

Electron energy loss spectroscopy at high spatial resolution: from elemental to orbital mapping

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With the development of aberration correctors and monochromators, electron energy loss spectroscopy (EELS) in the scanning transmission electron microscope (STEM) has become a widely used technique to combine both spatial and chemical information, via elemental mapping in crystals down to the atomic level. While for elemental mapping the full absorption edge can be selected, additional information on the electronic structure and properties can be obtained by selecting a specific feature in the fine structure (FS) of the energy loss near edge structure (ELNES). The unoccupied density of states probed in core-loss EELS contains valuable information on the electronic structure and related properties of the material investigated. Arising from transitions to unoccupied states of a particular energy, the ELNES FS allow for identification of localized states at the atomic scale. The relevance of localizing FS at the atomic scale is shown for the case of cuprate superconductors, providing insights into the long-standing problem of the localization of holes in these compounds. Support by inelastic channelling calculations proves to be necessary for a quantitative evaluation of hole concentrations. Furthermore, direct mapping of individual atomic orbitals in bulk specimens is demonstrated on rutile (TiO₂). The results presented here highlight some challenges in terms of data interpretation, with the need for numerical simulations for both qualitative and quantitative analyses.