電気材料技術雑誌 第14巻第2号
J.Soc.Elect.Mat.Eng. Vol.14, No.2, 2005

Transport Studies of Isolated Molecular Wires in Self-Assembled Monolayer Devices

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Abstract

We have fabricated novel molecular diodes based on self-assembled-monolayers (SAM) of solid-state mixture (SSM) of molecular wires (1,4 benzene-dimethane-thiol; Me-BDT), and molecular insulator spacers (1-pentanethiol; PT) with different concentrations, r of wires/spacers, which were sandwiched between two gold electrodes. We introduce new methods borrowed from Surface Science to confirm the connectivity between the Me-BDT molecules with the upper Au electrode, and count the number of isolated molecular wires in our devices.

The electrical transport characteristics of SSM SAM diodes fabricated with different r-values were studied at different temperatures. A potential barrier caused by the connectivity gap between the PT molecules and the upper Au electrode dominated the transport properties of the pure PT SAM diode (r = 0). The transport properties of SSM SAM devices, on the contrary are dominated for $10^{-8} < r < 10^{-4}$ by the conductance of the isolated Me-BDT molecules in the devices. We found that the temperature dependence of SSM SAM devices' resistance is much weaker than that of the PT SAM device that indicates the importance of Me-BDT molecules bonding to the two opposite Au electrodes. From the differential conductance spectra of the various devices we found that the energy difference, Δ between the gold electrode Fermi-level and the Me-BDT HOMO (or LUMO) level is ~1.5 eV; whereas it is ~2.5 eV for the PT molecule. We explained the weak temperature dependence resistance of the SSM SAM devices by the weak temperature dependence of Δ.

In addition, our measurements reveal that the conductance of the fabricated SSM SAM devices scales linearly with r, which shows that the charge transport in these devices is dominated by the sum of the isolated Me-BDT molecular conductance in the device. Based on this finding, and the measured number of the Me-BDT wire molecules in the devices we obtained the 'single molecule resistance', R_M. We measured $R_M = 6 \times 10^8\ \Omega$ for isolated Me-BDT molecules, which is consistent with previous measurements using other transport measuring techniques. A simple model for calculating R_M, where the transport is governed by electron tunneling through the Me-BDT molecule using the WKB approximation, is in good agreement with the experimental data thus validating the procedures used for our measurements.