Scattered photons tell us about the magnetic interaction between atoms

Measuring -or feeling- magnetic interactions looks simple at first glance: holding two magnets close to each other gives an immediate idea. How about the case when the 'magnets of interest' are tiny and amount to nothing more than atoms? X-rays generated at the Swiss Light Source allow 'zooming in' on magnetic interactions relevant at inter-atomic scale: we bring forward the first evidence of local spin flips of atomic moments in a 'photon-in photon-out' scattering experiment.

Driven by the development towards smaller, faster and cheaper electronic devices, scientists are searching for novel materials. Digital cameras which fit into a pocket or light-weight portable computers are some of the every day life examples made possible due these efforts. Like architects combining known bricks into new buildings, material scientists need to understand the way atoms interact when assembled together in a crystal. Therefore the precise experimental characterization of inter-atomic interactions plays a key role: it allows validating the theories describing materials at inter-atomic scale and sets reference points for future models. This study exemplifies how scattering of x-rays can help gaining such kind of information about a prototypical material, nickel oxide. The method is however applicable to a wide range of materials.

The idea behind

How can we 'zoom in' on the magnetic interactions between atoms? To give a very simplified view, in insulating materials the atomic magnetic moments are like tiny magnetic needles pinned on the carrying atoms, at their crystal sites. As for any other magnets their interaction depends on their orientation, so that changing their relative direction requires some extra energy. For example, in antiferromagnetic materials the local magnetic moments are oriented alternatively parallel and antiparallel to the magnetization axis: the net magnetization is zero despite a strong magnetic interaction between neighboring atoms. This is the case of nickel oxide at room temperature, as depicted in Figure 1. How strong is the magnetic interaction between the nickel atoms? Quantum mechanics helps spotting a simple way to measure it: flipping one of the atomic magnetic moments relatively to the neighboring moments increases the energy of the system by a certain quantified amount; in principle, measuring the energy difference between the ground state and the various spin-flipped states directly yields the magnetic exchange interaction. The idea of using x-ray scattering for this purpose was theoretically put forward in 1998 by de Groot et al. but its practical implementation was delayed by the relative weakness of the magnetic interaction: the experiment requires very precise measurement of the energy loss of x-rays after exciting such a spin flip excitation.

The Experiment

At the Surface/Interface: Spectroscopy (SIS) beamline, we were able to measure such local spin flip excitations in a 'photon-in photon-out' experiment. Incoming photons with well defined energy illuminate the sample (in our case the nickel oxide) and the energy of scattered (outgoing) photons is recorded with high energy resolution (see Figure 2). The difference between the energy of the incoming and outgoing photons gives the amount of energy transferred to the sample. The transferred energy results in local excitations, like the local spin flips. The SIS beamline provides a high flux x-ray beam and convenient photon energies for this kind of experiments. The detection is performed by employing a diffraction grating which separates the photons in space according to their energy.

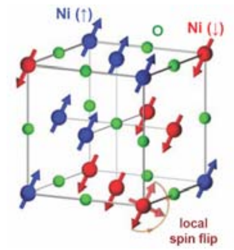

Figure 1: *Schematic representation of local spin flip excitations in nickel oxide: one nickel spin flips its relative orientation to the surrounding local spins.*

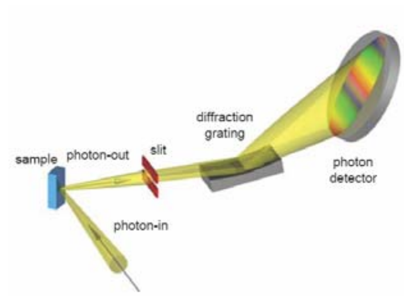

Figure 2: *Sketch of the experimental setup.*

The results

The spectra recorded for nickel oxide are summarized in Figure 3, showing the intensity of the scattered photons versus the energy transferred to the sample for incoming photon energies spanning the Ni M absorption edges. Besides elastically scattered photons (zero transferred energy), well defined losses are detectable. They essentially resemble reorganizations of the nickel valence electrons within the shell, when energy is transferred from the incoming x-rays (dd excitations). The fine details of spectral changes, when changing the incoming photon energy, can be explained based on theoretical calculations. The separation of the double structure visible in the high resolution spectra (Figure 3, lower panel, see spectrum depicted with magenta line) allows the determination of the magnitude for magnetic interaction between nickel atoms, based on the good agreement between measured and calculated data [1]: it takes at least 125 meV to flip one local nickel magnetic moment.

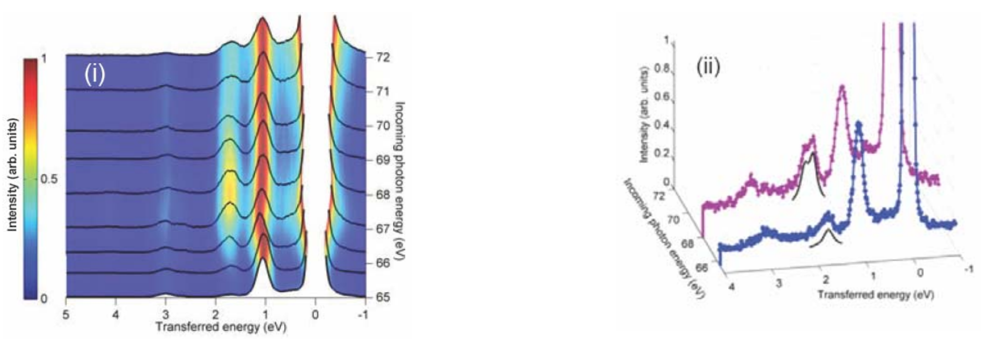

Figure 1: *X-ray scattering results for nickel oxide with incoming photon energies encompassing Ni M absorption edges. For the spectra shown in the lower panel (ii) the resolution was increased by accessing the second diffraction order of the grating.*

Publications

- **Publication title**
  S.G. Chiuzbaian, G. Ghiringhelli, C. Dallera, M. Grioni, P. Amann, X. Wang, L. Braicovich and L. Patthey*,
  Physical Review Letters, 95, 197402 (2005)
  http://dx.doi.org/10.1103/PhysRevLett.95.197402

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