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Modeling of charge injection in organic/polymeric diodes

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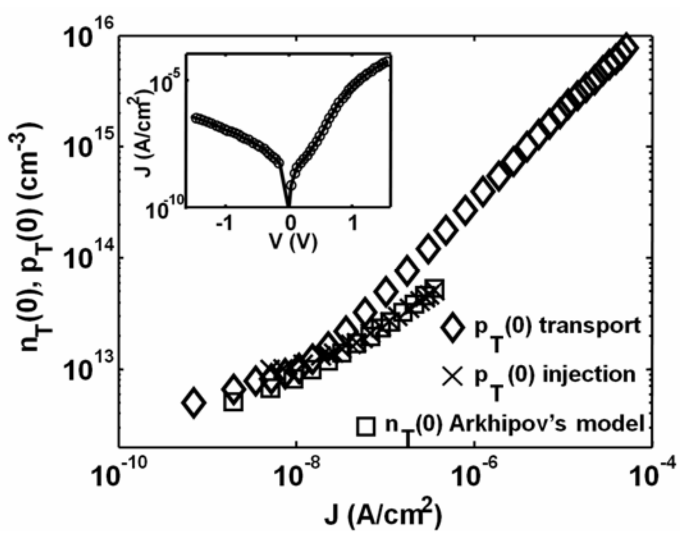
Abstract. We present a technique to model the injection of charge in metal-organic (or metal-polymeric) structures by means of an appropriate boundary value of the charge density at the metal-organic interface. Current-voltage curves of diodes with different energy-barrier heights can be interpreted by solving the transport equations with this boundary value. The value of the free charge density at the interface is related to results obtained by using appropriate injection models. At low energy barriers, where injection models give way to transport models, our model is still valid. It links different regions and explains transitions observed in current-voltage curves associated to different injection and transport mechanisms.

Motivation. The injection of charge depends on different factors such as the height of the injection barrier, the applied electric field, the temperature, chemical reactions leading to interface dipoles, band bending or Fermi level pinning. These different mechanisms present difficulties when studying the injection of charge in organic devices. However, the transport of charge also plays a key role in the performance of the device and must be properly accounted for. However, depending on the energy barrier height, one mechanism can dominate over the others. There are simple specific models for each mechanism and complex models that include both [1]. Despite these efforts, transitions in *I-V* curves from ohmic to space charge limited current (SCLC) or to injection limited current (ILC) are not well explained. Transitions from ILC to SCLC are sometimes interpreted by a variation of the charge density at the metal-organic interface from a finite value in ILC to an infinite value in SCLC [1]. However, a high value for the charge density is not in agreement with the ohmic behavior seen at low voltages in both ILC and SCLC regimes [2]. Therefore, we propose to use a realistic finite value for the charge density at the interface in order to characterize these transitions. At the same time, the value of the free charge density at the interface must be consistent with the injection mechanism for high energy barriers.

Procedure and results. In a previous work [2], we proposed a method to extract the charge density at the metal-organic interface from *I-V* curves measured in organic diodes with low energy barriers. The transition from ohmic to SCLC was explained by a realistic finite charge density at the interface $p(0)$. In this work, we present an explanation of the transition from SCLC to ILC also by using a finite value of $p(0)$. In that sense, the value of the charge density at the interface can be interpreted as the result of different physical mechanisms that occur during the injection. The proposed method is based on the solution of the transport equations including a well known mobility model and the use of a boundary value for the charge density at the interface. The comparison of *I-V* curves measured in organic diodes with our numerical results provides information of the parameters of the mobility model and the boundary condition. The mobility model used is the correlated Gaussian disorder model (CGDM) [3] that depends on electric field and temperature. The basic parameters that appear in this model are the mobility at low electric fields $\mu(0, \mathrm{T})$, the intersite spacing a and the width of the Gaussian distribution σ : $\mu_{\mathrm{CGDM}} = \mu_{\mathrm{CGDM}}(E, T, a, \mu(0, T), \sigma)$.

We apply this idea to organic diodes with different injection barriers (sweeping from SCLC to ILC regimes). We extract the total charge density at the interface $p_T(0)$ as a function of the current density. As an illustration, Figure 1 shows the analysis of experimental current-voltage curves (inset) measured in an ITO/CuPc/Au diode [3] (experimental, circles; our results solid line). At positive bias, the height of the injection barrier is low, 0.05 eV, while at reverse bias, the barrier is 0.6 eV. The charge density is extracted at negative (×) and at positive (◊) bias. It can be observed that at low voltages, the amount of injected carriers is low, compared to the existing thermally generated carriers; for this reason, the charge at the contact is constant in both cases. When the current density is increased, the charge density increases, making a transition from ohmic to ILC or SCLC ((×) and (◊), respectively). It is also observed that the electrode injects more holes when the barrier is lower, as expected. In order to check our model in the ILC region, we compare our results with an injection model developed by Arkhipov et al. [1] and extensively used by different authors (□). A good agreement is observed showing how our method provides the same information as more elaborate injection models.

Figure 1



Conclusions. We present a way to interpret and model current-voltage curves of organic diodes with different barrier heights. The solution of the transport equations with a proper boundary value for the charge density at the metal organic interface preserves the information of both ILC and SCLC regimes. Realistic transitions of this variable among ohmic, ILC and SCLC regimes are obtained.

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