

Electronic structure of spintronics materials studied by hard X-Ray Photoemission

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X-Ray Photoemission Spectroscopy is a powerful tool for the investigation of chemical states and the electronic structure of various materials [1]. The probing depth, however, is limited by the inelastic mean free path of the excited photoelectrons limiting the sensitivity of soft X-ray studies to the top few nanometers of the samples [2]. Using hard x-rays in the energy range of a few keV the inelastic mean free path is drastically increased to 5-15 nm, permitting more bulk-sensitive studies [3]. We have used the newly commissioned HAXPES (*Hard X-Ray Photoelectron Spectroscopy*) facility at beamline P09 of PETRA-III to study the bulk electronic structure of two systems relevant for future spintronics devices.

FeRh – temperature-dependence

Stoichiometric 50:50 FeRh consists of alternating monolayers of Fe and Rh atoms and has long been known to exhibit a transition from antiferromagnetic to ferromagnetic order (AFM-FM) that occurs on very short time scales which makes the system interesting for applications in magnetic storage systems [4]. We have carried out temperature-dependent measurements of core levels and the valence band to investigate the origin of this transition.

The bulk-sensitive core-level spectra of Fe 2p_{3/2} peaks (Fig. 1(a)) reveal changes in the intensity of the core-hole screening satellite ($E_{\text{Kin}} \approx 5245.0$ eV) relative to the main well-screened peak ($E_{\text{Kin}} \approx 5244.5$ eV) with the AFM-FM transition (at ~ 350 K). Atomic multiplet theory calculations by collaborator P. Krueger explain the observed phenomenon as the evidence of change in the Fe *d*-orbital occupation with the transition. Analysis of the valence-band spectra (Fig. 1(b)) which also undergo changes with the AFM-FM transition (work in progress) is being carried out to further understand the electronic mechanism behind the transition.

Growth conditions of EuO tunnel barriers

Europium Oxide (EuO) belongs to the rare group of materials that simultaneously exhibits insulating and magnetic properties [5]. Establishing high-quality EuO tunnel barriers for spin injection onto the technologically most relevant semiconductor, silicon, is the aim of our project. An important objective for obtaining single crystalline and stoichiometric EuO thin films is the careful control of growth parameters on the basis of molecular beam epitaxy (MBE): Too high oxygen pressure can result in the incorporation of stable, but nonmagnetic oxides, while too low oxygen pressure gives rise to oxygen vacancies limiting crystalline quality and degrading magnetic properties. In order to quantify the precise stoichiometry of EuO thin films, we performed HAXPES experiments on Al-capped EuO/Si(001) heterostructures with different EuO stoichiometries, i.e. (i) single-phase EuO and (ii) O-rich Eu_{1-x}O_x. The most direct information regarding the initial valency of insulating Eu compounds can be obtained from the 4f core-level

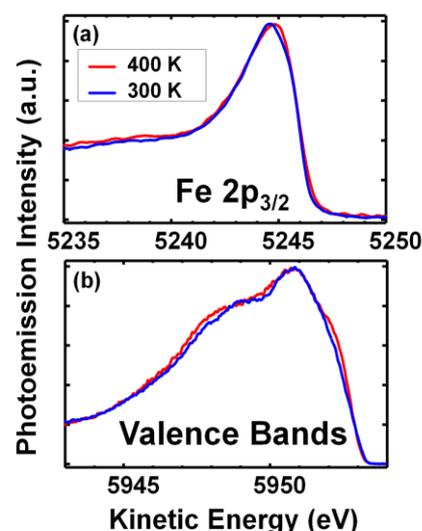


Fig. 1. Photoemission spectra of *Fe*₅₀*Rh*₅₀ above and below critical temperatures and below critical temperature (a) *Fe* 2p_{3/2} region, (b) valence-band region.

