

**Local Atomic
Environments
Studied By
Neutron Scattering**

J. L. Robertson

**Workshop on
“Single-Crystal Diffuse Scattering
at Pulsed Neutron Sources”**

June 16-17, 2003

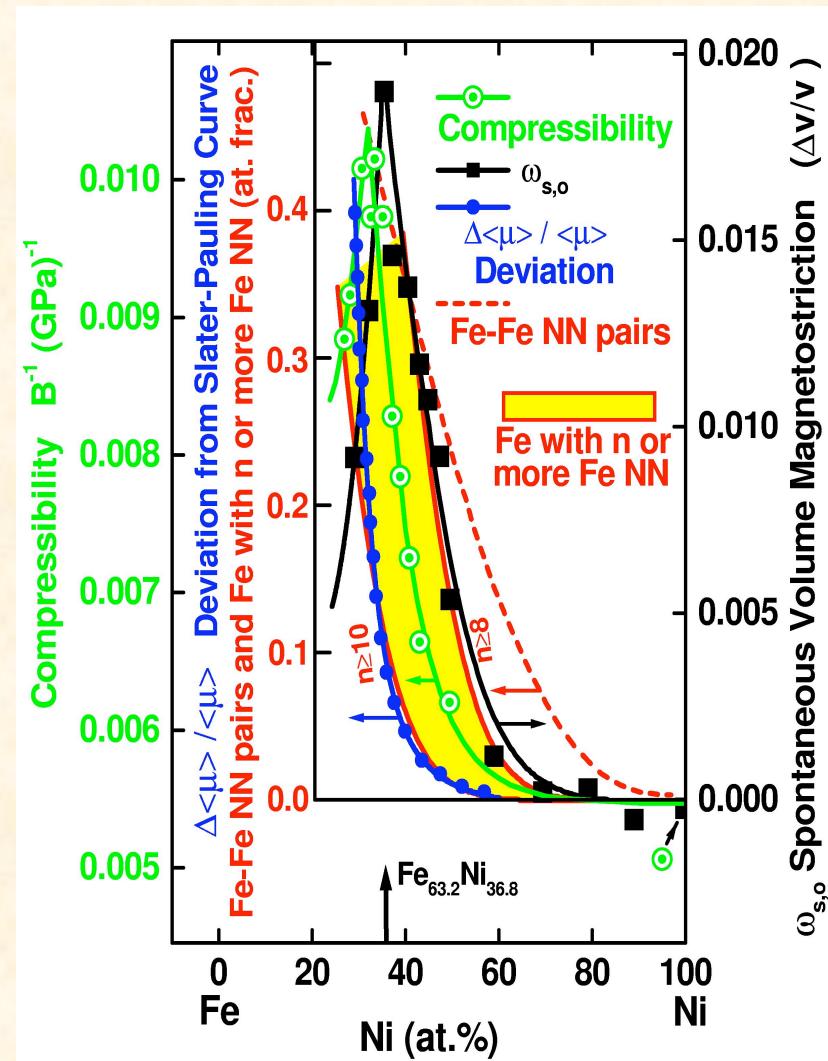
INVAR: Fe_{63.2}Ni_{36.8}

J. L. Robertson, C. J. Sparks and G. E. Ice, ORNL

What is an INVAR Alloy?

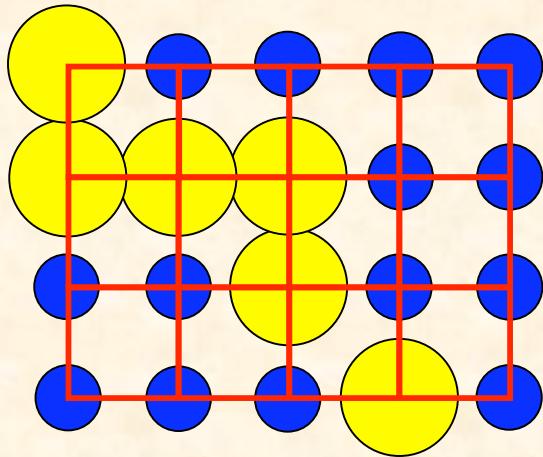
Magnetic alloys that exhibit:

- ◆ small coefficient of thermal expansion
- ◆ unusual variations of the magnetization, electrical resistivity, heat capacity, and elastic moduli with respect to composition, temperature, pressure and applied magnetic field
- ◆ strong correlation observed between the characteristic magnetic properties and lattice parameter (volume/atom) with concentration (i.e. number of Fe-Fe nearest neighbor pairs).



