distance a. Energy position of the transport level at the distance a from the contact with respect to the Fermi level in the metal of the contact is of crucial importance for the regime of carrier transport within the potential well. If the zero-field barrier Δ is high enough such that

$$U(a)-E_{tr}=\Delta-\frac{e^2}{16\pi\varepsilon_0\varepsilon a}-eFa-\sigma\sqrt{2\ln\left[\frac{9\sqrt{\pi}}{2\sqrt{2}}\left(\frac{\sigma N_t^{1/3}}{kT\gamma}\right)^3\right]}>0, \quad (18)$$

the first carrier jump from the contact into the insulator will be an upward jump implying immediate establishing of the regime of energetically upward carrier jumps within the bulk of the sample. As it was mentioned in the previous section this regime is similar to the trap-controlled carrier transport with E_{tr} substituting the mobility edge and carrier upward jumps from deeper states governing the kinetics of transport and energy relaxation. Since the coordinate dependence of E_{tr} follows the potential distribution $U(x)$ the probability for a carrier to cross the potential barrier via jumps around E_{tr} can be calculated as the Onsager probability ω_{esc} of geminate pair dissociation in one dimension

$$\omega_{esc}=\frac{\int_a^{x_0}dx\exp\left[-\frac{e}{kT}\left(Fx+\frac{e}{16\pi\varepsilon_0\varepsilon x}\right)\right]}{\int_a^{\infty}dx\exp\left[-\frac{e}{kT}\left(Fx+\frac{e}{16\pi\varepsilon_0\varepsilon x}\right)\right]}, \quad (19)$$

where x_0 is the distance of a first carrier jump from the contact into a hopping site. Averaging over the distance of the first jump and the energy of target sites E' yields the following expression for the injection current density j

$$j=e\nu_0\left\{\int_a^{\infty}dx\exp\left[-\frac{e}{kT}\left(Fx+\frac{e}{16\pi\varepsilon_0\varepsilon x}\right)\right]\right\}^{-1}\times\int_a^{\infty}dx_0\exp(-2\gamma x_0)\times\int_a^{x_0}dx\exp\left[-\frac{e}{kT}\left(Fx+\frac{e}{16\pi\varepsilon_0\varepsilon x}\right)\right]\times\int_{-\infty}^{\infty}dE'\,\mathrm{Bol}(E')g[U(x_0)-E']. \quad (20)$$

The physical meaning of Eq. (20) is very simple: the injection current is determined by the rate of first carrier jumps multiplied by the probability for a carrier to escape surface recombination if it has made an initial jump over the distance x_0 into a site with the energy E'. The rate of initial jumps exponentially decreases with increasing jump distance and most initial jumps are jumps into nearest available sites, i.e., jumps over the distance a. For a positionally ordered hopping system this corresponds to nearest-neighbor jumps. Since the Onsager escape probability is the same for both positionally ordered and disordered systems this implies a weak dependence of the injection current upon positional disorder.

At strong electric fields the distance from the contact to the maximum of the potential distribution may be comparable with the average intersite distance. For instance, at an electric field 2×10^6 V/cm in an insulator with dielectric constant 3 the maximum of the electrostatic potential is located at 0.8 nm away from the contact while the typical intersite distance is 0.6 nm. Under these conditions carriers can make initial jumps into the bulk behind the maximum of the potential distribution. The Onsager probability to escape surface recombination approaches unity for such carriers and, concomitantly, the injection rate is practically equal to the rate of initial jumps. At lower temperatures, carriers have low probability to cross the barrier if they make initial jumps over the distance $x<x_{max}$, where x_{max} is the coordinate of the maximum of the potential distribution. Therefore, carrier jumps through the barrier represent the main channel of the injection at strong fields and relatively low temperatures. With increasing field the initial jump distance through the barrier becomes close to the thickness of the barrier at the Fermi level of the electrode. Concomitantly, the current vs field curves resemble the Fowler-Nordheim field dependence of the injection current at strong electric fields[8] although long distant tunneling is neglected both in the analytic model and in Monte Carlo simulations.

