

SEMICONDUCTORS AND DIELECTRICS

Injection of Holes into Organic Molecular Solids

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Abstract—A model is proposed for injection of carriers (holes) from a metal into organic molecular solids. It is shown that the total injection current is restricted by the process of tunneling between the levels of a molecule and states in the metal. The role played by phonons in the tunneling transition is studied in detail, and the contribution from these transitions to the total injection current is estimated over a wide temperature range.

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1. INTRODUCTION

Organic compounds are presently considered to be promising materials for micro- and optoelectronics applications. They were employed to advantage in development of light emitting diodes and field transistors which are enjoying wide use. Their bandgap being fairly large (3 eV and larger), the concentration of intrinsic carriers in such materials is rather low, so that they behave as dielectrics in weak electric fields. Electric field injects carriers from the electrodes. The injection intensity is determined by the barrier forming at the metal–dielectric interface.

The injection (electron and hole) currents (j_i) from the metal into the corresponding bands of inorganic dielectrics or semiconductors are usually described by equations similar to those representing field and thermionic currents from a metal into vacuum [1]. At the same time, such equations are frequently employed, without any grounds whatsoever, to treat injection of carriers (both electrons and holes) into organic molecular solids (OMSs) [2–5], to which the concepts of the band theory of solids are inapplicable because of the weakness of molecular interactions involved, and of the conduction being of the hopping nature. This accounts for the increasing interest being focused in the recent years [6–11] on the problem of carrier tunneling from a metal to local states in organic materials which feature typically a high concentration of such states with a Gaussian distribution in energy.

The results obtained in an analysis of electron injection are usually applied to description of the injection of holes as well (see, e.g., [10]), an approach which, considering that the shape and height of barriers for injection of electrons and holes are different, does not appear justified enough.

The specific features of hole injection into an OMS were first discussed in [12]. Hole injection was treated

there as a consequence of ionization of molecules which are located close to the surface of a metallic anode in a tunneling transition of an electron from the higher occupied molecular orbital (the HOMO level) to a free electronic level in the metal. This was done under the assumption that the potential barrier at the metal–OMS interface is surmounted by the electron in one hop. With no field applied, the barrier is formed by Coulomb interaction of the electron and the hole with their mirror images in the metal. As a result of the increase in the barrier transparency near a metallic surface induced by the image forces the probability of ionization of organic molecules near metallic surfaces may be quite high, while in the bulk of a polymer it is negligible for the same field strength. The shape of the barrier in an electric field F is described in this case by the relation [13]

$$U(x, x_i, F) = E_F + \varphi + exF - \frac{e^2}{16\pi\epsilon\epsilon_0 x} - \frac{e^2}{4\pi\epsilon\epsilon_0(x_i - x)} + \frac{e^2}{4\pi\epsilon\epsilon_0(x_i + x)}, \quad (1)$$

where x_i is the distance from the anode, and E_F and φ are the Fermi energy and the work function of the electrode. The first two terms in Eq. (1) define the barrier height at the interface with no field applied, the third term allows for the effect of an electric field on the energy of a charge at a distance x from the anode, the fourth describes interaction of the electron with its image, the fifth, the energy of interaction of an ion with the electron, and the sixth term accounts for the interaction of the electron with the image of the ion. For $x = 0$ and $x = x_i$, this relation reduces to $-\infty$, and therefore one assumes conventionally that an electron with energy E is incident on the barrier not at points $x = 0$ and $x = x_i$.

but rather at points x_1 and x_2 which are roots of the equation $E - U(x, x_i, F) = 0$. Obviously enough, the barrier width in this case is $(x_2 - x_1)$. Figure 1 illustrates the shape of the barrier as calculated from Eq. (1) for $E_F = 5$ eV, $\phi = 5$ eV and $\epsilon = 3$, for different field strengths and distances from the anode. We readily see that in the case considered here, the barrier differs substantially in shape, for all values of F and x_i , from the one treated usually in an analysis of electron emission.

It was shown [12] that, in strong electric fields (high field strengths can occur, for instance, in the vicinity of micro-sized hillocks on the anode), regions can form close to the anode in which intense ionization of molecules can set in. Unfortunately, the $j_i(F)$ relation was in this publication not obtained. The authors [12] did not also take into account the energy distribution of local states in an OMS.

