Proceedings of the Fifth Vietnamese-German Seminar on Physics and Engineering, Hue, 25 February - 02 March, 2002

Application of thin molecular layers in hybrid inorganic/organic semiconductor structures

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Organic semiconductors have attracted increasing interests owing to their potential applications in various electronic and opto-electronic devices. The progress in the development of the organic molecular beam deposition (OMBD) has led to a monolayer-level control in the growth process of organic thin films under ultra-high vacuum (UHV) conditions. Here thin films of perylene derivatives, e.g. perylene tetracarboxylic dianhydride (PTCDA), were used as interlayers for the electronic modification of Ag/n-GaAs(100) Schottky contacts.

The electric transport properties and in particular the barrier height were investigated recording *in situ* current-voltage (IV) and capacitance-voltage (CV) characteristics as a function of interlayer thickness. Two differently treated GaAs substrates were used, first H-plasma treated, and secondly S-passivated surfaces. Chalcogen passivation of GaAs(100) reduces the number of chemically active sites on the surface and improves the structural properties of molecular films. For H-plasma treated substrates the effective barrier height is found to decrease from 0.81eV to 0.64 eV with increasing PTCDA layer thickness (see Fig.1).

In the case of sulfur passivated GaAs the effective barrier height first increases and then decreases, the overall range being 0.54 ~ 0.73 eV. This behaviour depending on substrate treatment can be explained by a different alignment between the band edges of GaAs and the molecular orbitals of PTCDA and the results of the electrical measurements allow the energy position of the lowest unoccupied molecular orbital (LUMO) to be estimated.

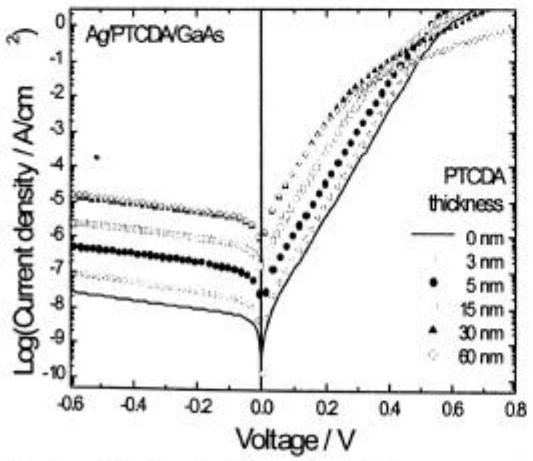

Fig. 1: IV characteristics of Ag/PTCDA/GaAs(100) Schottky contacts as a function of the interlayer thickness d_{PTCDA}. The contact area is 2.1×10^{-7} m^2.

For a complete description of device characteristics, however, a thorough understanding of the electronic structure at the organic/inorganic as well as metal/organic interfaces is essential. For this purpose ultraviolet photoemission spectroscopy (UPS) measurements were performed in order to determine the energy level alignment at the interfaces formed upon deposition of PTCDA on

differently treated n-GaAs(100) surfaces as well as for metal deposition onto the organic layer. Typical results are shown in Fig.2.

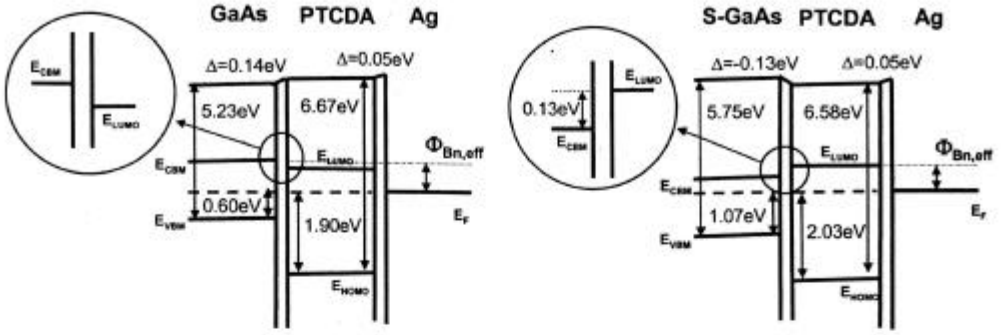

Fig. 2: Energy level alignment at Ag/PTCDA/GaAs(100) (a) and Ag/PTCDA/S-GaAs(100) interfaces (b)

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 (CBM) 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. This information is particularly valuable since in contrast to inorganic semiconductors the so-called transport gap is significantly larger than the gap which is obtained from optical absorption measurements due to the strong polarization effects and the high exciton binding energies in molecular materials.

This work was supported by the Bundesministerium für Bildung und Forschung (BMBF, No. 05 SE8OCA 7) and the EU funded Human Potential Research Training Network "DIODE" (contract no.: HPRN-CT-1999-00164). We also grateful to Freiberger Compound Materials for their support.

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