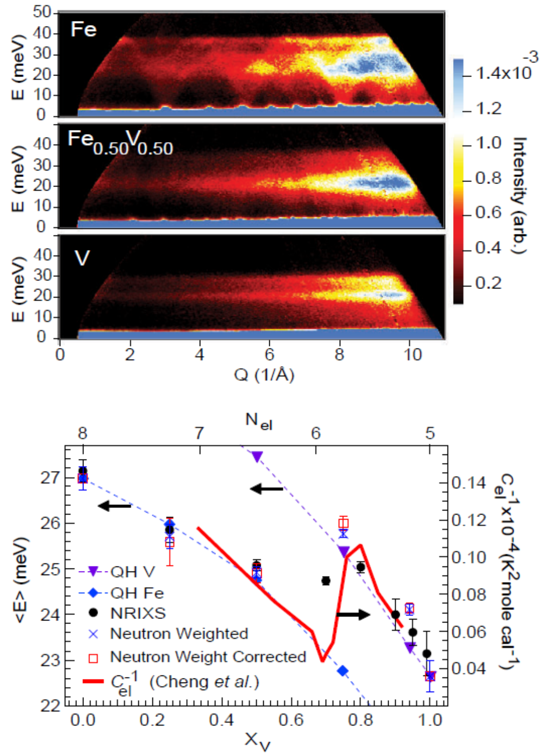
ARCS shows effect of ferromagnetism on phonons in FeV alloys

Researchers at ORNL, in collaboration with the California Institute of Technology, have investigated the properties of phonons in iron-vanadium, FeV, alloys. This effort was done to explore the effects of magnetism on phonons, and to determine the role of vibrational entropy on magnetic phase transitions. FeV alloys are technologically important in the processing of steel and are candidate materials for use in fusion reactors

Inelastic neutron scattering experiments on the Wide Angular-Range Chopper Spectrometer (ARCS, BL-18), carried out at the Spallation Neutron Source (SNS) at ORNL, were combined with isotope selective inelastic nuclear resonant x-ray scattering (NRIXS) measurements at the Advanced Photon Source (APS) at the Argonne National Laboratory. The NRIXS measurements were used to correct for the neutron weighting caused by the different thermal neutron scattering efficiencies of Fe and V.

Both the ARCS results and the NRIXS results showed a change in the average phonon energies as a function of composition across the ferromagnetic transition. The quasiharmonic (QH) model accurately captured the effects of changes in lattice volume with alloying for the Fe-rich ferromagnetic phase and the V-rich nonmagnetic phase.

At low temperatures the enthalpic term dominates the Gibbs free energy $G=H-TS$, where H is the enthalpy, T the temperature, and S the entropy. The energy versus volume curves for different magnetic states calculated from first principles showed that, for pure Fe, the ferromagnetic phase minimizes the energy. However, at moderate temperatures entropic effects begin to dominate. The figure at right shows that phonons in the ferromagnetic phase have lower average phonon energies than those in the nonmagnetic phase for Fe-V alloys. The vibrational entropy is larger for lower average phonon energies. At moderate temperatures the ferromagnetic phase is stabilized with respect to the nonmagnetic phase by the vibrational entropy, which is approximately 0.3 k_B/atom. In contrast, the electronic entropy destabilizes the ferromagnetic phase by 0.1–0.2 k_B/atom, as the number of states at the Fermi level is greatly reduced by spin polarization. The change in the average phonon energies across the magnetic transition follows the inverse of the electronic contribution to the low temperature heat capacity, indicating that increased electronic screening lowers the average forces in the ferromagnetic alloys.



Top: Phonon spectra for FeV alloys acquired on ARCS (beamline 18, SNS). The figure shows the coherent scattering of phonons in Fe, and the incoherent scattering of phonons in V. Bottom: Average energy of phonons on left hand side versus composition. The right hand side shows the inverse of the electronic coefficient of the low temperature heat capacity. There is a decrease in the number of electronic states at Xv=0.8 that is concomitant with the increase in the average energy of phonons.

The paper was recently published in *Physical Review B.*

"Effects of composition, temperature, and magnetism on phonons in bcc Fe-V alloys," M. S. Lucas, J. A. Munoz, O. Delaire, N. D. Markovskiy, M. B. Stone, D. L. Abernathy, I. Halevy, L. Mauger, J. B. Keith, M. L. Winterrose, Y. Xiao, M. Lerche, and B. Fultz, *Physical Review B* **82**, 144306, October 22, 2010. http://prb.aps.org/abstract/PRB/v82/i14/e144306

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