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Investigation of metal-insulator transition in Slater insulator, NaOsO3 using static and time-resolved resonant x-ray diffraction

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The metal-insulator transition in 5d transition metal oxide NaOsO3 which occurs concomitantly with antiferromagnetic order (TMIT=TN) has been proposed to be driven by Slater mechanism [1, 2] i.e. it is the onset of the antiferromagnetic order that drives the system into an insulating state [3]. However, there is no consensus and other mechanisms such as a Lifshitz transition have been proposed [4]. We employed static non-resonant and resonant x-ray single-crystal diffraction at the Os L2,3 edges in order to obtain details of the Os electron density deformation across TMIT and to investigate the microscopic mechanism of the phase transition. In the case of a Slater metal-insulator transition, there should be no change in the crystallographic symmetry and, indeed, our off-resonance single crystal x-ray diffraction experiments find no evidence of crystallographic symmetry breaking across the metal-insulator transition. In addition, using an incident x-ray energy corresponding to the Os L3 resonant edge, we observe the emergence of a diffracted intensity of the forbidden re-flection (300), also called ATS (anisotropic tensor of the x-ray susceptibility) reflection at TMIT=TN for a specific energy EA = 10.878 keV. The intensity of this ATS reflection increases continuously with decreasing temperature and is not of magnetic origin. We show that it is due to a change in the Os electron density associated to the onset of long range antiferromagnetic ordering. Thus, the main conclusions of our experimental results namely: the absence of crystallographic symmetry breaking and the presence of antiferromagnetic driven Osmium electron density reconstruction, support the first realization of a Slater insulator, NaOsO3.

We further observed that upon photo-excitation, ultrafast changes in the reflectivity takes place. In order to study the time-evolution of long-range ordering arising from structural, magnetic and electronic ordering, we employed time-resolved resonant x-ray diffraction at the Os L3 edge. From our preliminary data analysis, we observe a significant drop of the antiferromagnetic peak intensity after photo-excitation within the time resolution of the experiment, while the timescale associated with the drop of intensity of a structural reflection is in the order of several picoseconds. As a next step, we aim at comparing the ultrafast dynamics of long range ordering in this system with other transition metal oxides, in order to determine the existence of unified description of a universal time-dependent order parameter in transition metal oxides.

References
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Position

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