Beyond locating the atoms towards addressing the electronic structure of crystals using advanced transmission electron microscopy

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With the present focus on nanostructures, the role of the transmission electron microscope (TEM) as a research tool is becoming increasingly important. Among the major strengths of TEM are the capability of obtaining diffraction patterns and electron energy loss spectra (EELS) from nanometer sized areas. In addition, advanced TEM may serve as a supplement to synchrotron x-ray diffraction and absorption spectroscopy in efforts to study bonding and electronic structure of bulk materials. This is in particular the case when only small-grained polycrystalline samples are available, but TEM may also provide valuable input in studies of single crystals. For example, the near edge fine structure at EELS absorption edges was used to locate different valence states of Fe within the unit cell of a mixed valence crystal already two decades ago [1], and more recently precision convergent beam electron diffraction (CBED) was used in combination with x-ray diffraction to study the spatial distribution of valence electrons in Cu_2O [2].
In this presentation, we report our recent study of the MgB_2 where we use both EELS [3] and CBED [4] to gain insight into the electronic structure of this new superconductor with T_c=39K. Using angle-resolved EELS we studied the fine structure at the K-edge of boron in order to probe the empty boron p_{xy} and p_z states near the Fermi level in this anisotropic hexagonal crystal. Similar information can be obtained using polarized soft x-rays in absorption spectroscopy (XANES) if sufficiently large single crystals become available. Using quantitative CBED we determine the structure factors at short g-vectors. These structure factors at short g-vectors, which are strongly influenced by the valence electron redistribution, can be determined with very high accuracy using electron diffraction. For example, after converting to x-ray structure factors, we measure F_{001} of MgB_2 to be 2.15±0.03 electrons while the calculated structure factor for the procrystal differs 20 standard deviations from this value (2.75 electrons). We also did DFT calculations, and found good agreement between experimental and theoretical structure factors.

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