Diffuse Scattering from a Binary Alloy

$$I_{\text{Total}}(Q) = I_{\text{Bragg}}(Q) + I_{\text{SRO}}(Q) + I_{\text{1SD}}(Q) + I_{\text{Huang}}(Q) + I(Q)_{\text{HOT}} + I_{\text{TDS}}(Q)$$

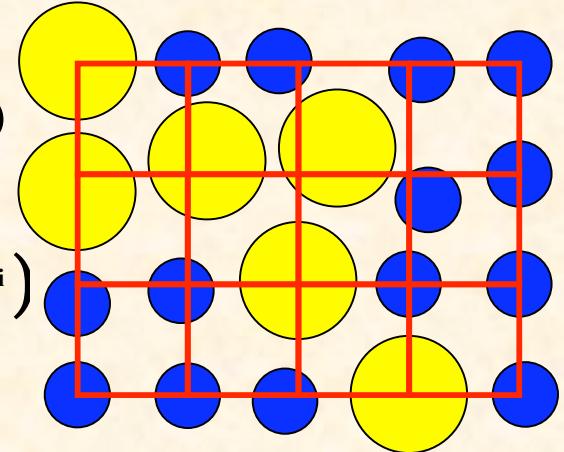


$$I_{\text{SRO}}(Q) = c_{\text{Fe}} c_{\text{Ni}} |f_{\text{Fe}} - f_{\text{Ni}}|^2 e^{-2M_0} \sum_{lmn} \cos 2\pi (q_x l + q_y m + q_z n)$$

$$\alpha_{lmn} = 1 - \frac{P_{lmn}^{\text{FeNi}}}{c_{\text{Ni}}} = 1 - \frac{P_{lmn}^{\text{NiFe}}}{c_{\text{Fe}}}$$

$$I_{\text{1SD}}(Q) = c_{\text{Fe}} c_{\text{Ni}} |f_{\text{Fe}} - f_{\text{Ni}}|^2 e^{-2M_0} \sum_{lmn} \tilde{a}_{lmn} \sin 2\pi (q_x l + q_y m + q_z n)$$

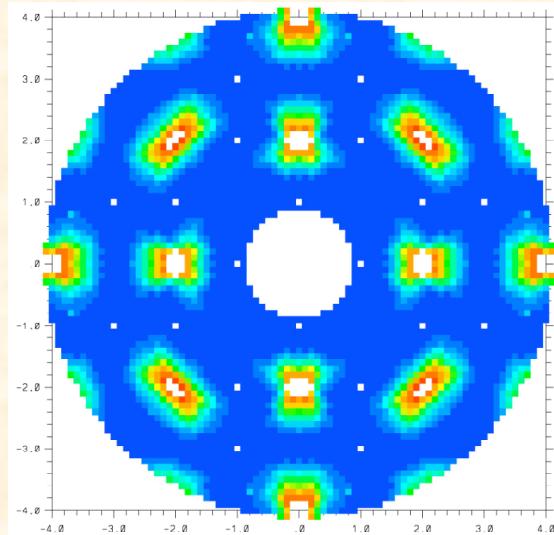
$$\tilde{a}_{lmn} = \frac{f_{\text{Fe}}}{f_{\text{Fe}} - f_{\text{Ni}}} \left[\frac{c_{\text{Fe}}}{c_{\text{Ni}}} + \alpha_{lmn} \left(Q \cdot \ddot{A}_{lmn}^{\text{FeFe}} \right) \right] \frac{f_{\text{Ni}}}{f_{\text{Fe}} - f_{\text{Ni}}} \left[\frac{c_{\text{Ni}}}{c_{\text{Fe}}} + \alpha_{lmn} \left(Q \cdot \ddot{A}_{lmn}^{\text{NiNi}} \right) \right]$$



