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# Interface formation of Mg with DiMePTCDI studied by Raman spectroscopy

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Abstract

Metal/organic interfaces play an important role in the performance of organic based devices. In this work the interface formation between Mg and N,N′-DiMethyl-3,4,9,10-Perylene Tetra Carboxylic DiImide (DiMePTCDI) films grown on sulphur-passivated GaAs (100) substrates is investigated *in situ* by Raman spectroscopy. The Raman spectra are taken in a backscattering geometry at room temperature under resonance conditions with the 488 nm (2.54 eV) $Ar^+$ laser line. They reveal that when Mg is deposited onto a 15 nm DiMePTCDI layer the external phonon modes are preserved up to large metal coverages. Since these modes are a fingerprint of the molecular crystal, their preservation indicates a low diffusion of Mg into the DiMePTCDI layer. Concerning the internal molecular modes, the Mg deposition induces a breakdown of selection rules which is proposed to originate from a dynamical charge transfer between the DiMePTCDI molecules and the metal. Above 0.3 nm nominal thickness of Mg the line-shape of the molecular breathing mode at 221 $cm^{-1}$ develops an asymmetric tail towards higher frequencies. A similar effect is observed for the bands that occur at 1291 $cm^{-1}$ and 1606 $cm^{-1}$ but the asymmetry appears at the low frequency side. This line-shape asymmetry is likely to be related to a Fano resonant coupling between the molecular vibrational modes and the electronic continuum of states of metallic clusters formed above 0.3 nm Mg coverage. (© 2005 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim)

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