The quantum-mechanical problem of electron transition from local states in a polymer into continuum in a semiconductor or a metal was considered [14]. The author calculated the probability of this transition under the assumption of the local states in a polymer being monoenergetic. It was also assumed that the HOMO level of macromolecules in a polymer in the absence of electric field lies close to the electrode Fermi level. In this energy region, there are always free states in a metal into which electrons can tunnel isoenergetically from OMS molecular orbitals (it may be added that this situation is not characteristic of OMSs with the ionization potential of macromolecules in excess of 6 eV, in particular, the majority of polymer OMSs). With this assumption, one obtained [14] an analytic expression for the density of the hole injection current. It differs from the well-known Fowler–Nordheim equation with a triangular barrier in the presence of a prefactor, but the close-to-linear pattern of the $\log[j_{inj}(F)F^{-2}]$ vs. F^{-1} relation (in the Fowler–Nordheim coordinates) is retained in this case as well.

The purpose of the present study was to consider electron transition from HOMO levels of molecules of organic materials (i.e., the hole injection process) under the condition that in the absence of electric field these levels lie substantially lower than the Fermi level in a metal. The idea was to use the concepts of the ionization mechanism underlying hole formation in an OMS proposed in [12], while considering HOMO levels as local states with a Gaussian distribution in energy, to derive appropriate expressions for the field and temperature dependences of the density of injection current in the presence of a strong electric field. Note in this connection that the average effective electric field strength in modern devices, for instance, in thin-film organic light-emitting diodes, is close to 10^6 V/cm. Because of the electrodes being nonuniform, local field strength may

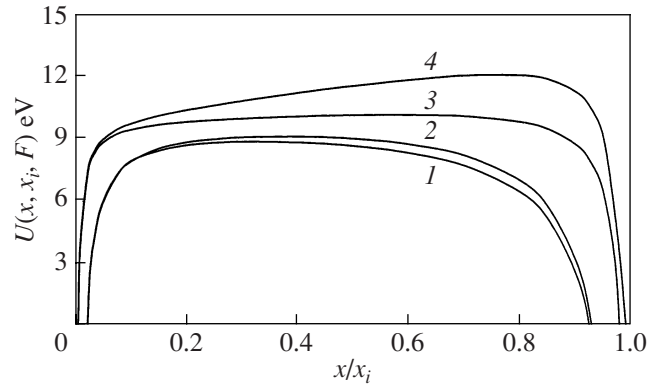


Fig. 1. Shape of the potential barrier mediating hole injection from a metal into an OMS. $F = (1, 3)$ 500 and $(2, 4)$ 2000 MV/m $(2, 4)$. $x_i = (1, 2)$ 0.6 and $(3, 4)$ 2.0 nm.

exceed this value by a few times. An analysis of the strong field region is particularly important also for the problem of electrical strength of organic materials [15].

2. THEORETICAL MODEL

The calculation of the tunneling injection current was performed in the frame of Bardeen's theory [16]. In this approach, the total Hamiltonian of a tunneling-coupled system is divided into a sum of Hamiltonians of the left- and right-hand subsystems, $H = H_L + H_R$, with each of them corresponding to the "unperturbed" case of the other subsystem being absent; said otherwise, the tunneling barrier is infinitely thick. The eigenstates $|L\rangle$ and $|R\rangle$ of the unperturbed Hamiltonians H_L and H_R can be identified with the energies E_L and E_R and the wave functions Ψ_L and Ψ_R . This approach describes formally a tunneling transition as a perturbation having a tunneling matrix element T . By the Fermi golden rule, the tunneling transition probability is defined as $w = \frac{2\pi}{\hbar} |T|^2 \delta(E_L - E_R)$. The tunneling matrix element T can be expressed through the wave functions of unperturbed states as

$$T = -\frac{\hbar}{2m} \int_{\Omega} (\Psi_R^* \nabla \Psi_L - \Psi_L \nabla \Psi_R^*) d\Omega, \quad (2)$$

