TECHNISCHE UNIVERSITÄT WIEN

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstr. 8-10/138, 1040 Wien
www.ifp.tuwien.ac.at

EINLADUNG zum IFP-SEMINAR

Optimization and Applications of Orbital Mapping Using TEM/EELS

Manuel Ederer

Institut für Festkörperphysik, TU Wien

Host: Stefan Löffler

Termin: Mittwoch, 14. Juni 2023, 16:00 Uhr

Ort: Institut für Festkörperphysik, TU Wien
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

Electronic states are responsible for the majority of macroscopic properties of the materials in our everyday lives. From the electrical characteristics to the type of chemical bonding, everything is ultimately determined by the specific state of the electronic orbitals. While models exist describing individual electronic states in bulk materials, directly observing them in real space was beyond reach until recently. Atomic resolution transmission electron microscopy (TEM) together with electron energy loss spectroscopy (EELS) has made this new achievement possible [1].
Probe electrons that inelastically interact with sample electrons can trigger a transition from an initial core state to the conduction band. Information about the transition to a specific final electronic state is contained in the EELS fine structure and can, thus, be mapped when a suitably small energy window is chosen. However, this so called orbital mapping pushes even modern transmission electron microscopes to their limits. The demanding needs for high spatial resolution and stability, together with the tiny energy windows of the spectrometer that result in a low signal-tonoise ratio, strongly limit the everyday use of this method. Thus, careful planning of experiments is of utmost importance to obtain usable data.
The first half of my talk will mainly deal with optimizing and improving orbital mapping as much as possible. We have employed extensive simulations in order to fully investigate orbital mapping of a transition metal system (rutile), a system comprised of a light element (graphite), as well as an interface. With the use of an image difference metric, specially adapted to TEM images [2], we find ranges of parameters (high voltage, sample thickness, …) that would result in the optimal experimental images. The second half of my talk will be about applying the method to a small selection of materials. In particular, I will present maps of spatially resolved π* and σ* orbitals of edge-on graphene [3] and maps of a 2D electron gas at the $TiO_2/LaAlO_3$ interface [4].

1 Löffler et al., Ultramicroscopy, 26 (2017), p. 177.
2 Ederer et al., Ultramicroscopy, 240 (2022), p. 112578.
3 Bugnet et al., Phys. Rev. Lett. 128 (2022), p. 116401.
4 Oberaigner et al., in preparation