Phase-Selective Spectroscopy Of Mixed 2D Oxides Using Diffraction Anomalous Near-Edge Structure

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Understanding catalysts is crucial if we wish to move our society towards green technology. Having 2D model catalysts on single crystals let us mimic the condition of industrial catalyst. Even with such simple systems as mono- or bi-metal oxides give valuable information when measured in operando. Nevertheless, we must not expect to have only one single 2D model catalyst in the real applications. Usually, a more complex combination of crystal phases will be found intertwined on real sample surfaces.[1] It is on these multiphase structures we wish to detangle the signals and get spectres of the individual phases

Obtaining X-ray absorption near edge structure (XANES) from a specific phase in a multiphase system is difficult under normal conditions, as the data is averaged over all different XANES signals.

However, by using surface diffraction we can separate the individual phases on the crystal and by performing anomalous surface diffraction we can get chemical spectra for the individual elements in their respective phases. Measuring the energy across the near-edge regions gives us the diffraction anomalous near-edge structure(DANES)[2]. Thus, DANES gives a complete picture of the individual crystal structures and their chemical composition.

We scanned the energy across the Co and Fe k-edge while recording the diffraction intensities on a 2D detector. This allows for the detection of the two elements in the individual phases on the sample. In our study we have looked at two different samples of ultrathin films of Co and Fe oxides.

The first sample was made purely with Fe deposit using molecular beam epitaxy (MBE) in an oxygen atmosphere on Ag(100) single crystals. On the sample surface we found Fe as Fe^{2+} in monolayers of FeO and Fe^{3+} in a trilayer of Fe_3O_4 simultaneously. Knowing that we could detangle the signal from two almost identically phases we proceeded to a more complex sample with a mixture of different phases. Those we made by co-deposition of Co and Fe in an oxygen atmosphere with MBE onto an Ag(100) crystal. We identified the oxidation states of Co and Fe together with their presence in a 2D Fe_3O_4-like film as well as Fe_3O_4 in bulk structure. Co was additionally found as FCC Co-nanoclusters. All coexisting on the same sample surface.

REFERENCES

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