where integration is performed over the surface Ω separating the tunneling subsystems and located somewhere inside the barrier, and $d\Omega$ is a vector oriented along the normal to this surface. Consider a transition from a localized state of an organic molecule described by a wave function $\psi_R(\mathbf{r})$ and energy E_R into a delocalized state in a metal with a wave function $\psi_L(\mathbf{r})$ and energy E_L . We shall assume the wave function of the localized state in an organic material to be spherically symmetric, and consider the dependence of the tunnel-

ing barrier height on coordinate in the quasi-classical approximation

$$\psi_L(\mathbf{r}) = \begin{cases} \frac{c_1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}}, & x < x_1 \\ \frac{c_1}{\sqrt{V}} e^{i\mathbf{k}_\parallel \mathbf{p}} e^{-\int_{x_i}^x k_x dx}, & x > x_1, \end{cases} \quad (3)$$

where $\kappa_x(x) = \frac{\sqrt{2m}}{\hbar} \sqrt{U(x) - E}$, $U(x, F, x_i)$ is the profile

of barrier (1), $E = \frac{\hbar^2 k_x^2}{2m}$, \hbar is Planck's constant, m is the

free electron mass, \mathbf{k} is the wave vector of an electron in a metal, \mathbf{k}_\parallel is the projection of the wave vector onto the barrier plane, k_x is its projection on the x axis which is perpendicular to the barrier, \mathbf{p} is the projection of the electron radius vector on the barrier plane, V is the volume of the metallic electrode, and c_1 is a normalization constant of order unity. The wave function of the localized state will be taken in the form

$$\psi_R(\mathbf{r}) = \frac{1}{\sqrt{\pi r_0^3}} e^{-\frac{|\mathbf{r} - \mathbf{r}_R|}{r_0}}, \quad (4)$$

where \mathbf{r} is the radius vector of the center of the localized state, and r_0 is its Bohr radius. For the energy of this state reckoned from the vacuum level, we have

$$E_0 = -\frac{e^2}{4\pi\epsilon\epsilon_0 r_0}. \quad (5)$$

For the surface Ω , one may conveniently take the yz plane located close to the center of the localized state. After some manipulation we obtain the following relation for the matrix element

$$T = \frac{\hbar^2 c_1}{2m\sqrt{V}} e^{-\kappa_{\text{eff}}(x_2 - x_1)} \frac{\kappa_{\text{eff}} \sqrt{r_0}}{\sqrt{\pi}} \frac{1}{1 + r_0^2 k_\parallel^2}, \quad (6)$$

where $\kappa_{\text{eff}} = \frac{1}{(x_2 - x_1)} \int_{x_1}^{x_2} \kappa dx$.

It is prudent to reckon the energy E from the bottom of the conduction band of the metal; in view of Eq. (5), we arrive now at

$$T = \frac{ec_1 \hbar^2 \kappa_{\text{eff}} e^{-\kappa_{\text{eff}}(x_2 - x_1)}}{2m\sqrt{\pi}\sqrt{V}} \times \left(1 + \frac{2me^4}{(4\pi\hbar\epsilon\epsilon_0)^2 (E_m - E)} \right)^{-1}, \quad (7)$$

where E_m is the vacuum level relative to the conduction band bottom of the metal; $E_m = ex_i F + E_F + \phi$. To calculate the total injection current, one has to perform

summation over all states of the metal and of the polymer, with due account of their occupation

$$I = e \frac{2\pi}{\hbar} \sum_{L, R} |T|^2 \delta(E_L - E_R). \quad (8)$$

The above reasoning suggests that the equation for the density of injection current of direct tunneling transitions can be cast in the form

$$J = e \frac{2\pi}{\hbar} V \int_0^\infty dE \int_a^\infty dx T(x)^2 Z(E) g(x, E) \times (1 - f(E)) f_{\text{loc}}(x, E), \quad (9)$$

where $Z(E)$ is the density of states in the metal, $f(E)$ is the Fermi function in the metal, $f_{\text{loc}}(x, E)$ is the function of local state occupation in the organic material, $g(x, E)$ is the energy density of local states in the organic material, and a is the minimum tunneling length, which in order of magnitude is a few r_0 .

