

High-resolution Non-resonant Inelastic X-ray Scattering Studies of $d-d$ Excitations in NiO

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Transition metal compounds with partially filled d -shells exhibit a large variety of interesting properties, ranging from metal insulator transitions, colossal magneto resistance, to superconductivity. These properties are believed to arise from the strong interplay between the orbital, charge, spin, and lattice degree of freedom observed in these materials. Simple transition metal oxides such as MnO, NiO, CoO and CuO are of particular interest as prototype systems for understanding these complex behaviors and have been subjected to numerous studies using various well-established spectroscopic techniques. The recent advance of non-resonant inelastic x-ray scattering (NIXS) has revived the interest in these simple compounds. The energy resolution achievable for state-of-the-art NIXS and yet still retaining sufficient intensity for observing charge excitations in these systems has been improved to the level comparable to optical techniques ($\leq 100\text{meV}$). The ability to obtain momentum (q)-resolved information compared to optical spectroscopies, where q equals zero, has made NIXS a particularly powerful tool in elucidating the charge dynamics of these systems as recent examples have shown [1-3].

In this experiment, we explore the capability of high-resolution NIXS in elucidating the detailed structure of $d-d$ excitations recently reported in NiO using NIXS [2]. We are interested further the temperature dependent behavior of the $d-d$ excitations as it carries important information about electron-phonon coupling in the system. The experiment was performed at BL12XU using one of the high-resolution configurations, where the incident beam was monochromatized using in-line Si(333) channel-cut crystals and Si(444) spherical diced analyzers, yielding a total instrumental resolution of 64 meV. The incident photon energy was scanned from $\sim 7913\text{eV}$ to just above the $d-d$ excitation. This energy is below the Ni K-edge, thereby avoiding absorption loss of the intensity.

In our previous run (2007A4264), we measured spectra at both room temperature and at 120K along the [111] direction at a momentum transfer (q) of 7Å^{-1} , which revealed two excited states at around 1.8 and 3.0 eV with unprecedented details. Both peaks showed broadening and splitting at the higher temperature (room temperature). Another state of much weaker intensity was also observed around 1.0 eV, which showed large energy shift to lower energy at higher temperature. This state was predicted to peak at [113] direction due to its symmetry [4].

In the present run, we confirmed the 1.0 eV feature by measuring along the [113] direction at 7Å^{-1} momentum transfer. Measurement was taken also at temperature above the Neel temperature of NiO ($T_N = 523\text{K}$). Again a clear shift of the peak towards lower energy was observed at the higher temperature. For the excited states at 1.8 and 3.0 eV, similar trend was

observed. Further analysis is underway. The data are believed to provide important information on electron-phonon coupling in the system.

References

- [1] Y. Q. Cai *et al.*, Phys. Rev. Lett. **97**, 176402 (2006).
- [2] B.C. Larson *et al.*, Phys. Rev. Lett. **99**, 026401 (2007).
- [3] N. Hiraoka *et al.*, Eur. Phys. J. B **70**, 157 (2009).
- [4] M.W. Haverkort *et al.*, Phys. Rev. Lett. **99**, 257401 (2007).

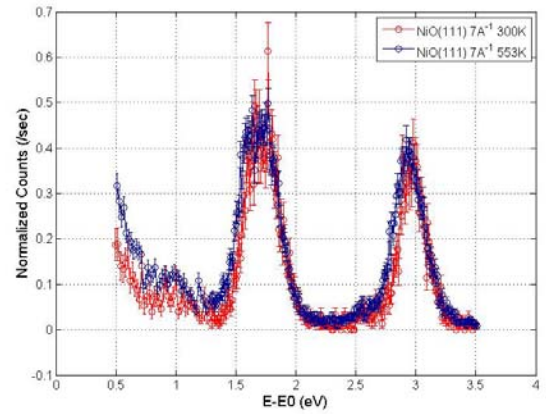


Fig. 1: Spectra showing the 1.8 and 3.0 eV feature taking along the [111] direction at $q = 7\text{Å}^{-1}$ at 300 and 553 K. Both features show broadening at the higher temperature and a clear shift to lower energy.

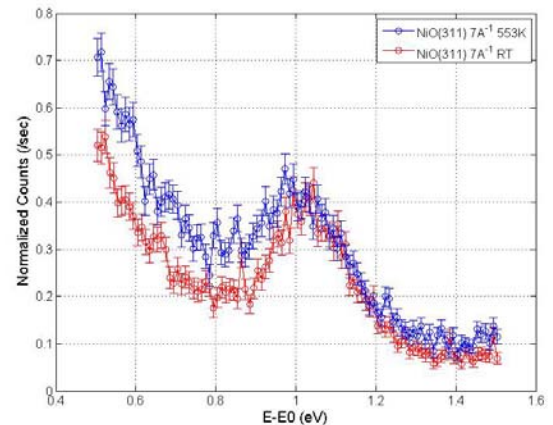


Fig. 2: Spectra showing the 1.0 eV feature taking along the [311] direction at $q = 7\text{Å}^{-1}$ at 300 and 553 K. As in Fig. 1, the feature shows broadening at the higher temperature and a clear shift to lower energy.