ROLE OF INTERFACES ON THE DIRECT TUNNELING AND THE INELASTIC TUNNELING BEHAVIORS THROUGH METAL/ALKYLSILANE/SILICON JUNCTIONS

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In molecular electronics, the role of interfaces remains the subject of many controversies. In fact, since the last ten years many works have reported the electrical properties in electrode/molecule/electrode junctions, but their role was not always taken into account, and frequently the interface can explain the electrical behavior measured in the molecular device.

In this work, we compared the dielectric behavior of metal/alkylsilane/silicon junctions by measuring their current density-voltage (J(V)) characteristics. For some junctions, depending on the chemical nature of the alkyl/metal interface, the results are in excellent agreement with the theory of Simmons [1] for tunneling current between dissimilar electrodes separated by a thin insulating film. With this model, we extracted the effective mass (m^*) and the barrier height (ϕ) of the junctions. For a deeper physical characterization of these junctions, we reported inelastic electron tunneling spectroscopy (IETS) measurements of the electrons-molecular vibrations coupling. Understanding vibronic interactions between electrons and nuclear motions in molecules is recognized as a key point in molecular electronic devices [2].

The metal/alkylsilane/silicon junctions were prepared on highly-doped silicon covered by an ultra-thin native dioxide (~1nm) films. Self-assembled monolayers constituted of alkylsilanes chains from 3 to 11 carbon atoms, and bearing different terminal groups (methyl, vinyl, bromide and thiol) were deposit by chemisorption in solution. Metal electrodes (aluminum or gold) were gently evaporated through a shadow mask to complete the junction. The metal/terminal group combinations were chosen allowing specific chemical interactions at the interface, to test their influence on the electrical behavior and IETS.

We demonstrated that the thiol group at the interface avoids diffusion of gold into the molecule even for a 3 carbons chain. For this short molecule, we observed pure tunnel conduction with barrier height at the monolayer/Si and monolayer/Au interfaces found to be respectively 2.14 and 2.56 eV, which are very large considering the small thickness of the monolayer (0.8 nm). These values are obtain using Simmons equation [1] with an effective mass parameter $m^* = 0.16\ m_e$ (m_e = mass of the electron).This extends the demonstration of the excellent tunnel dielectric behavior of organic monolayers down to 3 carbon atoms with a thiol/Au couple at the interface. Other SAMs without the thiol end-group (i.e. CH_3 terminated) do not follow a pure tunneling behavior.

IETS confirms the quality of the thiol-Au interface; we observed a strong S-Au vibration peak at 25.1 mV. Moreover for all the different systems, we are able to distinguish and identify the most intense vibration modes of the alkyl chains: (i) the δ-CH_2 rocking mode at 95.2 mV; (ii) the ν C-C vibration at 134.3 mV and (iii) the δ-s CH_2 vibration at 187.9 mV. These peaks are clearly distinguished from those of the Si and ultra-thin SiO_2 phonons [3].

In conclusion, we demonstrated that the thiol/gold couple at the interface avoids gold diffusion and damage creation in junctions during the evaporation of the metal for alkyl chains as short as 3 carbon atoms. For this device, the good electrical contact permits observing a perfect tunneling current behavior in the junction in agreement with Simmons's model.

References:

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