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First-principles Study Of The Residual Resistivity Of Single-Phase Ni-based Concentered Solid Solution and High Entropy Alloys

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Recent discoveries demonstrate that the remarkable electronic, magnetic, mechanical and radiation resistance properties of a novel class of multicomponent concentrated solid solution alloys (of which 5 or more component High Entropy Alloys are exemplars) can be tuned through control of the degree of chemical complexity – number and types of alloying elements. Residual resistivity (ρ_0) provides a direct measurement for the effect of chemical disorder on the Fermi surface. Here we use *ab-initio* KKR-CPA method to access the electronic structure and estimate ρ_0 from Kubo-Greenwood formula in a series of 2-5 component equiatomic alloys comprised of Ni and various combinations of other mid *3d*-transion metal elements. In agreement with experiment, for alloys without Cr or Mn elements, low residual resistivity is observed due to weak disorder scattering in one spin channel. On the contrary, Mn/Cr elements greatly raise ρ_0 due to smeared Fermi surface in both spin channels, resulted from the antiparallel spins on Cr/Mn. While chemically induced magnetic disorder is the dominant scattering mechanism, we present additional results that clarify the role of local lattice distortions and magnetic non-collinearity neglected in standard KKR-CPA based transport calculations. The effect from variation of the size of the local moment is also investigated.

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