The situation we are considering here corresponds to the case of the states in the polymer lying in energy substantially below the Fermi level of the metal. Accordingly, the direct tunneling transitions discussed above can be largely suppressed by the presence of the factor $(1 - f(E))$ in Eq. (9); in other words, the number of empty states in a metal may be not large enough to permit isoenergetic tunneling of electrons from the polymer. It appears therefore important to estimate the contribution of non-isoenergetic tunneling processes, primarily of those involving phonons. We shall perform now such an estimation in the particular example of one process in a metal in which acoustic phonons take part. The formulation of the problem reduces to a calculation of the rate of electron transitions from a localized state in an organic material into a delocalized state in a metal, with due allowance for absorption of an acoustic phonon in the metal. Such a perturbative calculation accounting for the tunneling term and electron-phonon coupling meets with certain difficulties associated with the fact that in the model of the Bardeen Hamiltonian tunneling transitions take place between states with the same energy and are actually not true quantum-mechanical transitions treated in the theory of time-dependent perturbations. This gives rise to the appearance of singular energy denominators in second-order perturbation theory. We invoked a different approach to calculate the rate of tunneling transitions involving phonons. In this approach, the role played by tunneling reduces to inversion splitting of eigenstates of the metal-organic-compound system by a quantity T . The subsequent calculation of the rate of phonon-mediated electron transitions is done by first-order perturbation theory.

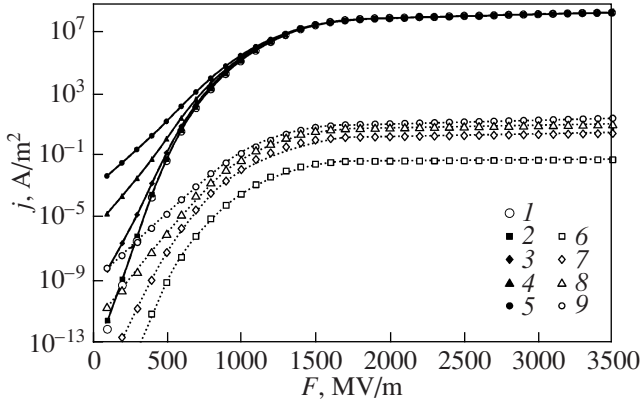


Fig. 2. Current density plotted vs. electric field strength for different temperatures and direct transitions (solid lines): and transitions involving phonon absorption (dotted lines). $T = (1) 0, (2, 6) 100, (3, 7) 200, (4, 8) 300$ and $(5, 9) 400$ K.

Rather than delving into details of these calculations, we shall present here only the final expression for the tunneling current density

$$J = V \frac{\pi^2 e \Xi^2 m^2}{s \rho \hbar^4} \int_0^\infty dE \int_a^\infty dx T(x)^2 Z(E) g(x, E) \times \frac{1}{e^{\frac{2\sqrt{2mEs}}{kT}} - 1} (1 - f(E + 2\sqrt{2mEs})) f_{\text{loc}}(x, E), \quad (10)$$

where Ξ is the deformation potential constant defining the efficiency of acoustic phonon coupling with electrons, s is the sonic velocity in the metal, and ρ is the density of the metal.

We note that $\int_0^\infty g(x, R) f_{\text{loc}}(x, E) dE$ describes the total hole concentration at a distance x from the anode and, hence, determines the conditions of current flow through the OMS. We will consider subsequently a particular case of relations (9) and (10) in which the current flowing through an OMS is mediated only by the electrode process; i.e., the holes forming in the OMS reach instantaneously the cathode to become neutralized there. In this case, we can accept $f_{\text{loc}}(x, E) = 1$.