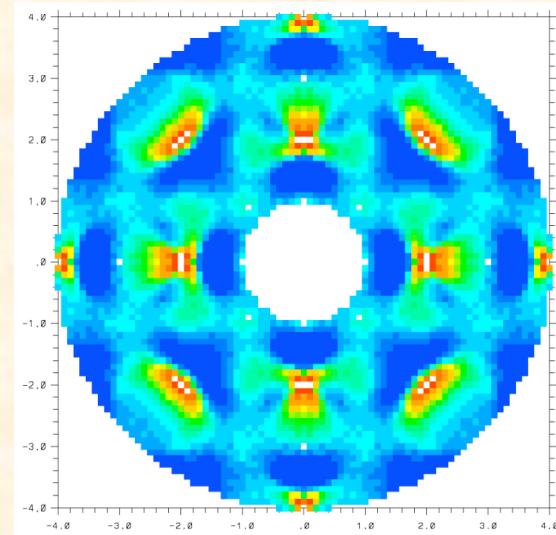
Diffuse X-ray Scattering

110 Plane : T=60K

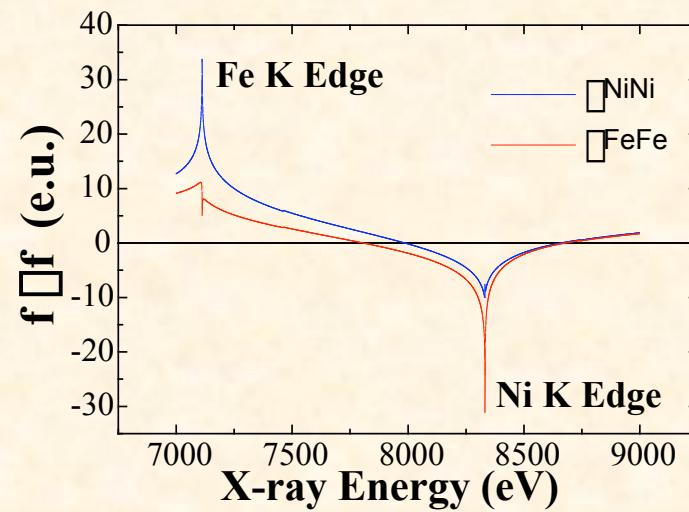
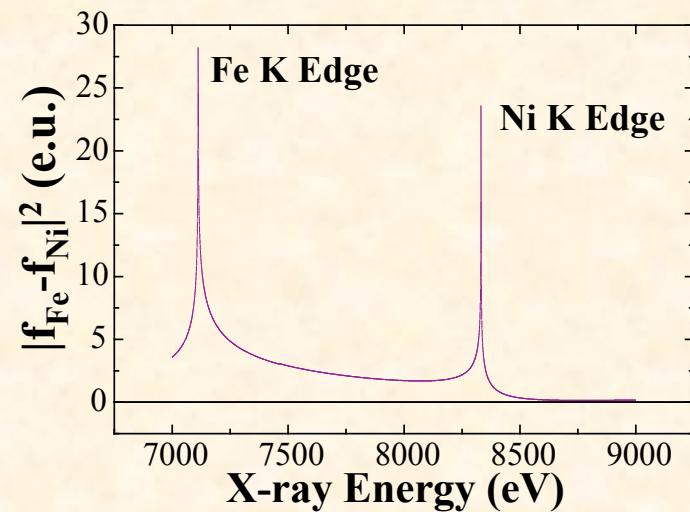
