Properties of Complex Inorganic Solids

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INVESTIGATION OF GALVANO-MAGNETIC PROPERTIES OF TRANSITION METAL ALLOY SYSTEMS USING THE KUBO-GREENWOOD EQUATION

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INTRODUCTION

The galvano-magnetic effects, i.e. the spontaneous magnetoresistance anisotropy (SMA) and the anomalous Hall resistivity (AHR) observed in spontaneously magnetized materials are used since decades in sensor technology [1]. Although it has been pointed out more than 40 years ago that these effects are caused by spin-orbit coupling, i.e. are of intrinsic origin and not due to an external magnetic field [2], a thorough theoretical description for them could be given only very recently by Banhart and Ebert [3]. Since then detailed theoretical investigations of the residual ($T = 0$ K) resistivity properties of disordered Fe_xNi_{1-x} [3], Co_xPd_{1-x} and Co_xPt_{1-x} [4] alloys have been performed. The theoretical approach of Banhart and Ebert is based on the Kubo-Greenwood-formalism with the underlying electronic structure described within the Dirac-formalism for magnetic solids. This ensures that the sources of galvano-magnetic effects – spin-orbit coupling and magnetization – are accounted for on the same level. As will be shown, additional insight into the mechanism giving rise to the SMA and AHR can be obtained by model calculations for which relativistic effects are manipulated. Furthermore it is demonstrated that performing scalar and fully relativistic calculations in parallel, it is possible to check the two-current model [2, 5, 6] that has been used so far to deal with the galvano-magnetic effects in magnetic solids.

THEORETICAL FRAMEWORK

Application of the Coherent Potential Approximation (CPA) alloy theory in connec-

tion with the multiple scattering or Korringa-Kohn-Rostoker (KKR) method of band structure calculation allows for a very accurate determination of the single-particle Green function at the Fermi energy E_F, $G^+(E_F)$, and that way also of the conductivity tensor σ via the Kubo-Greenwood equation [7]:

$$\sigma_{\mu\nu} = \frac{\hbar}{\pi V_{\text{cryst}}} \text{Tr} \left\langle j_\mu \, \text{Im}G^+(E_F) \, j_\nu \, \text{Im}G^+(E_F) \right\rangle_{\text{conf.}} \tag{1}$$

Here j_μ is the μ-th spatial component of the electronic current operator $\boldsymbol{j}$ and $\langle \ldots \rangle_{\text{conf.}}$ denotes the atomic configuration average for a disordered alloy.

Adopting the spin-polarized relativistic (SPR) version of the KKR-CPA method, the sources of the galvano-magnetic effects are properly included in the description of the underlying electronic structure. Furthermore, this approach accounts for the reduction in symmetry that is caused by the simultaneous occurrence of spin magnetism and spin-orbit coupling and is reflected by the form of the σ tensor. For example, for cubic systems with the magnetization along the z-axis, σ is - in contrast to the paramagnetic case - no more diagonal with identical elements, but has the form:

$$\rho = \sigma^{-1} = \begin{pmatrix} \rho_\perp & -\rho_H & 0 \\ \rho_H & \rho_\perp & 0 \\ 0 & 0 & \rho_\parallel \end{pmatrix} . \tag{2}$$

Here $\rho_\parallel$ and $\rho_\perp$ are the transverse and longitudinal resistivities with respect to the magnetization direction, respectively. The off-diagonal element ρ_H represents the spontaneous or anomalous Hall resistivity (AHR) [3]. Conventionally, the anisotropy of the resistivity is expressed by the SMA ratio

$$\frac{\Delta\rho}{\bar{\rho}} = \frac{\rho_\parallel - \rho_\perp}{\bar{\rho}} \tag{3}$$

where $\bar{\rho} = \frac{1}{3}(2\rho_\perp + \rho_\parallel)$ is the isotropic resistivity.

Campbell et al. [5] proposed the very simple expression

$$\frac{\Delta\rho}{\bar{\rho}} = \gamma \left(\frac{\rho^\downarrow}{\rho^\uparrow} - 1 \right) \tag{4}$$

for the SMA ratio that has extensively been used in the past for the interpretation of experimental data. This expression relies on the two-current model that assumes the existence of partial resistivities $\rho^{\downarrow(\uparrow)}$ for both spin subsystems with $1/\bar{\rho} = 1/\rho^\uparrow + 1/\rho^\downarrow$. Furthermore, spin-orbit coupling is represented by the phenomenological parameter γ, that is meant to describe the coupling of both spin subsystems.

