HIGH PRESSURE X-RAY ABSORPTION AT LOW ENERGY

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abstract: High pressure x-ray absorption spectroscopy has been extended to low energy using perforated diamond anvils and Be gasketst on the LUCIA beamline. Experiments at the Ti K edge (through the diamonds) on SrTiO₃ up to 10 GPa and at the Cl K edge (through the Be gasket on KCl up to 1.5 GPa have been performed. Modifications of the preedge features of SrTiO₃ are observed at 5 GPa in agreement with previously determined phase transformation. The variation of the K-Cl bond length determined by the modification of the EXAFS oscillations fits perfectly with the known equation of state of KCl.

High pressure is a thematic in progress, especially in synchrotron radiation centers, whatever is the scientific domain (geosciences, physics, chemistry, biology...). X-ray absorption spectroscopy¹ under high pressure is now a well established technique but, up to now, limited to high energy edges (above 7 kev) because of the absorption of the diamonds. Recently we have developed high pressure cells with perforated diamonds. The total thickness of the diamond anvils was reduced to 1mm which allows performing experiments down to 5 keV. To reach lower energies, different geometries have to be used. Between 3 and 5 keV, the x-ray beam goes through a partially perforated diamond (0.2mm wall remains) and the photons are detected in the fluorescence mode through a Be gasket. Below 3 keV both incoming and fluorescence photons go through a Be gasket. In this last geometry, because of the limited thickness of the Be gasket, close to 20-40 µm, we take a large advantage of the small size of the x-ray spot on the LUCIA beamline.

The figure 1 shows the absorption spectra of KCl at the Cl K edge at ambient pressure and at 1.6 GPa. The energy of the high pressure spectrum has been rescaled in order to take into account the bond length variation. The different oscillations show the same frequency. Consequently, the bond length variation fits well the known equation of state of KCl which validates the experiment.

The figure 2 shows the preedge part of the absorption spectrum of $SrTiO_3$ at the Ti K edge for different pressures. Each feature has been identified at room pressure². A clear reversible modification of the intensity of the different features is observed above 5 GPa. This corresponds to a phase transformation where the Ti atom goes to the center of the TiO₆ octahedron (peak labeled Ti-O in the figure) and where the cubic structure is slightly distorted (peak labeled Ti-Ti in the figure). The pressure transition is in good agreement with previous studies but this is the first time where the Ti atom motion is determined and where the Ti-Ti bond distortion is observed.

$B_{0} = 17.6 \text{ GPa}$

Fig. 1: X-ray absorption spectrum of KCl at the Cl K edge. The spectrum at 1.6 GPa has been rescaled using the known equation of state of KCl



Fig. 2: Preedge features of the Ti Kedge absorption spectrum for $SrTiO_3$ at different pressures.

REFERENCES

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Compressibility of KCI at the potassium K edge