Neutron Diffraction of NaBD$_4$: Phase Transition, Rietveld Structure Refinements, and Equation of State
Guillermo Esparza, Patricia Kalita, Professor Andrew Cornelius
Department of Physics and Astronomy
University of Nevada Las Vegas, NV 89154

BACKGROUND

NaBH$_4$ is a hydride with possible applications as a hydrogen storage material for future renewable energy technologies. Its dehydrogenation properties are enhanced with the mixture of particular catalysts through ball-milling techniques during which local pressures may exceed several GPa's. It is for this reason that understanding the behavior of pressure induced phase changes of its crystalline unit cell is an area of interest.

RESULTS

Analysis of the neutron diffraction data using Rietveld Refinement showed a phase transition occurring into the orthorhombic phase between 6.3 and 7.9 GPa. However, this appeared to occur from the cubic phase, as the intermediate tetragonal structure mentioned in other literature to appear between 6.3 and 8.9 GPa was not observed. Atom coordinates were determined for deuterium, demonstrating only a small amount of drift, and are showcased in Fig. 1 (a) for the cubic and orthorhombic structures. The Pressure vs. Volume data is also shown.

EXPERIMENTAL PROCEDURE & DATA ANALYSIS

This study makes use of neutron diffraction data collected from NaBD$_4$ up to about 12 GPa. The sample was held in a Paris-Edinburgh cell in non-hydrostatic pressure conditions. The program Topaz was used to perform Rietveld Refinement on the data, and external data on the structure and atom positions of Na and B was attained in order to determine the atom positions of hydrogen (in this case its isotope deuterium) within the unit cell. Volume vs. Pressure data was also collected in order to attain an appropriate equation of state and from it determine the compound’s bulk modulus.

CONCLUSIONS AND SUMMARY

When NaBD$_4$ is studied at high pressures up through 12.2 GPa, shifting of peaks to a higher 2θ in neutron diffraction patterns indicates a smaller d-spacing as the unit cell is compressed. The appearance of new peaks also indicates at least one phase transition to lower symmetry somewhere between 6.3 and 7.9 GPa, determined to be from a cubic Fm-3m space group to an orthorhombic Pnma one. The resulting pressure vs. volume data was used to fit a 3$^{rd}$ order Birch-Murnaghan equation of state to the cubic phase and a 2$^{nd}$ order one to the orthorhombic phase, with the determined values of B, B', and V$_0$ displayed in Fig. 2 (c).

REFERENCES


ACKNOWLEDGEMENTS

Guillermo Esparza would like to thank Professor Ravhi S. Kumar, Daniel Antonio, and Jason Baker from UNLV for constant support and encouragement. The UNLV High Pressure Science and Engineering Center was supported by the U.S. Department of Energy, National Nuclear Security Administration, under cooperative agreement number DE-FG52-06NA27684. Support from the REU program of the National Science Foundation under grant DMR-1005247 is gratefully acknowledged.