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Anisotropic X-ray Anomalous Dispersion in Ferroelectric $KNbO_3$

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Introduction: In the last decade major progress in theory of ferroelectricity has led to better understanding of electronic polarization in ferroelectrics, while experimental verification has lagged behind. Recently it was proposed by Egami [1] that x-ray anomalous scattering could directly probe electronic polarization in the ferroelectric state. In this experiment we demonstrate the potential of x-ray anomalous dispersion for studying the electronic structure of ferroelectric materials.

Methods and Materials: As a model system we chose a single-crystal potassium niobate, $KNbO_3$, a strong ferroelectric with a Curie temperature of 708 K, which therefore exhibits a strong directional bonding between niobium and oxygen. The measurements were performed near the Nb K-edge. The real and imaginary parts of the anomalous dispersion, f ' and f '', were determined by measuring the absorption coefficient and using the Kramers-Kronig analysis. In order to study the momentum transfer dependence of the f ' anisotropy we measured thermal diffuse scattering near several Bragg reflections.

Results: The anisotropy of f ' was determined by collecting the data at two different orientation of the sample, when the incident photon polarization was parallel to either crystallographic axis a- or b. In the first case, the electronic states formed due to Nb-O hybridization are accessible for the excitation of Nb 1s core electrons, whereas in the second case they are not accessible. Thus the anisotropy of the Nb-O bond results in the anisotropy of f '. At finite scattering momentum transfer (measurements near the Bragg peaks), the anisotropy was similar to that observed at zero momentum transfer, but larger in magnitude (see Figure 1). It also exhibited a Q-dependence: the crossover point of the anisotropy was shifting downward in energy with increasing Q. This indicates that anomalous scattering at the energy tuned to a metal absorption edge is capable of probing the band structure of the metal-oxygen hybridized states in ferroelectrics. Further experiments aimed at probing various Nb-O hybridized states in $KNbO_3$ are underway.

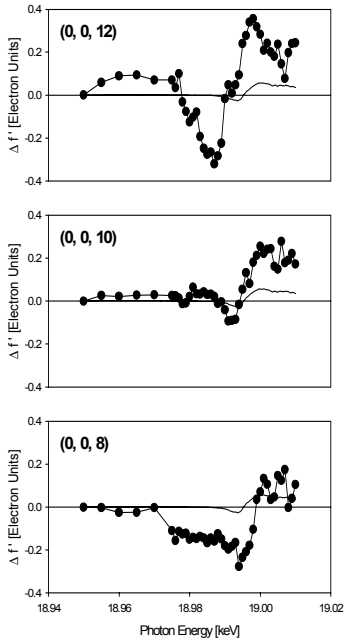

Figure 1. The polarization-dependent anisotropy of f ' at different momentum transfer obtained by subtracting the data collected when photon polarization was parallel to the a-axis from those collected with photon polarization along the b-axis. The anisotropy of f ' at zero momentum transfer is shown for comparison as the low-amplitude line with no symbols.

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References: [1] T. Egami, "Competing Interactions in Complex Ferroelectric Systems" in Fundamental Physics of Ferroelectrics 2000: Aspen Center for Physics Winter Workshop, edited by R.E. Cohen, p.16, AIP Conf. Proc. 535, Melville, NY, USA, 2000.