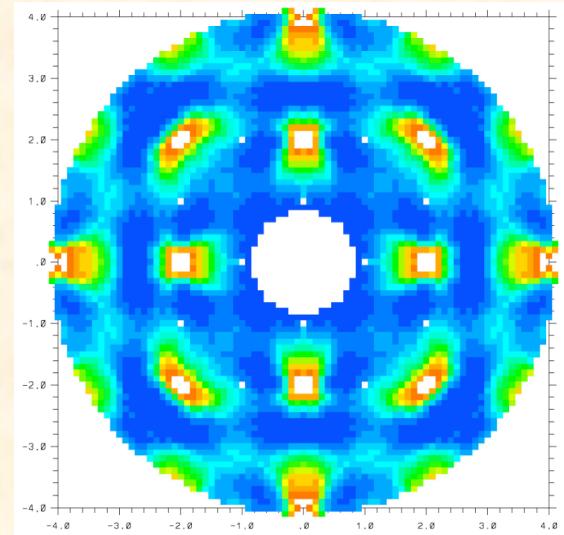
Minimum Contrast 8725eV



Fe K Edge 7092eV

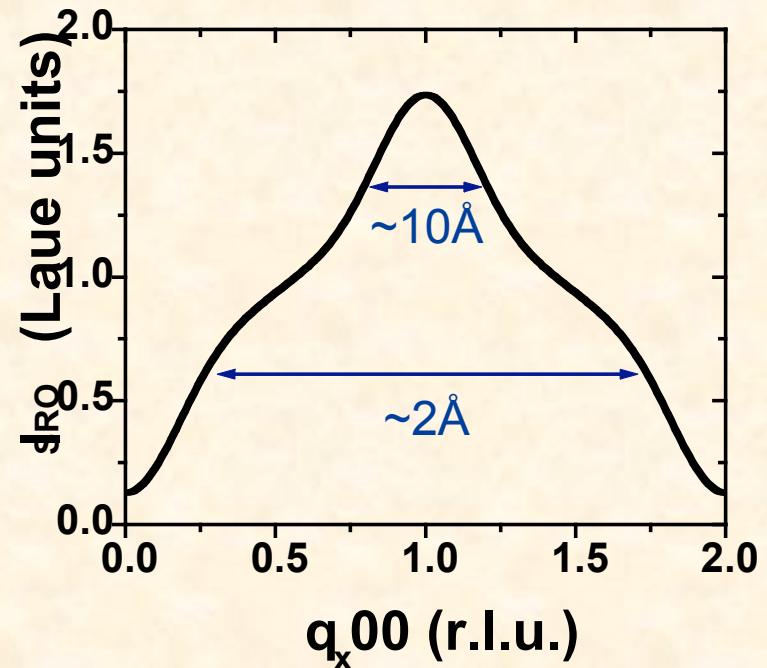
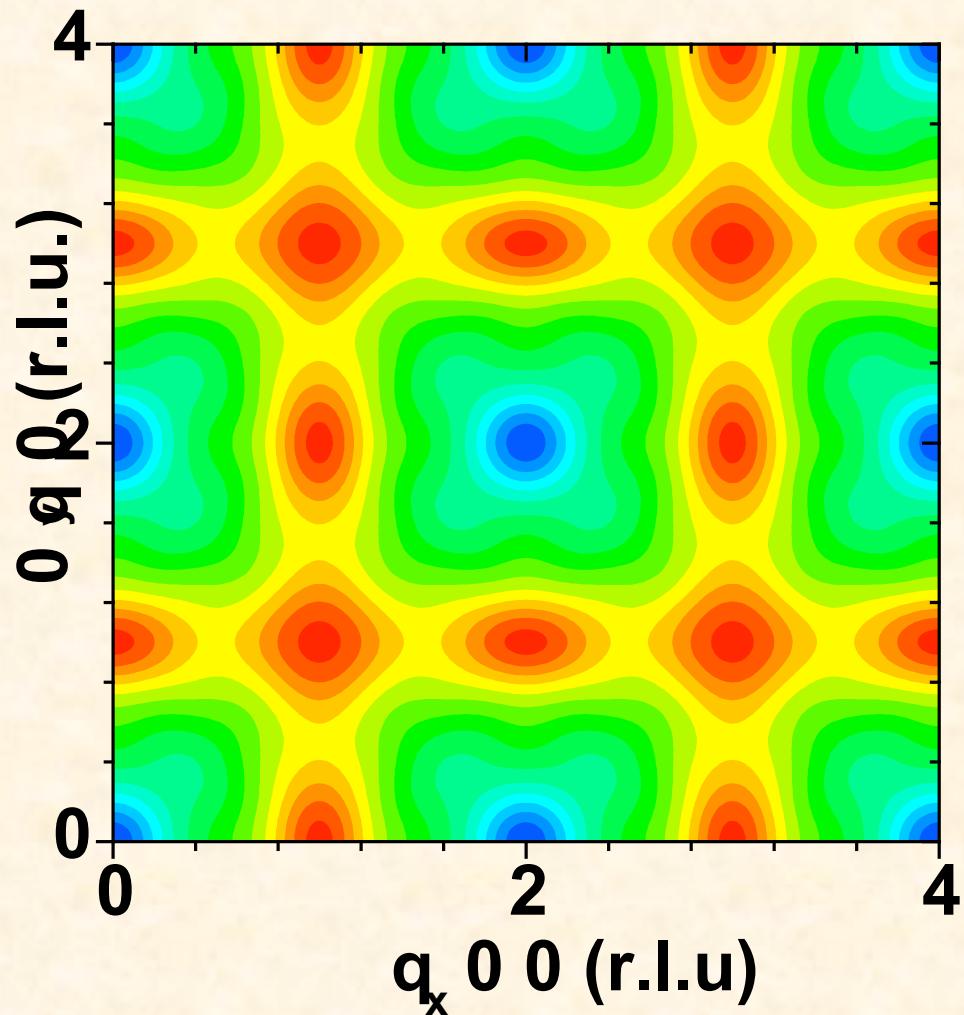