The condition of weak injection implies that fewer charge carriers will cross the potential barrier per unit time than the sample can transport. The rate-limiting step for charge transport in the bulk is the jump from sites populated in equilibrium into sites that belong to the transport level. The corresponding energy difference is E_0-E_{tr}. Note that, even if the barrier Δ is high enough and first carrier jumps from the contact are upward jumps, jumps through the interface will occur faster than in the bulk. In other words, more carriers may enter the sample than can be transported by virtue of field screening due to the space charge. However, under real conditions, only a minority of carriers, which have made first jumps from the electrode, can cross the potential barrier and contribute to the bulk current. Therefore, the current may be limited by charge-carrier injection even if the number of carriers making jumps from the contact per unit time is larger than the sample can transport.

B. Current injection under the regime of downward carrier jumps

Charge-carrier injection under the regime of downward jumps is possible if the Fermi level E_F in the electrode is sufficiently high that a carrier can cross the top of the potential barrier by making only downward jumps. In other words, the following condition must be fulfilled

$$U_{max}-E_{tr}=\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}-\sigma\sqrt{2\ln\left[\frac{9\sqrt{\pi}}{2\sqrt{2}}\left(\frac{\sigma N_t^{1/3}}{kT\gamma}\right)^3\right]}\leqslant0, \quad (21)$$

where U_{max} is the maximum of the potential energy distribution given by Eq. (1). Since a metal contact represents an infinite reservoir of carriers and the rate of downward jumps is much lower for deeper states — see Eqs. (2), (9), (11), and (13) — all hopping sites in the vicinity of the interface deeper than the Fermi level in the metallic contact will be filled. In other words, a quasi-Fermi level will be established close to the metal-polymer interface. Under these conditions the rate-limiting step for carrier injection must be the longest jumps between pairs of deepest states whose energies in the DOS distribution are equal to the quasi-Fermi level. This will be jumps below the top of the potential barrier. Substituting the energy

$$E=U_{max}=\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}, \tag{22}$$

into Eqs. (2), (11), and (13) yields the rate of such jumps, i.e., the density of the injection current

$$j=e\nu_0\exp\left\{-2\gamma\left(\frac{3}{2\pi N_t}\right)^{1/3}\times\left[\operatorname{erfc}\left(\frac{\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}}{\sqrt{2}\sigma}\right)\right]^{-1/3}\right\}, \tag{23}$$

$$j=e\nu_0\exp\left\{-2\gamma\left(\frac{9}{8\pi}\right)^{1/6}\left(\frac{\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}}{\sigma N_t}\right)^{1/3}\times\exp\left[\frac{\left(\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}\right)^2}{6\sigma^2}\right]\right\},$$

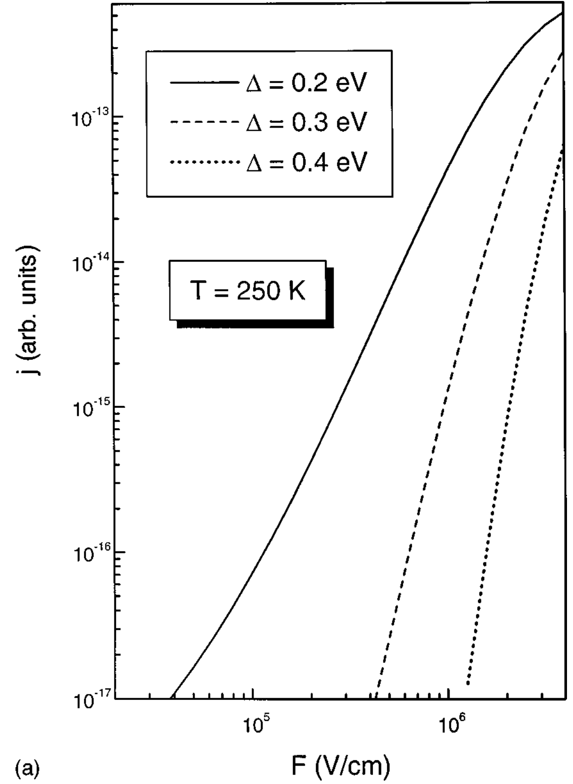
$$\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}\gg\sigma. \tag{24}$$