photoemission. Due to the strongly localized character of the 4f states, hybridization with ligand states is weak and photoemission from oxygen valence bands becomes well distinguishable. Fig.2 (a) and (b) show the 4f photoemission spectra of both EuO compounds (i) and (ii). From the integrated areal intensities A of the Eu^{2+} and Eu^{3+} components, we derived the Eu valence ratio, $r = A(\text{Eu}^{3+}) / (A(\text{Eu}^{2+}) + A(\text{Eu}^{3+}))$. For the stoichiometric EuO (i), a nearly integral divalent state of Eu cations was determined, whereas the O-rich Eu compound (ii) is of mixed divalent and trivalent initial-state. By changing the photoelectron emission angle from normal to grazing, information on the interface chemical state of EuO can be extracted from the photoemission data. Clearly, an interface chemical shift is observable in the lower panels of Fig.2 (a),(b), that is explained by the modifications in chemical bonding and atomic structure at the Eu/Al boundary. In summary, our HAXPES experiments on Al/EuO/Si(001) heterostructures yielded quantitative information on the initial-state valency of Eu cations, that permits determining the bulk EuO stoichiometry of different compounds, and further optimization of EuO growth on Si.

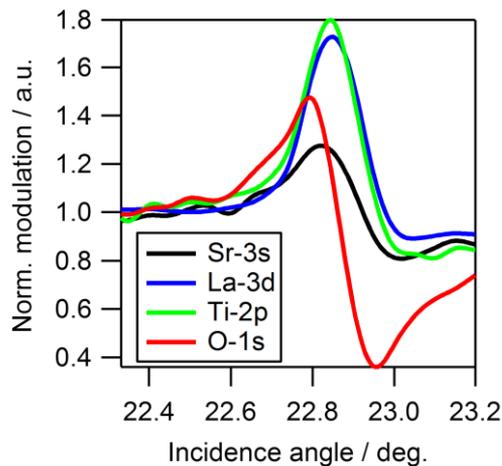


Fig. 3. Rocking curves of core-level photoemission intensities obtained by scanning over a Bragg reflection of the LSAT substrate, obtained with an x-ray energy of 4200 eV.

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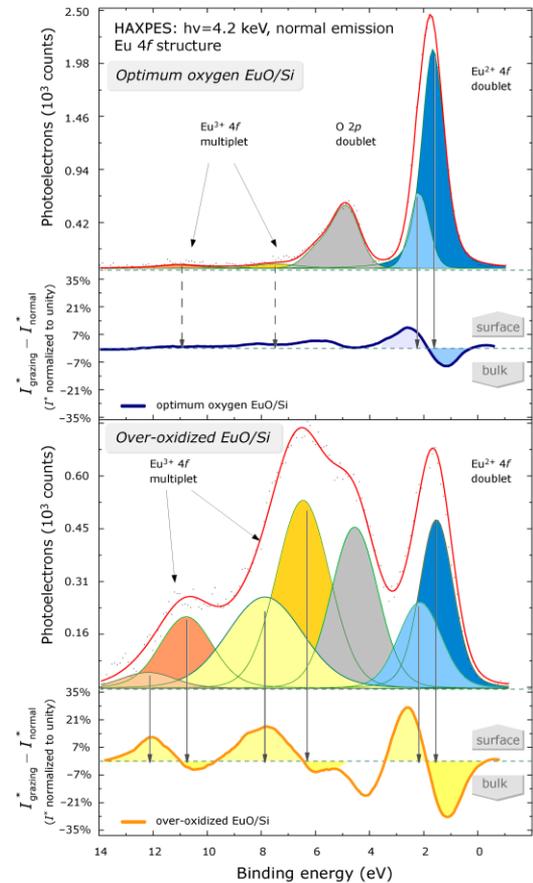


Fig. 2: HAXPES measurements of the 4f spectral region of EuO/Si samples (a) grown with optimum oxygen content and (b) over-oxidized.

Standing-wave excited photoemission from multilayers

We have also obtained a first set of standing-wave excited core-level photoemission results from an epitaxial multilayer of LaNiO_3 and SrTiO_3 grown by the Stemmer Group in Santa Barbara. These show anisotropy in multilayer rocking curve scans, as well as strong Bragg reflection peaks from the LSAT substrate crystal structure, as shown in Fig. 3, with both of these demonstrating the potential for future depth-resolved studies of the composition, electronic structure, and magnetic structure of such systems, at both the nm and sub-nm unit-cell scales. These studies will be continued in the future.