Ni K Edge 8313eV



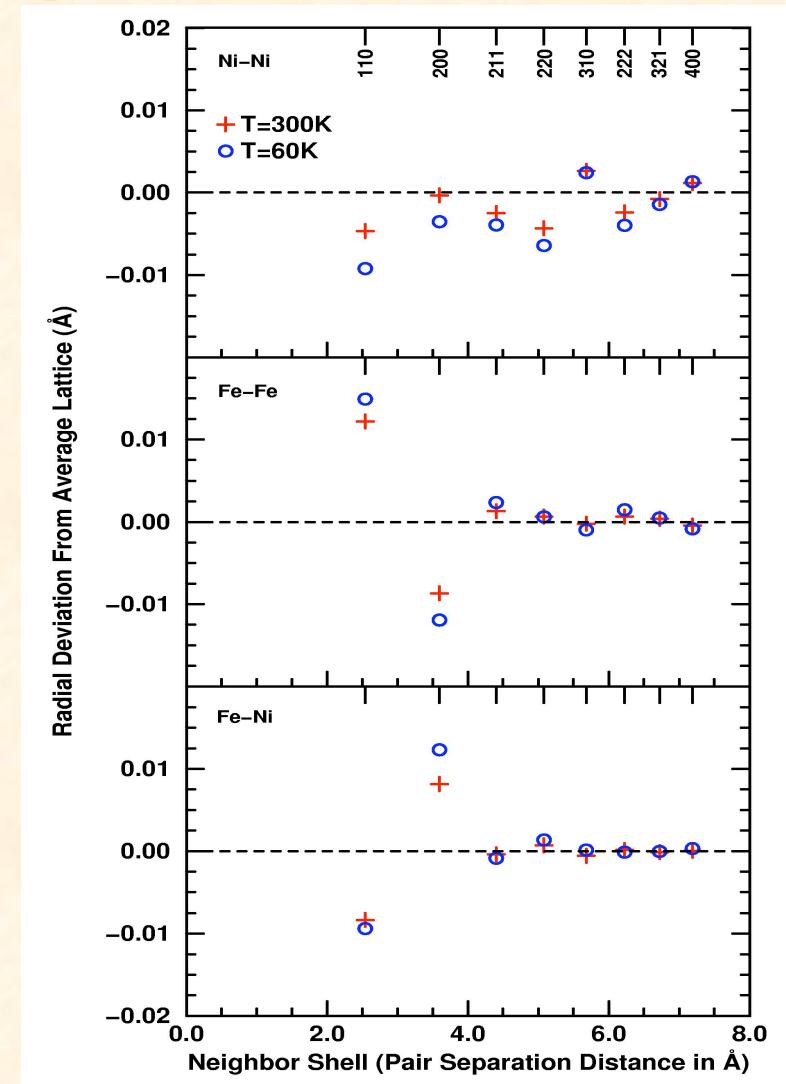
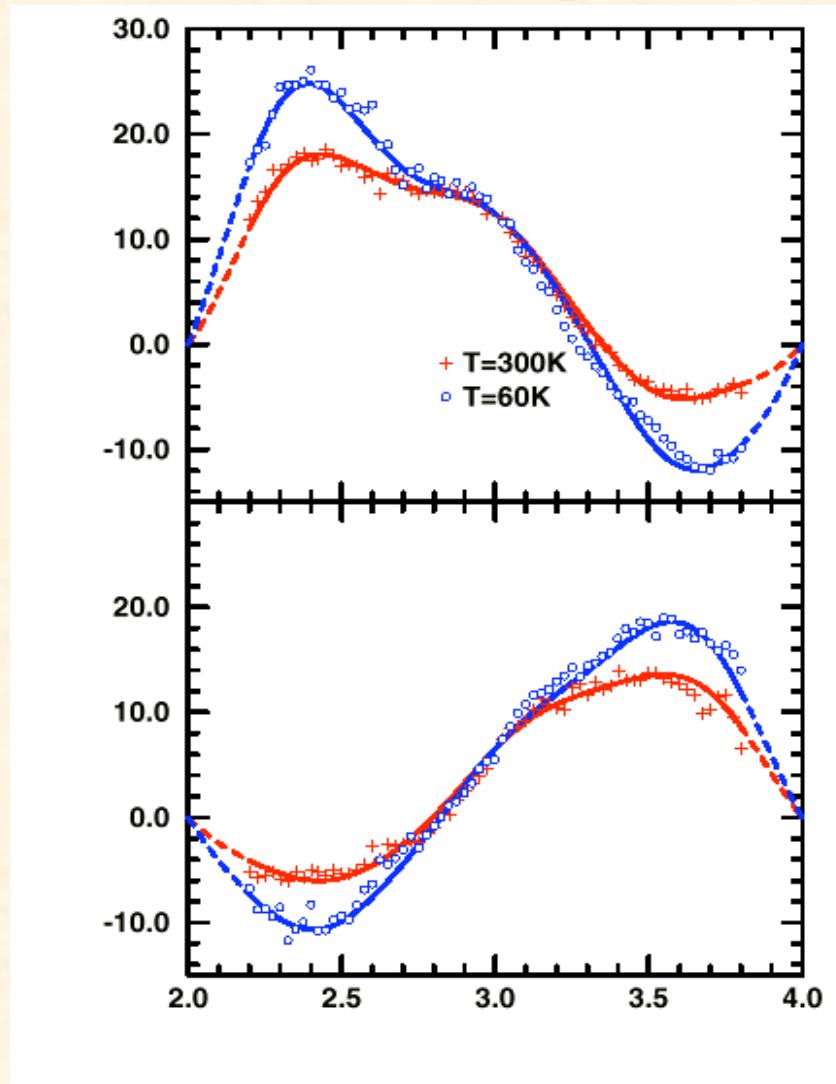
Chemical Short-Range Order

