Effect of magnetic short-range order on spin disorder resistivity.
ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska, USA, MARK VAN SCHILFGAARDE, Department of Chemical and Materials Engineering, Arizona State University, Tempe, Arizona, USA, JULIAN VELEV, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska, USA — Spin-disorder resistivity (SDR) of Fe and Ni is studied using the noncollinear density functional theory. The Landauer conductance is averaged over random disorder configurations and fitted to Ohm’s law. In the fully disordered state, SDR for Fe is close to the experiment, while for fcc Ni it exceeds the experimental value by a factor of 2.3. This indicates either strong magnetic short-range order (MSRO) or reduced local moment above $T_C$ for Ni. The temperature dependence of SDR for Fe was studied using the mean-field approximation and the Monte Carlo method applied to the classical nearest-neighbor Heisenberg model. Both methods give the same magnetization dependence of SDR that is in excellent agreement with the results for the isotropic s-d model. Further using the Reverse Monte Carlo method we generated disordered spin structures with strong MSRO. We found that resulting SDR is not significantly different than for Monte Carlo and mean-field methods. This result indicates that for Fe MSRO is not very important for SDR.