3. RESULTS OF THE CALCULATIONS AND DISCUSSION

The injection current density was calculated by numerical integration of Eqs. (9) and (10) with the use of the IMSL code library [17]. In calculation of the matrix element of tunneling in Eq. (7) we accepted $c_1 = 1$. In all cases we set $\varepsilon = 3$, $E_F = 5$ eV and $\phi = 5$ eV. The

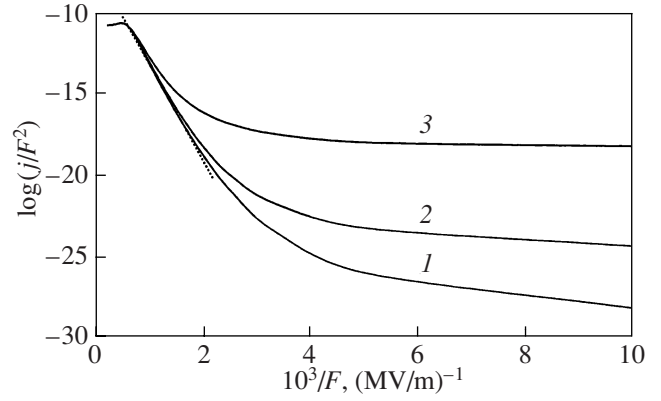


Fig. 3. Current density plotted vs. electric field strength (in the Fowler-Nordheim coordinates) for direct transitions at different temperatures: $T = (1) 0, (2) 200$, and $(3) 400$ K.

spectrum of local states (HOMO levels) in the molecular solid was assumed to be Gaussian, i.e.,

$$g(E, x_i) = \frac{N_{\text{loc}}}{\sqrt{2\pi}\sigma} \times \exp\left\{-\frac{[ex_i F + E_F + \phi - eI_C - E]^2}{2\sigma^2}\right\}, \quad (11)$$

where σ is the dispersion of the distribution, N_{loc} is the local state concentration, and I_C is the ionization energy of OMS molecules. The calculations were performed for $N_{\text{loc}} = 1 \times 10^{21} \text{ cm}^{-3}$ and $\sigma = 0.1$ eV.

Figure 2 presents plots of the injection current density calculated for $I_C = 6$ eV and $a = 0.6$ nm for different temperatures. The solid lines plot the currents calculated from Eq. (9) which takes into account only direct isoenergetic electron transitions from the HOMO levels into the metal, and the dashed ones, those calculated from Eq. (10) covering only indirect transitions involving phonon absorption. We readily see that at temperatures from 0 up to 400 K, throughout the range of electric fields studied, the current produced in direct transfer of electrons into the metal exceeds substantially that generated in indirect transitions. Hence, in an analysis of hole injection from metallic electrodes into an OMS, one may use for calculation of the current density only Eq. (9) and disregard the indirect transitions.

Two characteristic regions stand out immediately in the $j(F)$ graphs. At fairly moderate fields, $F \leq 1500$ MV/m, current density is seen to grow rapidly with increasing electric field, with the temperature exerting a noticeable effect on its magnitude. As the field strength increases, the rate of growth of j slows down, so that in a very strong electric fields the current density only weakly depends on the field and becomes practically temperature independent.

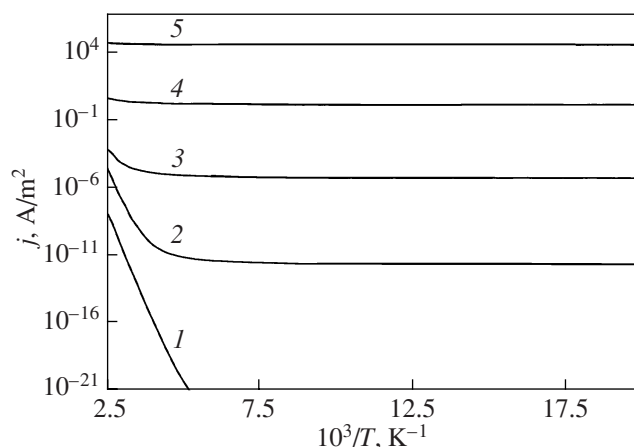


Fig. 4. Injection current density plotted vs. inverse temperature for different electric field strengths: $F = (1)$ 200, (2) 500, (3) 700, (4) 1000, and (5) 1500 MV/m.

In Fig. 3, the $j(F)$ relations calculated for direct isoenergetic transitions at $I_c = 6$ eV, $a = 0.6$ nm and temperatures of 0, 200, and 400 K (curves 1–3) are plotted in the Fowler–Nordheim coordinates. We observe a region of F variation (in strong electric fields) within which $\log[j_{inj}(F)F^{-2}]$ follows a close to linear dependence on F^{-1} . We note that its extent increases with decreasing temperature. Thus, we see that the current–voltage characteristic of an anode injecting holes into an OMS in a strong electric field may indeed be calculated using Fowler–Nordheim-type relation.