Tendency to Form $\langle 100 \rangle$ Platelets



First Order (Mean) Static Displacements

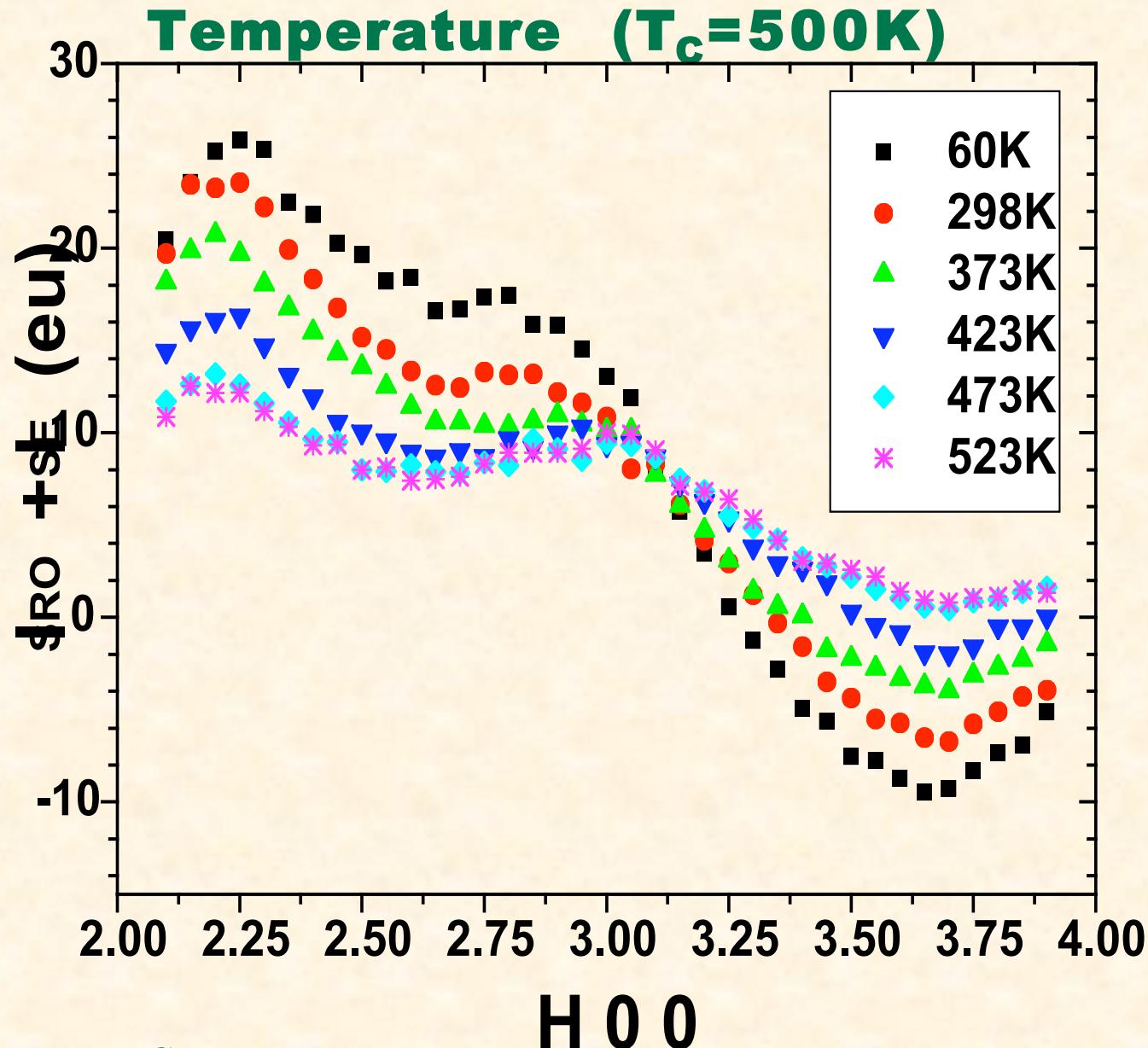
Temperature Dependence



What does this have to do with INVAR?

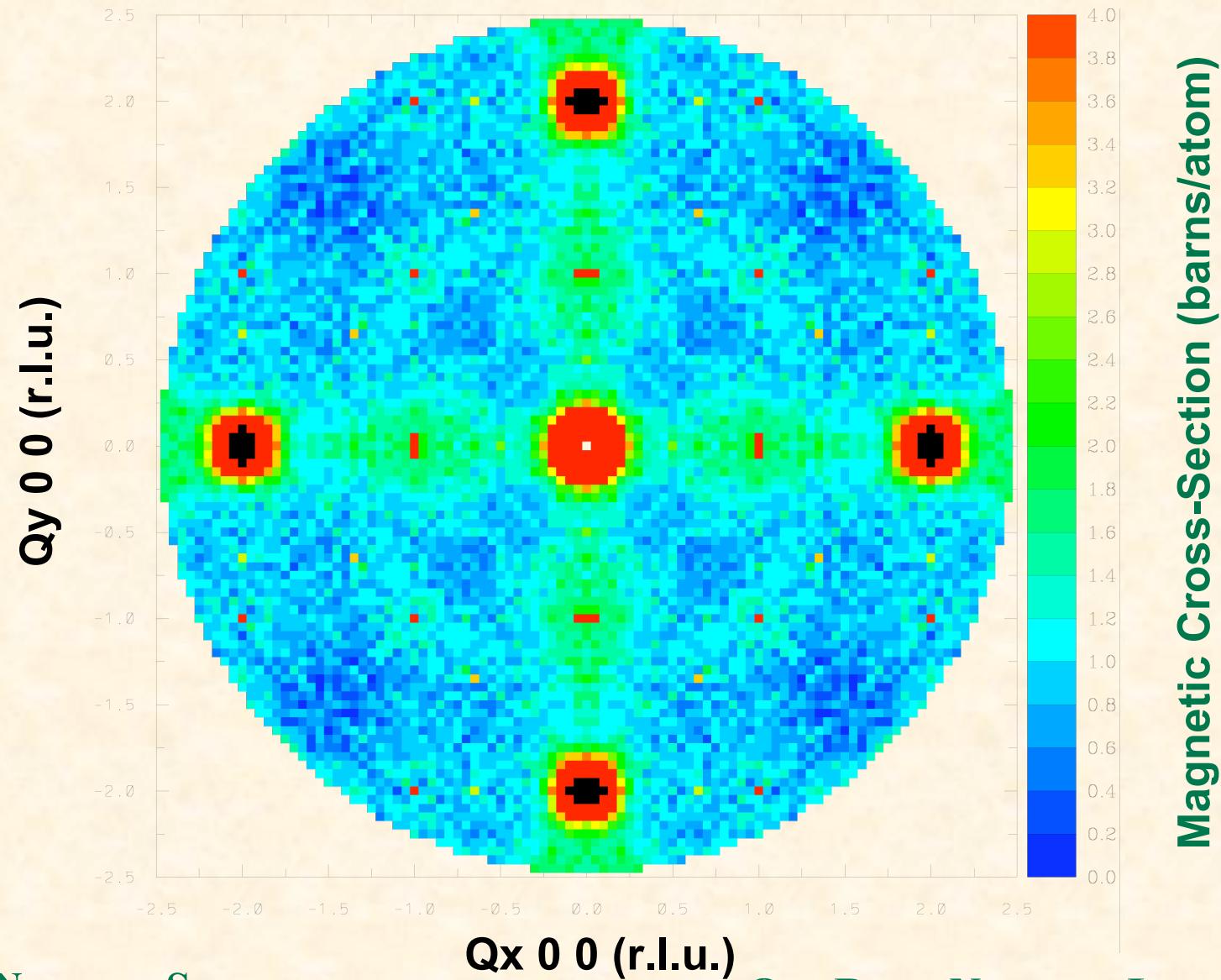
- ◆ The large Fe-Fe nearest neighbor spacing is associated with short-ranged ferromagnetic order in the alloy.
- ◆ The increase in the Fe-Fe nearest neighbor distance with decreasing temperature arises from both an increase in the local ferromagnetic alignment and an increase in the magnitude of the magnetic moments on the Fe atoms.
- ◆ The resulting increase in the volume occupied by the Fe atoms with decreasing temperature opposes the usual thermal contraction of the lattice giving rise to the anomalously small coefficient of thermal expansion.
- ◆ These results support the Large Moment / Large Volume explanation of the INVAR effect.

