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Local Distortions in MgCNi₃ Superconductor

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Beamline(s): X11B

Results: The local atomic structure of MgCNi₃ [1] has been determined over the temperature range of 3 to 300 K by Ni *K*-edge x-ray absorption fine structure measurements [2]. No anomalies were observed near $T_c \sim 7$ K. However the Ni-Mg and to a larger extent the Ni-Ni pair distributions are surprisingly broad over the entire temperature range. The correlations between these atomic pairs do not follow a simple harmonic model. Below $T^* \sim 70$ K the local structure is distorted from the perfect cubic *Pm-3m* crystalline structure determined by conventional neutron diffraction measurements. The symmetry of the Ni₆ octahedra is lowered to tetragonal, orthorhombic or possibly monoclinic space group. We suggest that the onset of local distortions could be closely related with the removal of the degeneracy in the electronic states dominated by Ni *d* bands. The results are discussed in relation to NMR, Raman scattering, and x-ray photoemission measurements as well as to the superconductivity.

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References:

[1] T. He *et al.*, *Nature* **411**, 51 (2001).

[2] A. Ignatov *et al.*, submitted to *Phys. Rev. B* (2002).

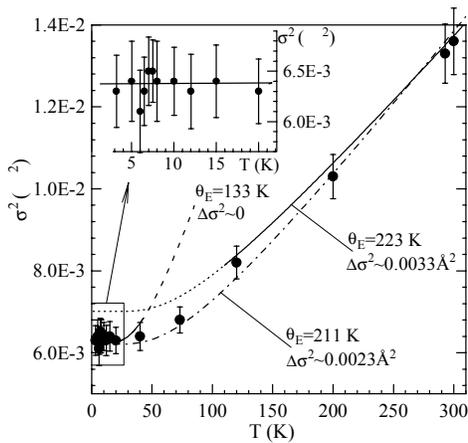


Fig. 1. DW factor of the Ni-Ni bond vs. T .

Model-1: Softening of vibration modes but preserving perfect *Pm-3m*;
 Model-2: Randomly distributed disorder (dotted-dashed line in Fig. 1);
 Model-3: Lowering of the symmetry with Ni motion in the $W(r)$ potential.

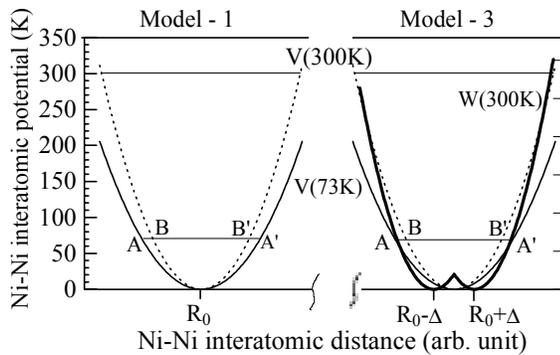


Fig. 2. Two possible sources of dynamic low- T broadening of the Ni-Ni PDF: $|AA'| > |BB'|$.