Note that Eqs. (23) and (24) do not depend upon temperature because downward jumps prevail. However, at fixed material parameters, these results are valid at sufficiently strong fields and at sufficiently low temperatures. The validity of Eqs. (23) and (24) is restricted by the condition that the energy $E=U_{max}$ does not exceed the transport energy E_{tr}. Therefore the inequality

$$\Delta-e\sqrt{\frac{eF}{4\pi\varepsilon_0\varepsilon}}\leqslant\sigma\sqrt{2\ln\left[\frac{9\sqrt{\pi}}{2\sqrt{2}}\left(\frac{\sigma N_t^{1/3}}{kT\gamma}\right)^3\right]} \tag{25}$$

must be satisfied. For $N_t=10^{21}$ cm^{-3}, $\sigma=0.15$ eV, $\gamma=10^8$ cm^{-1}, $\varepsilon=3$, $\Delta=0.25$ eV, and $F=10^6$ V/cm it yields $T<310$ K. For the same set of material parameters and $T=250$ K Eq. (25) requires the field to be above $F=1.6\times10^4$ V/cm. The field dependence of the injection current under the regime of downward carrier jumps is illustrated in Fig. 2.

If charge carrier injection occurs under the regime of downward jumps, the rate-limiting steps are also downward jumps in the vicinity of the maximum of the potential distribution. This implies the thermalization process is not finished when carriers cross the potential barrier and penetrates into the bulk of the sample. Since the effective carrier mo-



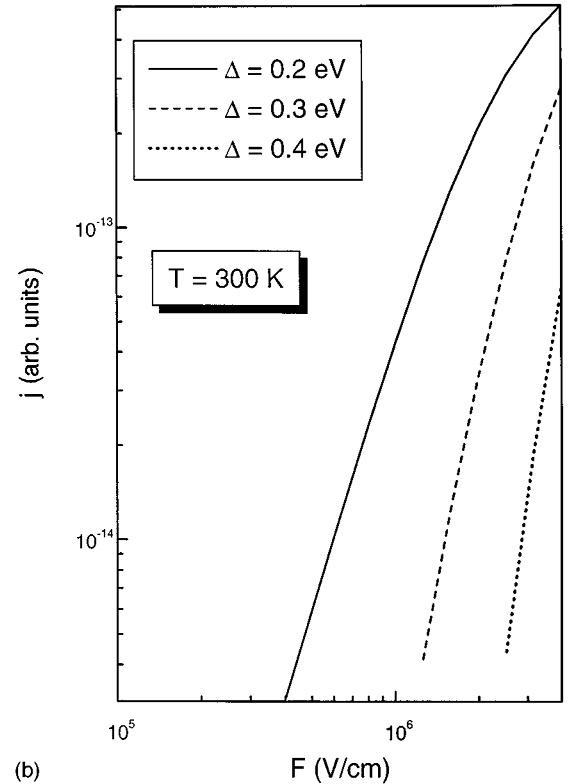


FIG. 2. Field dependencies of the dark injection current under the downward hopping regime for the following set of material parameters: $N_t=10^{21}$ cm^{-3}, $\sigma=0.15$ eV, $\gamma=10^8$ cm^{-1}, and $\varepsilon=3$.

