Residual resistivity and its anisotropy in random CoNi and CuNi ferromagnetic alloys

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Abstract. Residual resistivities of random CoNi and CuNi ferromagnetic alloys are calculated by a recently developed \textit{ab initio} technique based on the linear muffin-tin orbital (LMTO) method with perturbative inclusion of spin-orbit interaction. The obtained results compare well with those of existing fully relativistic techniques. Particular attention has been paid to the isotropic resistivity and the spontaneous magnetoresistance anisotropy; a high value of the resistance anisotropy is predicted for Ni-rich CoNi alloys.

1. Introduction
Recent development in magnetoelectronics and spintronics has stimulated intensive research activity in the theory of transport properties of bulk ferromagnetic alloys in presence of relativistic effects, especially the spin-orbit (SO) interaction [1–5]. The investigated galvanomagnetic phenomena can be classified according to their relation to the conductivity tensor $\sigma_{\mu\nu}$, where $\mu, \nu \in \{x, y, z\}$. For cubic alloys with magnetization pointing along $z$-direction, this tensor has three independent matrix elements, namely, $\sigma_{xx} = \sigma_{yy}$, $\sigma_{zz}$, and $\sigma_{xy} = -\sigma_{yx}$ [3]; the resistivity tensor $\rho_{\mu\nu}$ has a similar structure [1]. The non-diagonal elements give rise to the anomalous Hall effect; they have so far been studied mostly for model systems [3]. The diagonal elements, responsible for the isotropic resistivity $\rho = \frac{1}{3}(\rho_{xx} + \rho_{yy} + \rho_{zz})$ and the spontaneous magnetoresistance anisotropy $\Delta \rho = \rho_{zz} - \rho_{xx}$, have been studied for a number of random binary alloys on an \textit{ab initio} level [1, 2, 4, 5].

The latter studies were based on the Kubo-Greenwood formula evaluated using the Korringa-Kohn-Rostoker (KKR) method [6] and the fully relativistic Dirac (FRD) theory [7]; the alloy disorder was treated in the coherent potential approximation (CPA). Surprisingly, the effect of the SO interaction on the isotropic residual resistivity proved to be quite pronounced even for alloys of $3d$ elements, where the weak SO interaction leads to a failure of the well-known two-current model especially in systems with strongly spin-dependent disorder [2].

In this contribution, we investigate the residual resistivities of random face-centered cubic (fcc) CoNi and CuNi alloys as calculated by the tight-binding (TB) linear muffin-tin orbital (LMTO) method [8]. The weak SO interaction is treated as a simple perturbation of the TB-LMTO Hamiltonian in the scalar-relativistic approximation (SRA) [9, 10], while the diagonal elements of the conductivity tensor are formulated similarly to our previous transport studies within the SRA and the TB-LMTO-CPA [11, 12].
2. Theory and computational details

The TB-LMTO Hamiltonian including the SO interaction can be represented in an orthonormal LMTO-SRA basis by a matrix \[ H = C + \xi + \sqrt{\Delta} S^0 \left( 1 - \gamma S^0 \right)^{-1} \sqrt{\Delta}. \] (1)

The basis is labelled by a composed \( RLs \)-index, where \( R \) is the site index, \( L \equiv (\ell, m) \) is the orbital index, and \( s = \uparrow, \downarrow \) is the spin index. The \( C, \Delta, \) and \( \gamma \) in (1) denote \( RLs \)-diagonal matrices of the LMTO-SRA potential parameters, and the \( S^0 \) denotes the canonical LMTO structure-constant matrix [8]. The SO interaction is described by a site-diagonal matrix \( \xi \) in (1) with elements given explicitly by \( \xi_{RLs,RLs'} = \delta_{RR'} \delta_{\ell\ell'} \xi_{LLs's'} \langle Ls \mid \mathbf{L} \cdot \mathbf{S} \mid L's' \rangle \), where the \( \xi_{RLs's'} \) denote atomic-like SO parameters [9, 10].

