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Calculations of spin-disorder resistivity from first principles[1]
ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, JULIAN VELEV, Department of Physics and Astronomy, University of Nebraska Lincoln, MARK VAN SCHILFGAARDE, Department of Chemical and Materials Engineering, Arizona State University — Spin-disorder resistivity of Fe and Ni is studied using the non-collinear density functional theory. The Landauer conductance is averaged over random disorder configurations and fitted to Ohm's law. The distribution function is approximated by the mean-field theory. The dependence of spin-disorder resistivity on magnetization in Fe is found to be in excellent agreement with the results for the isotropic s-d model. In the fully disordered state, spin-disorder resistivity for Fe is close to experiment, while for fcc Ni it exceeds the experimental value by a factor of 2.3. This result indicates strong magnetic short-range order in Ni at the Curie temperature. We suggest that the analysis of calculated and measured spin-disorder resistivity provides a powerful method to extract information on the temperature dependence of the magnetic short-range order parameter in ferromagnetic metals.

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Aleksander Wysocki
Department of Physics and Astronomy, University of Nebraska Lincoln

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