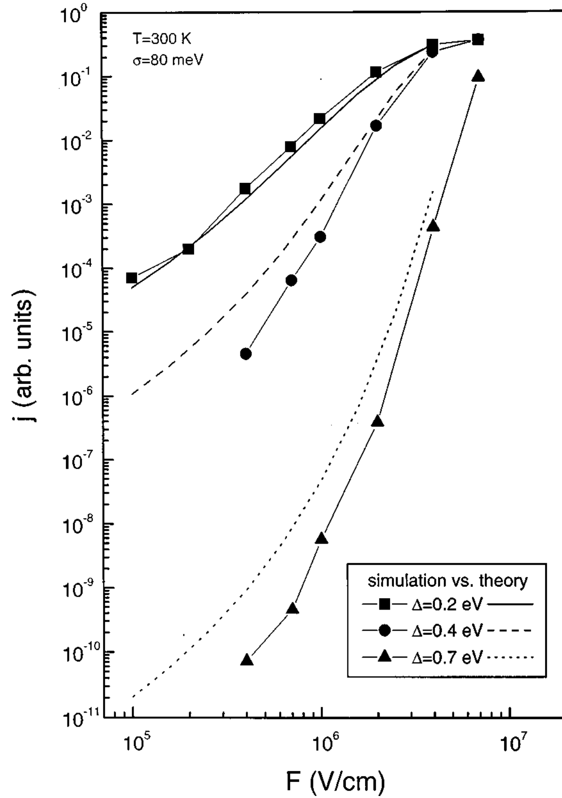


FIG. 3. Field dependencies of the injection current density derived from simulation and analytic theory parametric in the injection barrier Δ. The analytic data were normalized by a prefactor to fit the simulation data at a field of $F=4\times10^{6}$ V/cm and a barrier of $\Delta=0.2$ eV.

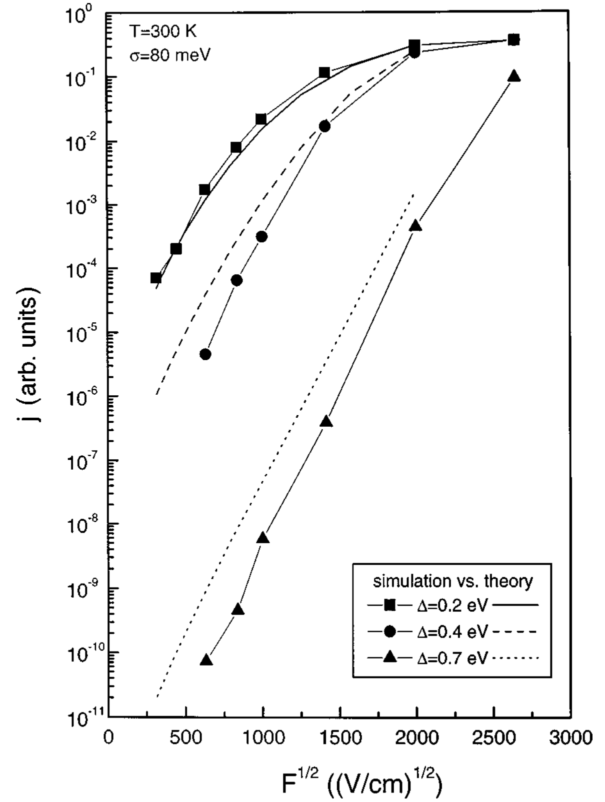


FIG. 4. Injection current densities from simulation and analytic theory parametric in barrier plotted versus $F^{1/2}$.

bility decreases in the course of thermalization the bulk current may, under these conditions, be less then the injection current at the same external field F. Carrier injection and transport in the bulk will be balanced again if the field at the interface is reduced compared to its value in the bulk. As a limiting case the regime of space charge limited current can be established.

IV. COMPARISON WITH MONTE CARLO SIMULATION AND DISCUSSION

Field dependencies of the injected current calculated from Eq. (20) are shown in Fig. 3 together with the results of Monte Carlo simulations for the injection efficiency for different heights of the zero potential barrier. A numeric prefactor is chosen such that the absolute values of analytic and simulated currents coincide exactly for the field $F=4\times10^{6}$ V/cm and $\Delta=0.2$ eV. After this normalization, the difference between any analytic curve and correspondent simulation data is less than one order of magnitude covering more than ten decades. Note that for higher barriers there will be some discrepancy between the predictions of the analytic model and the simulation data increases with decreasing electric field. The origin of this discrepancy is the following.