It appears only natural to assume that the complex pattern of the $j(F)$ relation is connected with the conditions of electron tunneling from the HOMO levels into a metal changing with increasing electric field and temperature.

At absolute zero, when all states in the metal with energies $E < E_F$ are occupied by electrons, they can undergo direct tunneling transitions to the metal only from the HOMO levels with energies $E_{\text{HOMO}} \geq E_F$. In our model, OMS molecules are located at a distance $x \geq a$ from the metal surface. For $x = a$, the maximum in the density of states $g(E, x)$ for the values of E_F , ϕ and I_c used in the calculations will lie about 1 eV below E_F . Therefore, at such a distance from the anode the concentration of states with energies in excess of E_F will be very low. It grows sharply only for the molecules located at distances from the anode larger than $x_0 \approx (I_c - \sigma - \phi)/eF$. For $F = 100$ MV/m, $x_0 \approx 10$ nm. Tunneling of electrons into a metal from such distances is obviously hardly probable. As the electric field strength increases, we will have, on the one hand, a shift (on the energy scale) of the maximum in the density of states $g(E, x)$ toward the Fermi level, which will entail a strong growth in the concentration of states with $E_{\text{HOMO}} \geq E_F$ in the region of the OMS adjoining the anode. On the other hand, a decrease in x_0 brings about

an increase in the barrier transparency in tunneling of electrons from molecules located at a distance x_0 from the anode, thus giving rise to a noticeable growth of their tunneling probability.

As the electric field is increased still further, an ever larger number of electrons will be able to transfer from the HOMO levels into the metal. The electric field strength at which the peak in the Gaussian distribution at $x = a$ will lie above the Fermi level in the metal may apparently be considered as the borderline field separating the first from the second region in the $j(F)$ dependence. In our case, it will be ~ 1800 MV/m. As the field strength continues to grow, the increase in the density of states will originate from the insignificant growth of the concentration of local states with energies $E_{\text{HOMO}} \geq E_F$ (through states in the distribution tail) and an increasing density of electronic states in the metal, in accordance with Eq. (11), which brings about, by Eq. (9), growth of j .

At a nonzero temperature, empty states with energies $E < E_F$ appear in the metal, to which electrons can tunnel. Hence, at a distance $x_i < x_0$ from the anode a certain number of electrons will appear which can tunnel into it from molecules whose HOMO level lies below the Fermi level in the metal. The number of such electrons depends on temperature, and this is what accounts for its effect on the injection current density in the first region of the relation under study. Significantly, the tunneling barrier width in this case does not depend on electric field, because the number of electrons which can transfer to the anode is not determined by x_0 . Indeed, as the temperature increases, electrons from molecules located increasingly closer to the anode will be able to tunnel into it, which will give rise to a sharp increase in the tunneling probability.

At fields above the borderline strength (i.e., fields F in the second region in the $j(F)$ dependence), HOMO levels of practically all molecules will lie above the Fermi level at any temperature, and, therefore, temperature will no longer influence the injection current density. Figure 4 plots the density of injection current vs. inverse temperature for different electric fields. The calculations were performed for $I_c = 6.5$ eV. We readily see that for fields $F \leq 700$ MV/m (curves 1–3 in the figure) the $j(1/T)$ plots can be divided into two regions, namely, the low temperature region where the temperature affects only weakly the injection current density (i.e., where the $j(1/T)$ graph is practically horizontal) and the region of relatively high temperatures where $j(1/T)$ follows a close to linear course.

