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Tuning Schottky barrier heights by organic modification of metal-semiconductor contacts

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Abstract

The initial stage of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) adsorption on Se passivated n-type GaAs(1 0 0)-(2×1) surface was investigated using high-resolution soft X-ray photoemission spectroscopy (SXPS). The thickness of the film was precisely controlled using previous results of core level intensity evolution and additional valence band spectra. A very small amount of PTCDA ($\ll$1 ML) is sufficient to induce a reduction of inhomogeneous band bending at the surface as judged from the sharpening of the core level spectra. This is interpreted in terms of preferential sticking of the organic molecules to surface defects. Thin films of PTCDA were then used as an interlayer for the electronic modification of Ag/n-GaAs(1 0 0) Schottky contacts. The electronic properties were investigated recording in situ current–voltage (*IV*) and capacitance–voltage (*CV*) characteristics. For H-plasma-treated substrates the effective barrier height decreases from 0.81 to 0.64 eV as a function of the PTCDA layer thickness (d_{PTCDA}). In the case of the sulphur-passivated GaAs the effective barrier height first increases and then decreases, the overall range being 0.54–0.73 eV. The substrate treatment leads to a different alignment between the band edges of the GaAs and the molecular orbitals of the PTCDA, making it possible to determine the energy position of the lowest unoccupied molecular orbital (LUMO) transport level. The latter is also derived from ultraviolet photoemission spectroscopy (UPS) measurements and the investigation of the electronic structure formed upon deposition of PTCDA on differently treated n-GaAs(1 0 0) surfaces. Interface dipoles are found to form according to the electron affinities (EA) of the substrates and PTCDA films at the interfaces and, consequently, the vacuum level alignment rule does not hold. The results demonstrate that the energy offset between the conduction band minimum of n-doped inorganic semiconductors and the LUMO of organic molecular films at the interfaces can be obtained using UPS by systematically varying the EA of substrates with a known band gap.

Author Keywords: Metal-semiconductor contacts; Schottky barriers; Organic layer modifications