The diagonal elements of the conductivity tensor at zero temperature based on the Hamiltonian (1) can be given a form identical to that obtained in the SRA [11], namely,

\[ \sigma_{\mu\mu} = -\frac{e^2}{\pi \hbar V_0 N} \text{Tr} \left( 3g^a(E_F) [X_{\mu}, S^a] 3g^a(E_F) [X_{\mu}, S^a] \right), \] (2)

where \( V_0 \) is the volume of the primitive cell, \( N \) is the number of cells in a finite crystal with periodic boundary conditions, and \( \langle \ldots \rangle \) denotes the configuration averaging. The superscript \( \alpha \) refers to the screened TB-LMTO representation, \( 3g^a(E_F) = [g^a(E_F + i0) - g^a(E_F - i0)]/(2i) \) denotes the anti-Hermitian part of an auxiliary Green’s function at the Fermi energy \( E_F \), \( S^a \) is the screened structure-constant matrix, \( [A, B] = AB - BA \) denotes a commutator, and \( X_{\mu} \) is a coordinate operator [10, 11]. The latter operator has been represented by a diagonal matrix \( (X_{\mu})_{RLs,RLs'} = \delta_{RR'} \delta_{\ell\ell'} \delta_{ss'} X^\mu_R \), where \( X^\mu_R \) denotes the \( \mu \)-th component of the vector \( \mathbf{R} \) [11].

The averaging in (2) including the CPA vertex corrections has been described elsewhere [11–13].

Selfconsistent electronic structures were obtained by employing the LMTO valence basis comprising \( s-, p- \) and \( d- \)type orbitals, both in the SRA [8] and with inclusion of the SO interaction (SRA+SO) [10]. Particular attention was paid to convergence of the conductivities (2) with respect to the number \( N \) of \( k \) vectors sampling the whole fcc Brillouin zone: \( N = 1.7 \times 10^9 \) and \( N = 1.7 \times 10^8 \) were necessary for the CoNi and CuNi alloys, respectively.
3. Results

3.1. CoNi alloy

The CoNi alloys are characterized by a very strong spin dependence of the alloy disorder, as documented in figure 1 for the Co$_{0.55}$Ni$_{0.45}$ alloy treated in the SRA: the majority spin channel exhibits negligible disorder, whereas sizeable disorder is found in the minority spin channel, in particular for energies close to the alloy Fermi level. As a consequence, the majority spin conductivity in the SRA (two-current model) is two orders of magnitude bigger than the minority one and the total resistivity is given essentially by the weak majority spin scattering [2]. However, the SO interaction affects the isotropic resistivity $\rho$ dramatically, especially for Ni-rich systems, leading to its enhancement by one order of magnitude, see figure 2(a). For alloy compositions around Co$_{0.25}$Ni$_{0.75}$, the resistivity anisotropy $\Delta\rho/\rho$ exceeds 50% of $\rho$, see figure 2(b).

3.2. CuNi alloy

The CuNi alloy exhibits a phase transition from a ferromagnetic state to a paramagnetic state at Cu content slightly above 50%. This transition is manifested by a sharp maximum on the calculated concentration dependence of the isotropic resistivity $\rho$, see figure 3(a). In the ferromagnetic state, the majority spin conductivity in the SRA exceeds its minority counterpart by one order of magnitude, especially for Ni-rich alloys. However, inclusion of the SO interaction does not change the isotropic resistivity $\rho$ appreciably throughout the whole concentration interval, see figure 3(a). The calculated values of $\rho$ are smaller than the measured ones, probably due to clustering effects in prepared alloy samples [4]. The resistivity anisotropy ratio $\Delta\rho/\rho$ amounts to about 10% at the Ni-rich end and it decreases with increasing Cu content until it vanishes in the paramagnetic state, see figure 3(b).
4. Conclusions
The developed TB-LMTO approach to residual resistivities of random 3d alloys leads to results in reasonable agreement with those of existing fully relativistic KKR techniques. The high predicted spontaneous magnetoresistance anisotropy of the random Co$_{0.25}$Ni$_{0.75}$ alloy calls for experimental verification; however, sensitivity of theoretical results with respect to neglected off-diagonal elements of the conductivity tensor has to be checked as well.

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