X-Ray Diffraction and Spectroscopy at High Pressures: Recent Studies

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Introduction

We have used infrared, nuclear inelastic, and Raman spectra and X-ray diffraction at high pressures to search for a predicted dense phases of HFNX an energetic material; to characterize structures and lattice dynamics of several Fe-Sn intermetallic compounds and alloys; [1] and to understand the shear-induced structural transition of PETN. [2] Selected results of these studies are described here.

Methods and Materials

X-ray diffraction and nuclear inelastic scattering experiments were performed at the HPCAT Sector of the Advanced Photon Source and NSLS Beam Line X7A. Infrared and Raman spectra were collected at NSLS Beam Line U2A and with a Jobin-Yvon U1000 spectrometer with CCD detection, respectively. PETN and HFNX were kindly provided by Drs. David Moore (Los Alamos National Laboratory) and Robert Chapman (Naval Air Warfare Center, Weapons Division, China Lake, CA). Fe-Sn alloys and compounds were synthesized by vacuum arc melting mixtures of isotopically enriched ^{57}Fe (95%) and ^{115}Sn (93%); the structures of the products were confirmed by x-ray diffraction. Samples were loaded for studies at high pressures is various of HiPSEC's diamond-anvil cells.

Two Particular Results

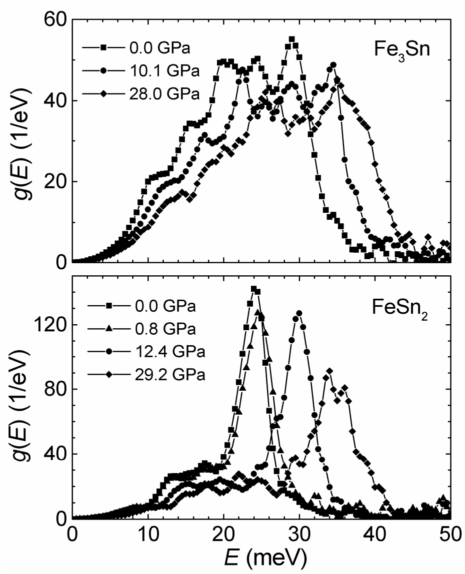

Fig.1. Phonon DOS of Fe_3Sn and $FeSn_2$ at selected pressures.

The derived partial phonon DOS spectra for Fe-rich Fe_3Sn and Sn-rich $FeSn_2$ at high pressures are shown in Fig. 1. Notice that, for the Sn-rich material, the higher-energy phonons are more heavily weighted in the Fe phonon DOS.

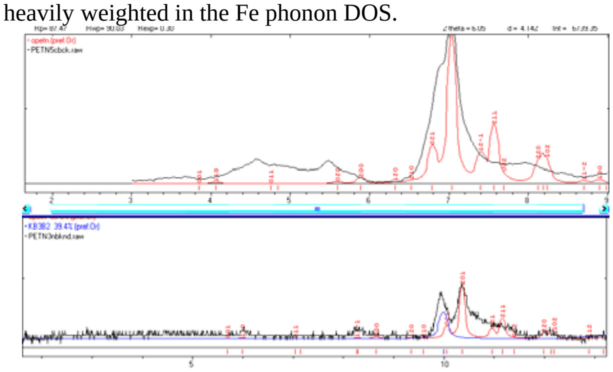

Fig .2 Experimental diffraction patterns (dark lines) and simulations of these patterns (red lines) for PETN collected at HPCAT (upper trace, focused beam) and NSLS X7A (lower trace, unfocused beam).

Although the lower pattern is less intense, it is more easily resolved and can be indexed; however, many peaks are too weak to provide reliable atomic coordinates. The structure of the shear-induced phase was determined by combining these data and results of *ab initio* calculations for likely structures. These calculations show that the transition is ferroelastic from a tetragonal ($P42_1c$) to an orthorhombic ($P2_12_12$) structure and does not change molecular conformations.

Discussion

The great variety of synchrotron radiation sources adaptable to high-pressure diamond-anvil cell research opens many avenues for forefront materials research under extremes of pressure as well as temperature and time.

References

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