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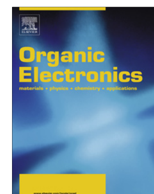

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Structural ordering versus energy band alignment: Effects of self-assembled monolayers on the metal/semiconductor interfaces of small molecule organic thin-film transistors

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ABSTRACT

A model describing the influence of self-assembled monolayers on the contact resistance of bottom-contact organic thin-film transistors is presented. The model takes the contact geometry, the energy level alignment and the structural order of the organic films into consideration when describing the contact effects of organic transistors. The treatment of the metal source/drain electrodes of the transistors by self-assembled monolayers allows for tuning the work function of the metal contact and an improved ordering of the organic molecules on top of the source/drain contacts. The results reveal that the contact resistance is mainly determined by the molecular ordering, rather than the tuning of the work function. The model is compared to experimentally measured contact resistances for different self-assembled monolayers.

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1. Introduction

Organic electronics has been in the focus of intensive research due to their possible application in large area and flexible display media [1]. Often the device performance is limited by the contact resistance, R_C, in particular for short channel transistors [2–4]. The main source of the contact resistance is attributed to the poor charge injection into the channel of the transistor. Understanding the chemical properties, the electronic structure and the electrical behavior of the metal/organic interfaces plays a crucial role in improving the organic devices' performance. Many authors have shown that the OTFTs' performance in terms of contact resistance strongly depends on the device geometry [5,6]. Top source/drain contact (TC) structures exhibit ten to hundred times smaller contact resistance than the bottom-contact (BC) structures [5,6].

Although, TC structures exhibit lower R_C, the downscaling of the transistor's dimensions is usually limited by the resolution of the fabrication technique, which typically involves shadow masking [6,7]. Standard lithography (generally used for obtaining high resolution small channel lengths) cannot be employed, because the semiconductor is deposited before the S/D electrodes, which will involve an exposure of the organic film to solvents degrading its performance [7]. Therefore, we will focus on transistors with bottom-contact geometry, whose cross-section and equivalent resistive network are shown in Fig. 1. The key to improving the performance of BC structures lays in understanding the properties of the metal/semiconductor interfaces. Since the energy band alignment at these

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interfaces is usually dependent on the metal work function, modifying it with self-assembled monolayers (SAMs) has drawn a considerable attention and has proven to be an effective way of reducing the contact resistance in BC thin-film transistors [5,6].

When a metal is brought in contact with a semiconductor, a barrier will be formed at the metal/semiconductor interface arising from the difference between the metal work function and the ionization energy (IE) or the electron affinity (EA) of the semiconductor [8]. The first model that described the nature of the metal/semiconductor contacts was the Schottky–Mott model [9,10]. A schematic energy band diagram of an ideal Schottky–Mott metal/semiconductor interface is shown in Fig. 2(a). According to this model, the barrier height at the interface is determined by the difference of the metal work function and the HOMO/LUMO levels of the semiconductor assuming vacuum level alignment. However, this model turned out to be insufficient in describing the experimental data [11,12]. As a consequence, the energy level alignment should consider a vacuum level discontinuity, which is related to an interface dipole Δ (i.e. vacuum level offset), resulting from charge rearrangement upon the interface formation. A schematic of an energy band diagram of such interface considering the created dipole is shown in Fig. 2(b).

In literature, the effect of the contact resistance on the transistor's characteristics is usually described purely by a barrier model as discussed above [13,14]. However, this model can be used only to explain the effect of the SAM treatment on the injection barrier, disregarding its effect on the growth morphology. On the other hand, in Ref. [5] a model describing the contact resistance with focus on the effect of SAM on the molecular ordering was presented. In this model, the influence of the SAM on the metal work function was not considered. In the following manuscript, a model describing the contact resistance of bottom-contact coplanar TFTs, considering both the morphology and the energy level alignment at the contacts, will be presented with a focus on gold (Au)/pentacene (Pn) interfaces. Moreover, the model will give insights on how SAM treatment reduces the contact resistance of the devices, although the work function of Au is reduced increasing the barrier height for holes.

2. Modeling of the contact resistance

In order to describe the contact resistance of the BC devices, the resistive network depicted in Fig. 1 was used. The contact resistance is determined by the specific contact resistance, ρ_C, of the metal/semiconductor interface. The specific contact resistance of a rectifying Schottky contact is given by:

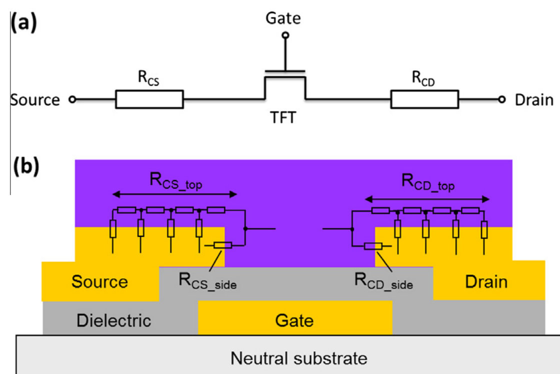

Fig. 1. (a) Equivalent circuit of a thin-film transistor including the contact resistances. (b) Schematic cross-section of a bottom-contact coplanar pentacene thin-film transistor.

$$\rho_c = \frac{k}{q \cdot A^* \cdot T} \cdot \exp\left(\frac{q \cdot \phi_b}{k \cdot T}\right) \quad (1)$$

with k being the Boltzmann constant, q being the elementary charge, A^* is the Richardson constant and ϕ_b is the barrier height. Moreover, the model takes into account the Schottky-barrier lowering, which is a mechanism causing image-force-induced lowering of the barrier height for charge carrier emission in the presence of the an electric field [15]. The change of the barrier height as a function of the applied electric field can be described by [15]:

$$\Delta\phi_b = \sqrt{\frac{q \cdot E}{4 \cdot \pi \cdot \varepsilon_0 \cdot \varepsilon_r}} \quad (2)$$

For simplicity, the electric field, E, is usually described by the maximum electric field at the junction and the ε_0 and ε_r are the vacuum and the semiconductor permittivity, respectively. More details regarding the image-force-induced barrier lowering can be found in Ref. [15]. As a consequence, the barrier height in Eq. (1) is given by $\phi_b = \phi_{b0} - \Delta\phi_b$, where ϕ_{b0} is the initial barrier height defined by the work function of the metal, the HOMO/LUMO level of the semiconductor and the interfacial dipole.

Furthermore, the contact geometry has to be considered. Charges injected both from the edge of the source/drain contact and from the top of the contact contribute to the charge injection, as indicated by the resistive network in Fig. 1(b). The normalized resistance r_{C_side},

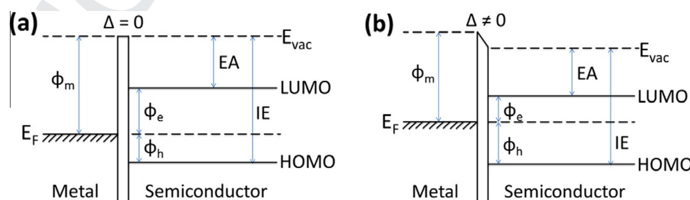

Fig. 2. Schematic energy band diagram of (a) an ideal Schottky–Mott metal/semiconductor contact and (b) a non-ideal metal/semiconductor contact with dipole created at the interface, shifting the energy levels of the semiconductor.

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