At moderate electric fields, the maximum of the $g(E, x)$ function lies substantially below E_F (for $F = 200$ MV/m and $I_c = 6.5$ eV, the HOMO levels of most of the molecules located close to the anode will be ~ 1.5 eV below the Fermi level), and, therefore, the appearance in the metal of unoccupied states, primarily with an energy $E \approx E_F - kT$, should not bring about a pro-

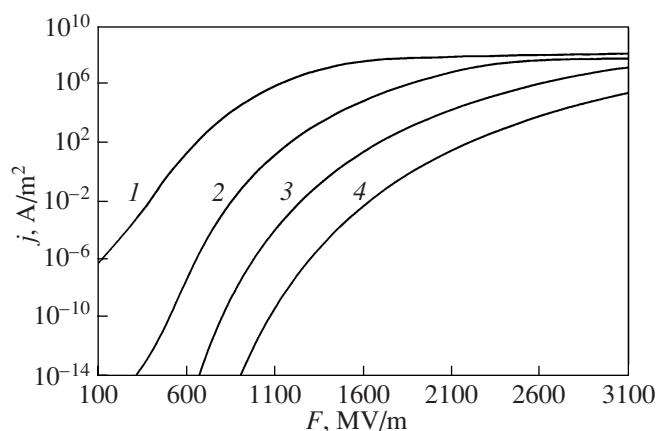


Fig. 5. Injection current density plotted vs. electric field strength for different values of the ionization potential of the molecules: $I_c = (1) 6.0$, $(2) 6.5$, $(3) 7.0$, and $(4) 7.5$.

nounced increase in the transition rate. However, as the temperature continues to grow, this effect will predominate, which is corroborated by the close to linear course of the $j(1/T)$ graph. We note that for $F = 200$ MV/m the effect of temperature becomes noticeable for $T > 200$ K (curve 2 in Fig. 4). It appears prudent to assume that as the field strength increases, another mechanism resulting in a growth of the injection current density will play an ever increasing role; it consists essentially in the number of local states with energies $E_{\text{HOMO}} \geq E_F$ for molecules located close to the anode increasing, and in a decrease in x_0 . As a result, the transition to the linear $j(1/T)$ pattern with increasing electric field strength will take place at ever higher temperatures. For instance, at $F = 700$ MV/m (curve 3 in Fig. 4) it is observed to set in at ~ 375 K. Finally, in fields $F > 1000$ MV/m the increase in the number of local states with energies $E_{\text{HOMO}} \geq E_F$ will play a predominant role, and temperature will no longer affect the density of the injection current (curves 4 and 5 in Fig. 4).

The ionization potential of molecules I_c affects substantially the injection current density. Figure 5 displays in graphic form $j(F)$ relations calculated for different values of I_c for $T = 250$ K. We readily see that while the injection current density decreases noticeably with increasing I_c , the relations under study do not undergo any qualitative changes.

One of the parameters used in calculations of injection current density was a , a quantity defined as the minimum tunneling transition length (associated with molecular size). Note that the value of a not only determined the lower integration limit in Eqs. (9) and (10) but set also the minimum tunneling barrier width at which the probability of electron transition from the HOMO level into the metal was the highest. It is instructive to analyze its effect on the character of the $j(F)$ relation.

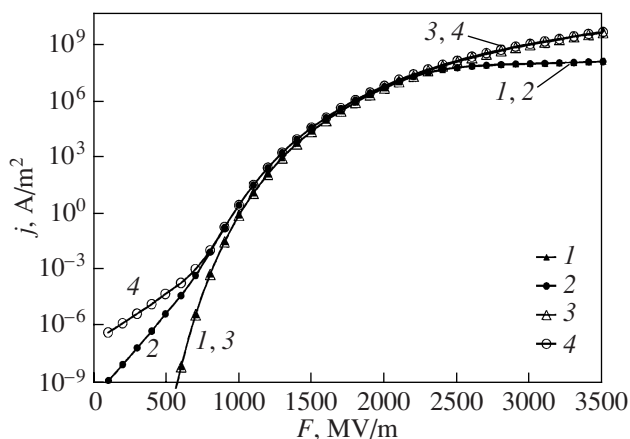


Fig. 6. Injection current density plotted vs. electric field strength for different temperatures and minimum tunneling transition lengths. $T = (1, 3) 100$ and $(2, 4) 400$ K. $a = (1, 2) 0.6$ and $(3, 4) 0.3$ nm.

