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Pressure-induced electronic Mott transition in MnO

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Mott's seminal work on how insulating character may arise out of the electron-electron repulsion used a *3d* transition metal monoxide, NiO, as an example and suggested its pressure-induced metallization, the Mott transition [1]. Yet for 55 years the Mott transition in these archetypal Mott insulators MnO, FeO, CoO, and NiO has eluded detection at room temperature due to the high pressures required. Recent resistivity measurements using "designer" diamond anvils, however, have seen this insulator-metal transition in MnO, a five order of magnitude decrease in resistance between 90 and 106 GPa [2]. In this paper, we present x-ray emission spectroscopy and x-ray diffraction data which not only suggest that the Mott transition in MnO is a far richer phenomenon than just the onset of metallization, but that it also exhibits profound similarities to transitions in the lanthanides and actinides as has been predicted [3] and thus furthers our general understanding of electron-correlation driven phase transitions.

MnO is a paramagnetic (PM) insulator in the B1 (rock salt) structure at ambient pressure and temperature, transforms to an antiferromagnetic (AFM) rhombohedral distortion (denoted dB1) at 30 GPa, then to an unknown "intermediate" phase at 90 GPa, and then to the B8 (NiAs) structure at around 120 GPa [4]. In the present x-ray emission experiments (Fig. 1), we found that MnO undergoes at least two first-order electronic transitions: one at the onset of the B1 (PM)-dB1 (AFM) transition at 30 GPa and the other in the middle of intermediate phase at around 105 GPa. Furthermore, our subsequent x-ray diffraction experiments found that the intermediate phase is consisted of a mixture of dB1 (AFM) and B8 (PM) phases and the B8 (PM) phase further transforms to an iso-structural diamagnetic B8 (DM) at around 105 GPa.

The present spectral and diffraction data together with the recent resistance data [2] provide a coherent picture of the Mott transition in MnO, which concurrently manifests (1) significant loss of magnetic moment, (2) large isostructural volume collapse and (3) the insulator-metal transition. The magnetic and structural sequence

we suggest is consistent with the available data for FeO [5,6] in a great geophysical importance and may shed light on the later *3d* monoxides as well. Furthermore, although similarities between the electron-correlation driven transitions in the *3d* monoxides and the 4*f*- and 5*f*-electron metals were predicted years ago [3], it is truly striking that these three signatures observed here for the archetypal Mott transition in MnO are *all* observed at the volume-collapse transitions in the lanthanide and actinide metals.

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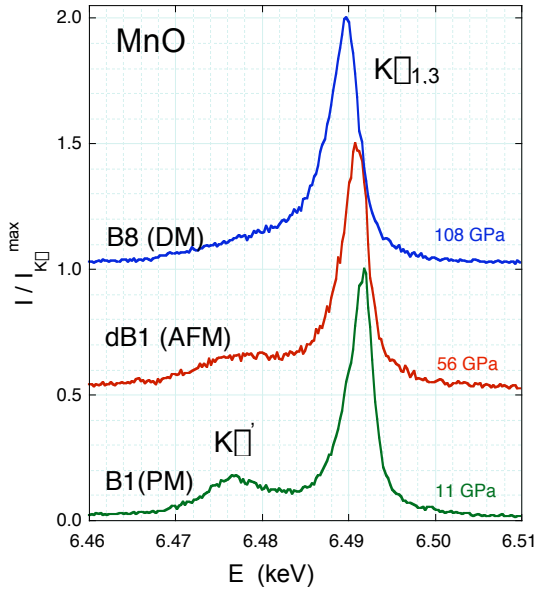

Figure 1. Mn K-edge x-ray emission spectra of MnO at high pressures showing a significant modification of magnetic moment evident from the changes in Kβ' as pressure increases. These spectral changes occur abruptly at 30 GPa and 105 GPa suggesting the first-order electronic phase transitions.

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