Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-principles investigation of deviations from Matthiessen's rule due to the interplay of phonon and spin disorder scattering in iron and gadolinium JAMES GLASBRENNER, KIRILL BELASHCHENKO, University of Nebraska - Lincoln — Magnetic materials contain an anomalous contribution to the electrical resistivity due to thermal spin fluctuations, which saturates in the disordered phase and is called the spin-disorder resistivity (SDR). Experimental determination of the SDR involves fitting to high-temperature resistivity data and extrapolating to T=0 K. Recent calculations of the SDR of the heavy rare-earth metals revealed strong underestimations of this quantity, particularly for Gd, while the results for transition metals were in good agreement with experiments. In order to understand this discrepancy, here we evaluate the mutual effects of phonon and spin-disorder scattering in Fe and Gd. Calculations are performed using the supercell approach within the linear muffin-tin orbital method. The atomic positions are displaced according to the Gaussian distribution, and the resistivity is evaluated as a function of the mean-square displacement $\Delta^2 \propto T$. The deviations from Matthiessen's rule (DMR) are large in Gd and moderate in Fe. Fitting the linear region of ρ vs Δ^2 in Gd yields an intercept ~ 2.5 times larger than the "bare" SDR, significantly improving the agreement with experiment. Large DMR suggest large variations of the relaxation time on the anisotropic Fermi surface.

James Glasbrenner
University of Nebraska - Lincoln

Date submitted: 09 Nov 2012 Electronic form version 1.4