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Phonon density of states of iron solid solutions at ambient and high pressures using nuclear inelastic X-ray scattering (NRIXS)

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Density of States of Iron Solid Solutions at Ambient and High Pressures using Nuclear Resonant Inelastic X-ray Scattering

Nuclear resonant inelastic x-ray scattering (NRIXS) of synchrotron radiation uses the energy transferred during the inelastic nuclear absorption of photons to determine phonon density of states for solid Mössbauer isotopes. This type of experiment can be conducted at ambient and high pressures with the use of a diamond anvil cell (DAC) and a rhenium gasket. Here, we are concerned with the phonon DOS of α-FePt 10% at pressures up to 30 GPa, as well as FeAl 4.3%, 6.4%, and 27.1% at ambient pressures. The iron samples used are doped in order to increase the pressure at which the alpha to epsilon phase transition for iron occurs. As the most abundant element within Earth's core, the study of iron is fundamental in geophysics and in terms of thermodynamic modeling.

^{57}Fe is the most common Mössbauer isotope, and its lattice dynamics have been greatly studied. The phase transition of magnetic α-Fe, body-centered cubic structure, to nonmagnetic ε-Fe, hexagonal close-packed structure, (see figure 1) occurs around 13 GPa [1]. We recently conducted experiments at the APS on beamline 16-IDD to determine how doping Fe samples with Pt and Al affects the Fe α-ε transition. As iron is the most abundant element within Earth's core, understanding how doping changes its transition is especially important in geophysics and in terms of thermodynamic modeling.

Phonon Density of States of Iron Solid Solutions at Ambient and High Pressures using Nuclear Inelastic X-ray Scattering (NRIXS)

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Background

^{57}Fe is the most common Mössbauer isotope, and its lattice dynamics have been greatly studied. The phase transition of magnetic α-Fe, body-centered cubic structure, to nonmagnetic ε-Fe, hexagonal close-packed structure, (see figure 1) occurs around 13 GPa [1]. We recently conducted experiments at the APS on beamline 16-IDD to determine how doping Fe samples with Pt and Al affects the Fe α-ε transition. As iron is the most abundant element within Earth's core, understanding how doping changes its transition is especially important in geophysics and in terms of thermodynamic modeling.

Figure 1: BCC structure of α-Fe and HCP structure of ε-Fe [2]

NRIXS

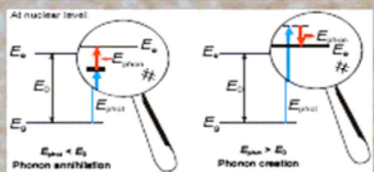


Figure 2 [3]: ^{57}Fe has a nuclear resonant energy of 14.413 keV [1]. When not at this energy, a phonon must either be created or annihilated to emit a photon and excite the nucleus.

Experimental Procedures

The NRIXS experiments were performed at ambient and high pressures using a Paderborn-type diamond anvil cell (DAC), figure 4. $Fe_{0.9}Pt_{0.1}$ was loaded into the cell with a rhenium gasket [4], figure 5, along with several rubies to measure the pressure and a methanol ethanol 4:1 liquid pressure transmitting medium. Solid solutions of $Fe_{1-x}Al_x$ 4.3%, 6.4%, and 27.1% were placed between two pieces of tape for ambient pressure measurements.

- Beamline: 16-ID-D
- High Resolution Monochromator: 4 bounce nested (Diamond (111))
- Focusing: K-B mirror (35x 25μm)
- Data Collection: 2 APD's
- Energy Range Scanned: ± 80meV in steps of 0.25meV
- Pressures Tested: 0, 11, 16, 21, 30 GPa

