Near Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS) and a few case studies

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Abstract

Electronic and structural properties are of utmost importance for the fundamental understanding of the macroscopic and microscopic behavior of materials. Surface properties play a particularly important role since they determine the interaction of an object with its environment. Basic knowledge of the structure and electronic characteristics of the surface of a material is therefore crucial for many applications. The technique called near-edge X-ray absorption fine structure spectroscopy (NEXAFS), a synchrotron based technique, was devised in the 1980s, mainly in order to resolve the structure of molecules and their electronic properties bonded to surfaces. NEXAFS involves the excitation of electrons from a core level to partially filled and empty states of a molecule. The decay of core hole states occurs through the emission of Auger electrons from valence molecular orbitals. This results in a NEXAFS electron yield spectrum. Hence, the peak positions and spectral line shape in a NEXAFS spectrum are directly related to the nature of these unoccupied electronic states. Decay of core holes may also occur via the emission of fluorescent photons, which originate from the top 200 nm of the film as opposed to Auger electrons, which arise from the top 10 nm. Thus, this technique is both surface and bulk sensitive. The transition matrix elements have an angular dependence on the angle made by the orbital with respect to the electric field vector of the incident-polarized X-rays. Since the light from the synchrotron source used is linearly polarized, the intensity of the transitions will be sensitive to the orientation of the orbitals with respect to the polarization vector. Therefore, changes in the intensity of resonances upon rotating the sample in the plane of incidence of the beam provide structural information. We will discuss the NEXAFS spectroscopy and some of our experimental studies using this method in the conference.