Nanoobjects microscopy

Effect of O_2 exposure on optical reflectance anisotropy of Bi/Si(001) interfaces

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Electronic excitations play an important role in surface physics, because it can be used as promoters of some chemical reactions or photodesorption. So the investigation of excited states provides important information about the properties of adsorbed surface layers. The aim of the work was in theoretical and experimental investigations of the excitation spectra of the Si(001) surface, covered with submonolayer Bi films.

Optical properties of Bi/Si(001) interfaces were investigated in a wide spectral range (1–4eV). The results are shown on the Fig. 1.

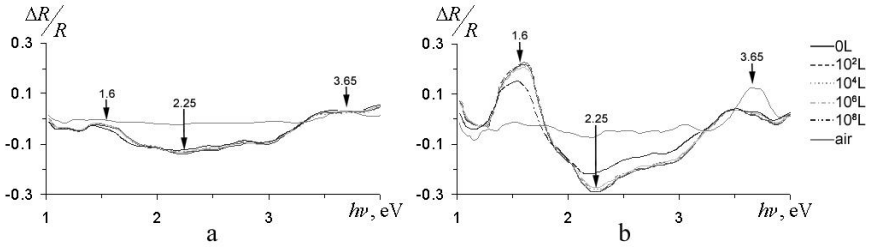

Fig.1. The spectral dependence of the reflectance anisotropy of Bi/Si(001) interfaces: 0.5ML (a) and 1ML (b).

As one can see there are no peaks at 1.4 and 1.84 eV associated with the transition on the π surface states of clean Si(001) surface for different reconstructions. Bi/Si(001) surface with a coverage of 0.5 and 1 ML exhibits interesting results: RA spectrum contains peaks at 1.6 and 2.25 eV, which could be formed by transitions between silicon surface dimer state and backbond Bi–Si state. The oxidation of the Bi/Si(001) surface in the air is completely removes low energy transitions of RA spectrum and exhibit new peak with energy of 3.65 eV, which could be formed by transitions in bulk oxidized Si. Electronic excited states were studied using time–dependent density functional theory (TDDFT) with B3LYP method in the SBK++ and N31-6/SBK++ basis sets. The absorption edge shifts towards higher energies with the bismuth coverage increasing from 0.5 to 1ML because of modification of the Bi/Si(001) surface structure.