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Revealing Electronic, Structural and Magnetic Phases in NdFeAsO with Electron Energy-Loss Spectroscopy

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The new iron-based family of high-Tc superconductors has generated interest in the scientific community because these materials present hybrid properties from both classical BCS and high-Tc superconductors [1]. Iron pnictides, quaternary compounds of the form (ReFeAsO, Re=rare-earth elements), present structural and magnetic phase transitions in the temperature range between 120 K to 150 K. Here, we report momentum transfer-dependent and temperature-dependent electron energy-loss spectroscopy (EELS) studies of the parent compound NdFeAsO using (scanning) transmission electron microscopy and density functional theory.

Z-contrast images were taken at 300 kV in a FEI Titan 80-300 S scanning transmission electron microscope (STEM), equipped with a CEOS probe aberration corrector, and in a dedicated STEM NION UltraSTEM at 100 kV, equipped with a NION probe aberration corrector. Both microscopes are located in Oak Ridge National Laboratory. The EEL spectra were acquired in the NION STEM microscope and in a JEOL 3000F operated at 300 kV, located in Brookhaven National Laboratory.

We find that both the Fe L_{23}-ratio and the Nd M_{45}-ratio change for different crystallographic orientations (Fig. 1). Additionally, the Fe L_{23}-ratio and the Nd M_{45}-ratio increase, while the intensities of the Fe L_1-edge and Nd M_3-edge reduce as the temperature decreases (Fig. 2). Using a combination of experiments and total-energy first-principles calculations within density functional theory, we will show that the changes of the EELS Fe and Nd fine structure can be directly correlated with changes on the electronic structure of NdFeAsO and Fe and Nd magnetic moments [2].

References:
[1] Y. Kamihara, et al. *J. Am. Che. Soc*, 128 (2006) 10012.
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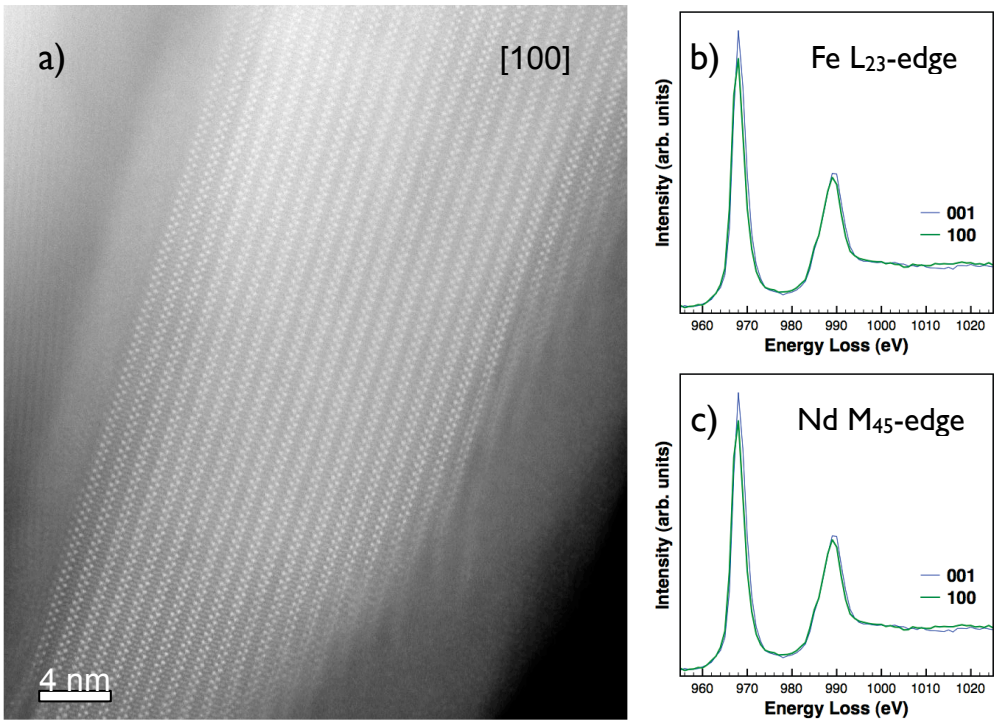

FIG. 1. (a) Z-contrast image NdFeAsO grain along the [001] crystallographic orientation. EEL spectra of (b) Fe L_{23}-edge and (c) Nd M_{45}-edge acquired in the 001 and 100 crystallographic orientations. Image obtained in the FEI Titan 80-300 S at 300 kV. Spectra collected in the NION UltraSTEM at 100kV.

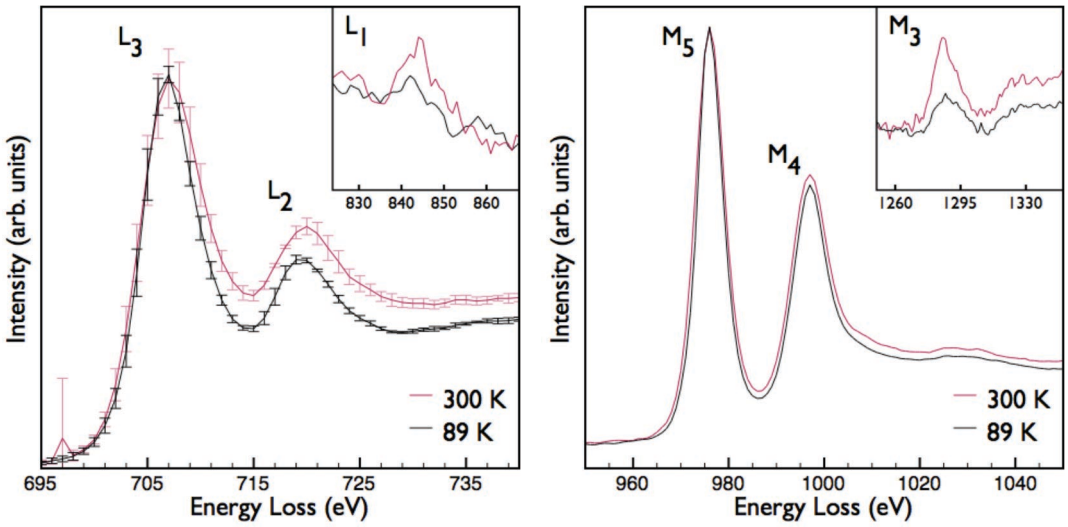

FIG. 2. Iron L-edge and Nd M-edge spectra taken from a NdFeAsO grain along the [001] crystallographic orientation. The spectra was taken at two different temperatures, 89 K and 300 K. Both Fe L_{23} ratio and Nd M_{45} ratios and the intensities of the Fe L_1-edge and Nd M_3-edge reduce as the temperature decrease. Spectra collected in TEM mode in the JEOL 3000F operated at 300 kV located in Brookhaven National Laboratory.

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