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Recoil effect in hard x-ray photoelectron spectroscopy from metal hydrides: a probe for hydrogen-related densities of states

The idea was to look for recoil effects in valence band spectra of a hydrogen containing crystalline solid. The proposal had referred to a complex borohydride of composition $NaBH_4$, based on its high hydrogen content and the low masses of the other two constituents. Unfortunately, test experiments carried out at ELETTRA in the period between proposal acceptance and the beamtime showed that charging effects from these insulating samples in the x-ray beam prevented the measurement of reasonable photoemission spectra.

Within a short time frame new hydrogen containing solids were considered and samples were obtained through collaborations: well ordered pentacene thin films from ETH Zürich, and single crystal samples of a hybrid organic-inorganic layered compound $(C_2H_5NH_3)_2CuBr_4$ (EACuBr4) which shows metallicity and can be readily cleaved. During our beamtime it turned out that we were not able to observe photoemission spectra from the pentacene films under hard x-ray irradiation. Nice spectra were obtained on the EACuBr4 samples. However, the samples were severely damaged after prolonged irradiation, and spectra remained stable for periods of a few minutes only. Therefore, protocols were developed to do automatic scans across the samples, but reproducibility remained an issue throughout the beamtime.

Preliminary analysis of the spectra did not show significant and reproducible recoil effects in the valence band region. Nevertheless, HAXPES valence band spectra from EACuBr4 could be measured for the first time. Experimental studies of this material are scarce, and we have initiated a density functional theory study of the compound as well as a careful XRD study to establish its crystal and electronic structure.

In any case, we found excellent experimental conditions at ID16 with the VOLPE spectrometer and regret that the samples were not more cooperative.