Magnetic Component of the Static Displacements Vanishes near the Curie Temperature ($T_c=500\text{K}$)



Magnetic Diffuse Neutron Scattering

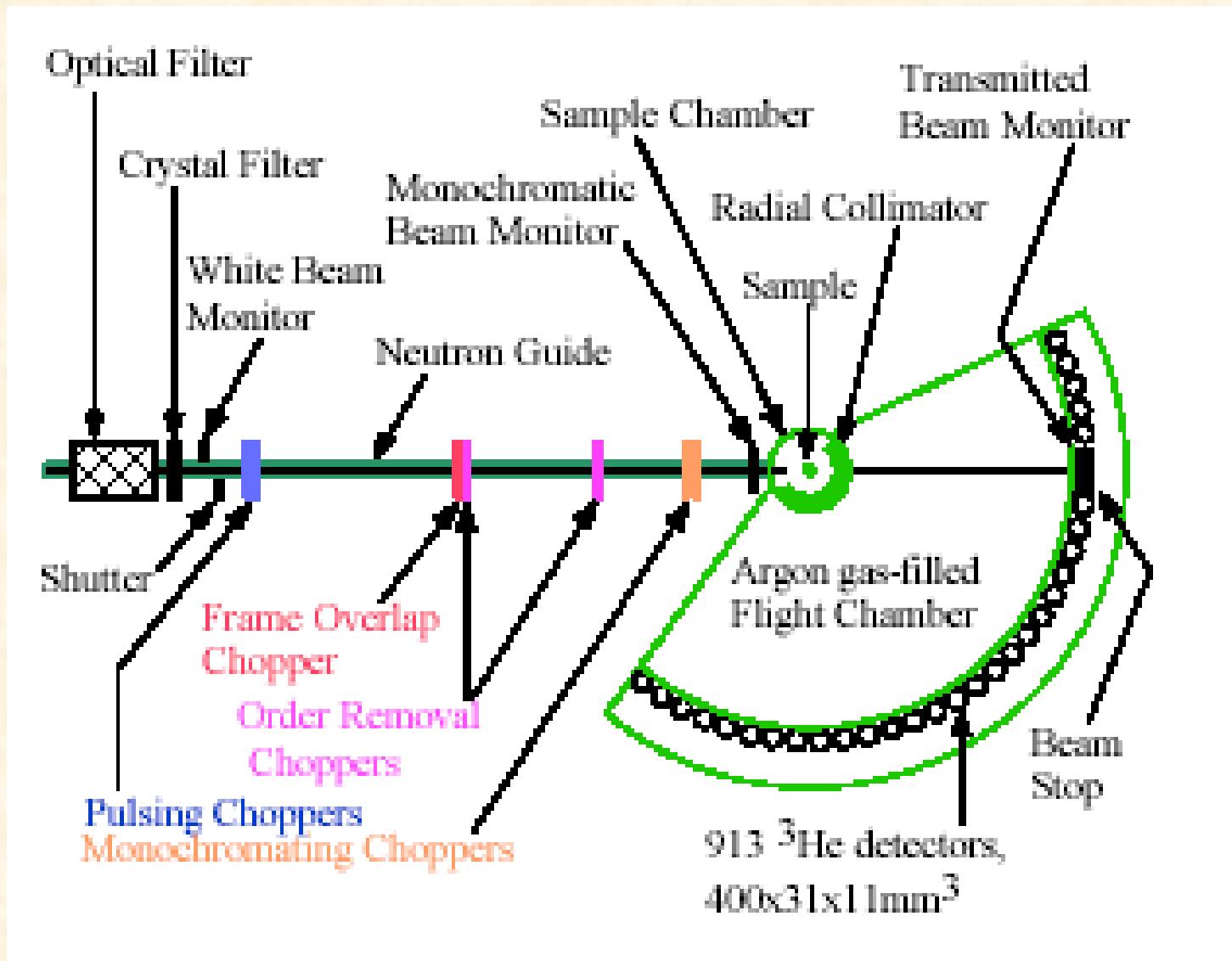
FeNi INVAR T=300K



CENTER FOR NEUTRON SCATTERING

OAK RIDGE NATIONAL LABORATORY

NIST Disk Chopper Spectrometer (DCS)