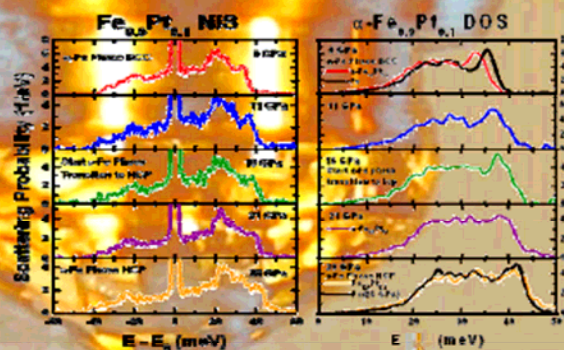
Figure 3: APDs

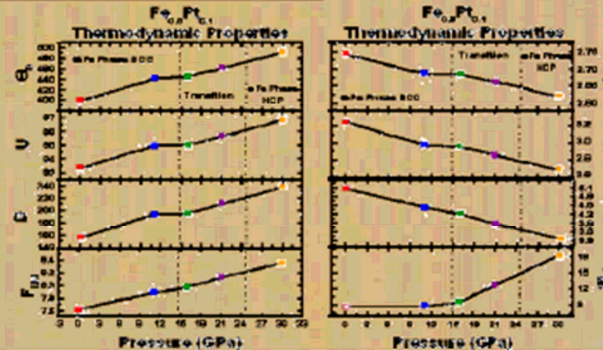
Figure 4: DAC

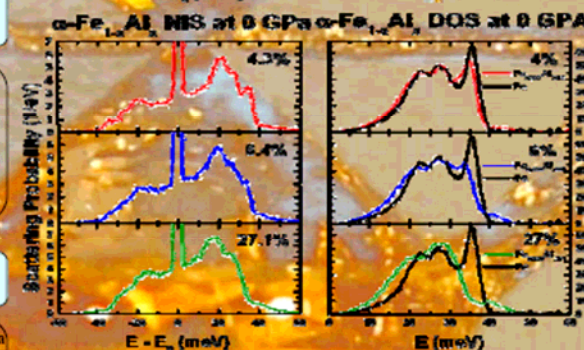
Figure 5: rhenium gasket

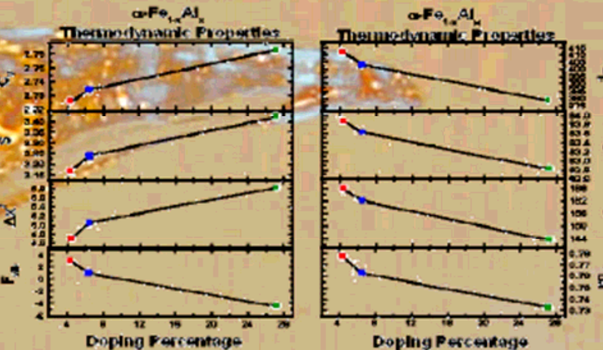
Figure 6: EDM

Data









Debye Temp. (Θ_D), Internal Energy (U), Force Constant (D), Lamb-Mössbauer Factor (F_{LM}), Specific Heat (C_V), Entropy (S), Mean Square Disp. (Δx^2), Helmholtz Free Energy (F_{vib}).

**Connecting line meant only to guide the eye.

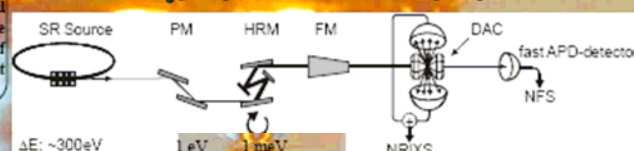
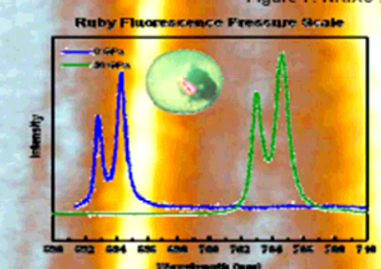


Figure 7: NRIXS setup [5]



$$P(GPa) = \frac{19.04}{B}\left[\left(\frac{\lambda(nm)}{\lambda_o(nm)}\right)^B - 1\right]$$

B = 7.665 (quasi hydrostatic) [6]

Figure 8: blue laser (401 nm)

References

[1] R. Lübbers et al., Science (287), 1250, 2000.

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Acknowledgements

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