Figure 6 plots $j(F)$ relations calculated for $I_c = 6.5$ eV and different values of a and different temperatures. In different regions of F variation the effect of a on j is seen to be different. For relatively weak fields ($F < 1000$ MV/m) and $T = 100$ K, a decrease in a from 0.6 to 0.3 nm (curves 1, 3) does not entail a marked change in current density. For this temperature, it is observed only for $F < 2500$ MV/m, where a decrease in a brings about an increase in the current density, this increase being the larger, the higher is the field strength. This suggests that the transitions dominant at comparatively low fields and low temperatures are those from local states for which $x_i \geq x_0$ and $x_0 > a$. At higher temperatures, for instance, at $T = 400$ K (curves 2, 4), a decrease in a leads to an increase in current density for $F < 1000$ MV/m, which may suggest that it is transitions from the molecules closest to the anode (at the distance a) that provide the dominant contribution to the injection current. As the field strength increases, however, variation in the value of a affects no longer the value of j (for $1000 \leq F \leq 2400$ MV/m, curves 1–4 practically merge). This should apparently be assigned to the fact that in this region of field strength variation the main contribution comes from transitions from molecules with $x_i \geq x_0$ and $x_0 > a$. Finally, for $F > 2500$ MV/m decrease in a again brings about an increase in the current density; i.e., electron transitions into metal from molecules closest to the anode become again predominant.

4. CONCLUSIONS

Thus, we carried out a theoretical consideration of the hole injection current from a metal into organic materials, allowing for the real shape and height of the barrier at the metal–OMS interface. Analytic expressions for the tunneling injection current were derived that describe the hole injection from a metal into an

OMS over wide ranges of temperatures and electric fields strengths.

We analyzed in considerable detail the role played by the processes involving phonon absorption. It was shown that the injection current is mediated primarily by direct electron transitions from HOMO levels of molecules into empty states in the metal. The contribution to the injection current due to transitions involving phonon absorption was found to be negligible.

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REFERENCES

1. A. G. Chynoweth, Usp. Fiz. Nauk **75**, 169 (1961) [Prog. Semicond. **4**, 95 (1960)].
2. P. Yan, Y. Zhou, and N. Yoshimura, Jpn. J. Appl. Phys. **39**, 3492 (2000).
3. D. Liu and K. C. Kao, J. Appl. Phys. **69**, 2489 (1991).
4. N. R. Tu and K. C. Kao, J. Appl. Phys. **85**, 7267 (1999).
5. C. Ganzorig, M. Sakomura, K. Ueda, and M. Fujihira, Appl. Phys. Lett. **89**, 263501 (2006).
6. M. A. Abkowitz, H. A. Mizes, and J. S. Facci, Appl. Phys. Lett. **66**, 1288 (1995).
7. H. Bässler, Phys. Status Solidi B **175**, 15 (1993).
8. U. Wolf, V. I. Arkhipov, and H. Bässler, Phys. Rev. B: Condens. Matter **59**, 7507 (1999).
9. V. I. Arkhipov, U. Wolf, and H. Bässler, Phys. Rev. B: Condens. Matter **59**, 7514 (1999).
10. V. I. Arkhipov, E. V. Emelianova, Y. H. Tak, and H. Bässler, J. Appl. Phys. **84**, 848 (1998).
11. V. I. Arkhipov, H. von Seggern, and E. V. Emelianova, Appl. Phys. Lett. **83**, 5074 (2003).
12. V. A. Zakrevskii and N. T. Sudar', Fiz. Tverd. Tela (St. Petersburg) **34** (10), 3228 (1992) [Sov. Phys. Solid State **34** (10), 1727 (1992)].
13. A. L. Suvorov and V. V. Trebukhovskii, Usp. Fiz. Nauk **107**, 657 (1972) [Sov. Phys.—Usp. **15**, 471 (1972)].
14. T. Quisse, Eur. Phys. J. B **22**, 415 (2001).
15. V. A. Zakrevskii and N. T. Sudar', Fiz. Tverd. Tela (St. Petersburg) **47** (5), 931 (2005) [Phys. Solid State **47** (5), 961 (2005)].
16. J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).
17. O. V. Barten'ev, *FORTRAN for Professionals: Mathematical Library IMSL* (Dialog-MIFI, Moscow, 2001), Part 3 [in Russian].

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