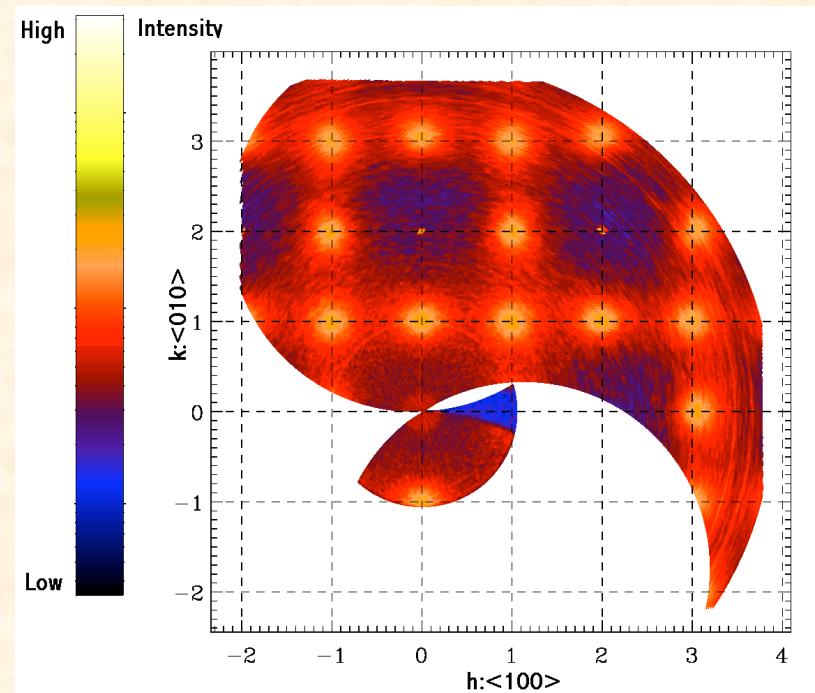
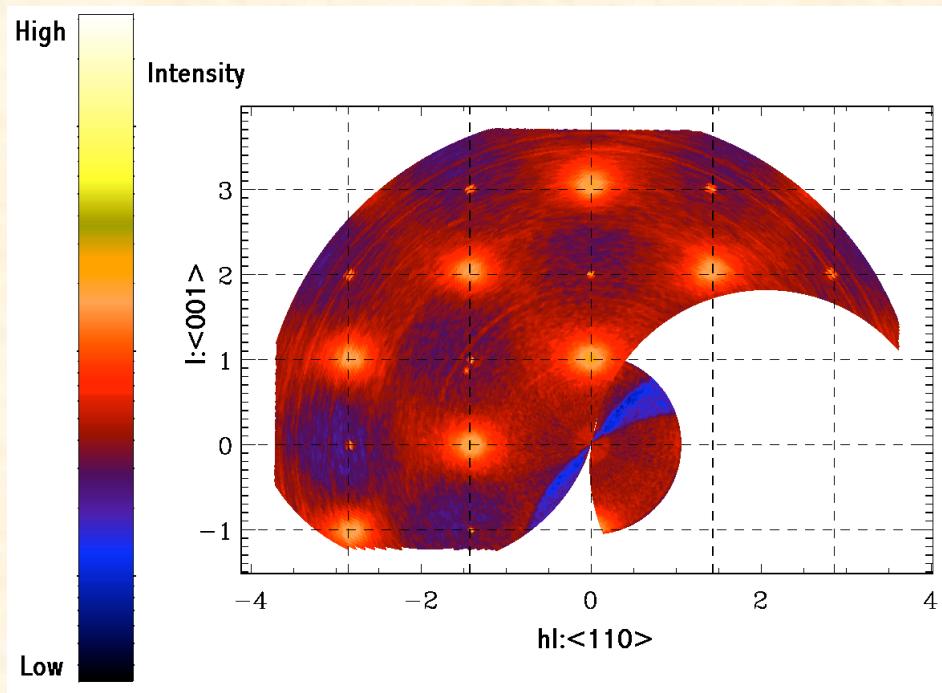
Neutron Scattering Studies of Short-Range Order and Atomic Displacements in a Null-Matrix $^{62}\text{Ni}_{0.52}\text{Pt}_{0.48}$ Single Crystal

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J. L. Robertson, ORNL

J.R.D. Copley and D. A. Neumann, NIST

J. Major, H. Reichert and H. Dosch, MPI für Metallforschung-Stuttgart



Neutron Diffuse Scattering Study of a $\text{Si}_{0.93}\text{Ge}_{0.07}$ Single Crystal

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