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**Local Lattice Instability in MgCNi<sub>3</sub> Superconductor Determined by Ni K-edge EXAFS and *ab-initio* Linear Response LDA.**

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**Results:** We have reported on Ni *K*-edge x-ray absorption fine structure measurements of newly discovered MgCNi<sub>3</sub> superconductor [1]. Band structure calculations indicate that Ni *d* electronic states are degenerate about many points of high symmetry in cubic BZ. The degeneracy could be lifted through *local* lowering of the symmetry from the cubic *Pm-3m*. No anomalies were observed near  $T_c \sim 7$  K. However, the Ni-Ni pair distributions are surprisingly broad for metallic compounds. Below  $T^* \sim 70$  K the local structure is distorted from the perfect cubic *Pm-3m* crystalline structure determined by conventional diffraction measurements. The symmetry of the Ni<sub>6</sub> octahedra is lowered to tetragonal, orthorhombic or possibly monoclinic. Remarkable correlation between temperature dependence of anharmonic broadening estimated from EXAFS and temperature dependence of nuclear relaxation rate deduced from NMR experiment supports the picture of nickel-reside local charge/spin density waves (LCDWs/LSDWs) removing the degeneracy of electronic states in MgCNi<sub>3</sub>.

To gain a deeper insight to the origin of the unusually large broadening of the Ni-Ni PDF we performed *ab-initio* calculations of phonon dispersion curves, phonon density of states and electron-phonon coupling strength of MgCNi<sub>3</sub> superconductor by using a full potential all-electron linear-response approach based on the LMTO method in the local density approximation. The GGA-96 approximation was used for the exchange-correlation potential. Assuming the *Pm-3m* structure numerous negative phonon frequencies were obtained, implying that the perfect structure is unstable. Frozen-mode calculations are under way.

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**References:** [1] A.Yu. Ignatov, L.M. Dieng, T.A. Tyson, T. He, and R.J. Cava, "Observation of a low symmetry crystal structure for superconducting MgCNi<sub>3</sub> by Ni *K*- Edge x-ray absorption measurements", (Submitted to Phys. Rev. B).

[2] A.Yu. Ignatov, T.A. Tyson, and S.Yu. Savrasov. " Lattice dynamic of MgCNi<sub>3</sub> determined by linear-response LDA " (unpublished).