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Spin-disorder resistivity of heavy rare-earth metals from Gd to Tm: An ab-initio study JAMES GLASBRENNER, KIRILL BELASHCHENKO, University of Nebraska - Lincoln — Electrical resistivity of heavy rare-earth metals has a dominant contribution from thermal spin disorder scattering. In the paramagnetic state, this spin-disorder resistivity (SDR) decreases through the Gd-Tm series. Models based on the assumption of fully localized 4f states treated as S or J multiplets predict that SDR is proportional to S^2 (S is the 4f shell spin) times a quantum correction (S+1)/S or (J+1)/J. The interpretation of this correction using experimental results is ambiguous. Since the 4f bandwidth is not small compared to the multiplet splitting, it is not clear whether the 4f shells in rare-earth metals behave as if they were fully localized and have a good quantum number S or J. To address this issue, in this work we calculate the paramagnetic SDR of the rare-earth metal Gd-Tm series using a non-collinear implementation of the tight-binding linear muffin-tin orbital method. The conductance is found using the Landauer-Büttiker approach applied to the active region of a varying size, averaging the conductance over random spin-disorder configurations and fitting its size dependence to Ohm's law. The results are compared with experiment and discussed. The sensitivity to basis set and the treatment of the 4f electrons, as well as the role of exchange enhancement in the conduction band is considered. The issue of the quantum correction is examined in light of the new results.

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