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RESONANT X-RAY SCATTERING AT METAL INSULATOR TRANSITIONS

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Results of resonant X-ray scattering on materials exhibiting metal-insulator transitions are presented. In a first example, Yb_4As_3 is studied, which shows a first order transition at 290 K into a quasi 1-dimensional charge ordered state. It is shown that the temperature dependence of the charge order parameter is significantly different compared to that of the structure. This shows that bond valence sum calculations would fail to correctly describe the temperature dependence of the valence. In a second example, $NdNiO_3$ is studied. Below the metal insulator transition the Ni ions are found in two different distinct sites with different electronic states. In combination with X-ray absorption, the site selective electronic states (valences) of Ni are determined. A significant difference in the order parameter of the structure, the charge and the magnetic moment of Ni is observed.

Keywords: METAL-INSULATOR TRANSITIONS, CHARGE ORDER, RESONANT X-RAY SCATTERING

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RESONANT X-RAY SCATTERING FROM ORBITALLY ORDERED SYSTEMS

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Orbital degree of freedom plays important roles in electric and magnetic properties in some transition metal oxides and f-electron systems. The experimental method to observe the orbital ordering, however, has been limited so far. Recently it has been pointed out that synchrotron x-ray diffraction is a very powerful tool to observe the ordering. In particular the resonant x-ray scattering (RXS) technique has been developed to detect the orbital ordering for last few years.[1] We have studied the orbital ordering of manganites, vanadates, titanates, and some f-electron systems by using this technique.[2] However, the microscopic mechanism of RXS still remains controversial. In order to elucidate the mechanism we have systematically examined the RXS from some manganites films and titanates. It has been found that Jahn-Teller distortion is mainly responsible for the RXS of manganites, while Coulomb interaction between 3d and 4s electrons become effective in the RXS of titanates.

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Keywords: RESONANT SCATTERING, ORBITAL ORDERING, QUADRUPOLE ORDERING

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ANISOTROPY IN RESONANT ANOMALOUS SCATTERING

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Even within the electric-dipole approximation, anisotropy in resonant photon scattering can lead to sizeable effects, including magnetic scattering and space-group forbidden Bragg diffraction. We outline the background to these effects, illustrated with results from recent experiments with synchrotron radiation.

Keywords: RESONANT SCATTERING SYNCHROTRON

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ON THE IMPORTANCE OF THE 'SMOOTH' ENERGY VARIATION IN RESONANT DIFFRACTION SPECTRA

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Near absorption edges, atomic scattering factor may be split in smooth and oscillatory parts. The non-oscillating smooth contribution can be used for contrast measurement using its chemical sensitivity. The oscillating contribution contains the short range order information, thus anomalous scattering is used for: (i) structure factor phase solution (M.A.D. method), (ii) element selective diffraction (Contrast method), (iii) selective site spectroscopy (D.A.F.S. method).

In this contribution, using different multilayer, powder and single crystal examples like spin-ladder oxides, we will focus on the part played by the smooth variation versus energy of diffracted intensity. Near an absorption edge, this contribution gives access for each reflection to a phase difference between the net phase contribution of all non anomalous atoms and those of anomalous atoms, and to the relative anomalous contribution itself. Therefore this smooth variation gives important and precise information on the crystallographic structure and determines the shape of the DAFS spectrum. In substituted samples, fits of the smooth spectra allow to extract occupancies of mixed sites. The sensitivity to smooth contribution is also important for DAFS analyses and for studies using the tensor properties of DANES spectra, since for 'forbidden' or superstructure reflections, the smooth contribution is highly sensitive to distortions. Phenomenon like orbital ordering or charge ordering are generally associated to lattice distortion, thus DANES is not a so simple and direct probe to study these orders and it is essential to select several superstructure or satellite reflections sensitive to different sites, atoms and aspects of the concerned transition.

Keywords: RESONANT DIFFRACTION DAFS CONTRAST METHOD