Reflectance anisotropy spectroscopy of CdTe(001) surfaces

RAUL VAZQUEZ, NORBERTO ARZATE, BERNARDO MENDOZA, Centro de Investigaciones en Optica, A. C. — The spectroscopical reflectance anisotropy (RA) response of (001) surfaces of CdTe, which exhibits a $(2 \times 1)$ and $(2 \times 1)$ surface reconstructions, is studied using two theoretical approaches: an *ab initio* pseudopotential calculation in the framework of the density functional theory and within the local density approximation (DFT-LDA) is used to obtain the relaxed atomic positions, and a microscopic formulation based on a semi-empirical tight binding (SETB) approach which includes spin-orbit (SO) interactions[1] is used to obtain the RA spectra. We show RA spectrum of each surface reconstruction and compare our theoretical results with experimental results[2]. We find a good agreement between experimental and theoretical spectra. We show how the RA changes when SO is taken into account and compare our theoretical results with experimental measurements of Ref. 2. [1] R.A. Vázquez-Nava, B.S. Mendoza and C. Castillo, Phys. Rev. B 70, 165306 (2004). [2] R. E. Balderas-Navarro, K. Hingerl, W. Hilber, D. Stifter, A. Bonanni and H. Sitter, J. Vac. Sci. Technol. B 18, 2224 (2000).

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