Interplay of the drift and diffusion is normally introduced into the Onsager problem by using Einstein relation between the mobility and the diffusivity. For a hopping system this implies neglecting the field dependence of μ, which may be justified only in weak electric fields. At stronger fields, the diffusivity is smaller than predicted by the Einstein relation for a given value of the mobility.[9] The total electric field in the sample is a superposition of the Coulomb field of the image charge and the external field. Close to the interface it increases with decreasing external field and forces a carrier to return to the contact. Under these circumstances, the Einstein relation leads to overestimating the rate of injection at weak external fields and at high barriers.

In Fig. 4 the curves shown in Fig. 3 are replotted on a $\log(j)$ vs $F^{1/2}$ scale, appropriate to test the validity of Richardson-Schottky (RS) theory of thermionic emission.[8] The comparison indicates that thermally assisted hopping injection does, in fact, resemble RS theory except that the slope, $\partial \ln j/\partial F^{1/2}$, approximately is larger by a factor of 2. The reason for that similarity is that, at higher temperatures, the energy of the transport level approaches the mean of the Gaussian DOS distribution. Therefore, the height of the potential barrier formed by the transport level is practically equal to that of the electrostatic barrier and carrier injection is mainly due to carriers which cross the barrier by thermally activated jumps. Under these conditions the probability to cross the barrier is determined by the probability to obtain the necessary thermal energy. The latter is governed by the Boltzmann distribution independent of whether a carrier acquires this energy as a single portion or as a sum of smaller portions. This is the essential assumption of the RS model, that a carrier can be injected from a metal into the bulk of a dielectric once it has acquired a thermal energy sufficient to cross the potential barrier. Deviations occur at lower fields and temperatures due to the stochastic carrier motion in the vicinity of the barrier as discussed in Sec. I.

Analytical approaches to the problem of carrier transport in disordered hopping systems normally imply that the drop of the electrostatic potential energy over a typical jump distance is small. This simplification allows us to consider hopping transport as a diffusion-type motion within a given potential landscape. However, this assumption becomes doubtful as long as the problem of carrier injection is concerned. In this case, the jump distance $\cong 1$ nm is comparable to the characteristic scale of the potential distribution close to the interface. Since the distance from the interface to the top of the potential barrier may be 4 nm and less at strong fields applying the concept of diffusion-assisted carrier release from the 1D Coulomb potential well is a rough approximation.

Another aspect of the analytic model not accounted for in a proper way is that the intermediate regime of carrier injection when carriers enter the sample via mostly downward first jumps while the transport regime is reversed before carriers cross the top of the potential barrier. This case can be described neither as temperature-independent carrier injection due to downward jumps nor within the framework of the Onsager type model of carrier upward jumps via hopping sites that belong to the transport level.

In summary, we checked the assumptions involved in the analytic approach for hopping injection into a random hopping system against the ''exact'' Monte Carlo simulations. The most serious of these is the neglect of disorder as far as the escape of a charge carrier across the Coulombic image potential is concerned. That process has been treated in the framework of the 1D version of Onsager's approach of geminate recombination. It implies the validity of Einstein's relation for diffusion and drift in the vicinity of the Coulomb barrier. The obvious success of the theory rests upon the fact that the rate-limiting step is the initial injection event from the metal into the dielectric described in terms of the general hopping approach involving the concept of transport energy. Once having recognized that the primary injection event is crucial one can elaborate upon that idea to improve injection by structural and/or chemical modification of the interface.[10]

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*On leave from Laboratorium voor Halfgeleiderfysica, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Heverlee-Leuven, Belgium.

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