RESULTS AND DISCUSSION

To investigate the connection between $\Delta\rho/\bar{\rho}$ and ρ_H and the various relativistic effects two types of model calculations were performed: i) the speed of light c and that way all relativistic effects have been varied artificially, ii) the strength of the spin-orbit coupling has been manipulated separately [8].

Results for the SMA $\Delta\rho$ of permalloy $Fe_{0.2}Ni_{0.8}$ as a function of the scaling parameters $(c_0/c)^2$ (c_0 the proper speed of light) and ξ, scaling the spin-orbit coupling strength, are shown in Fig. 1. First of all one notes that the fully relativistic calculations with $(c_0/c)^2 = 1$ or $\xi = 1$, are in very satisfying agreement with experiment.

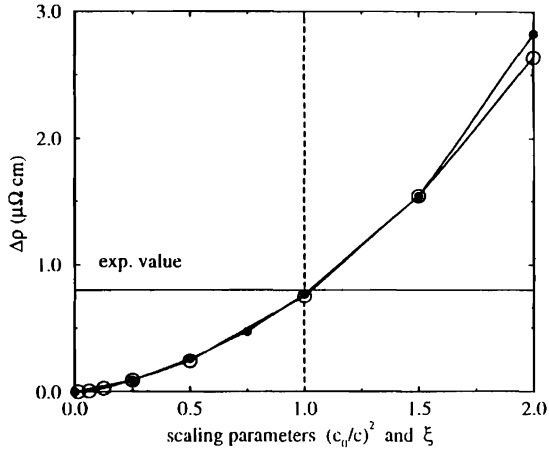

Figure 1: Spontaneous magnetoresistance anisotropy $\Delta\rho$ of $Fe_{0.2}Ni_{0.8}$ as a function of the scaling parameters $(c_0/c)^2$ (o) and ξ (•). The experimental value is that from to Jaoul et al. [9].

As expected, $\Delta\rho$ vanishes if the strength of the spin-orbit coupling is reduced to 0 by reducing $(c_0/c)^2$ or ξ, respectively. Both sets of model calculations give nearly the same results indicating that the so-called scalar relativistic effects due to the mass-velocity and Darwin-term, are of minor importance for the absolute value of $\Delta\rho$.

Very similar results are found for the Hall resistivity ρ_{H} (not shown here). Again, the fully relativistic value is in rather good agreement with experiment. Varying the strength of the spin-orbit coupling, ρ_{H} varies nearly quadratically with $(c_0/c)^2$ or ξ, respectively, in the range from 0 to 1. However, for higher values, i.e. in the super-relativistic region, both theoretical data sets deviate stronger than in the case of $\Delta\rho$. This means that scalar relativistic effects may have quite an appreciable influence on the absolute value of ρ_{H}.

As could be demonstrated by both types of model calculations spin-orbit coupling may also have a very strong impact on the isotropic resistivity $\bar{\rho}$ of a magnetic solid. For example, for $Fe_{0.2}Ni_{0.8}$ it was found that $\bar{\rho}$ decreases by a factor of 3 when the spin-orbit coupling is suppressed. This finding is obviously not compatible with the simple two-current model. Because the influence of the spin-orbit coupling is the more pronounced the higher the spin-polarization at the Fermi energy is, the use of the two-current model can be justified only for systems with a rather low spin-polarization at the Fermi energy. While for Fe_xNi_{1-x} this condition is far from being met, the use of the two-current model can be justified to some extent for the alloy systems Co_xPd_{1-x} and Co_xPt_{1-x} as it is demonstrated by Fig. 2.

For both alloy systems the theoretical results for ρ obtained in a fully relativistic are found in very satisfying agreement with the corresponding experimental data. In addition to these calculations a second set of calculations has been done making use of the two-current model. This means the partial resistivities $\rho^{\downarrow(\uparrow)}$ have been calculated by performing scalar relativistic calculations for every spin subsystem separately. As can be seen, the resulting total isotropic resistivity $\bar{\rho}$ is reasonably close to the fully relativistic result. Furthermore, one notes that the relative deviation of both sets of theoretical data is more pronounced for Co_xPd_{1-x} than for Co_xPt_{1-x}. This has to be

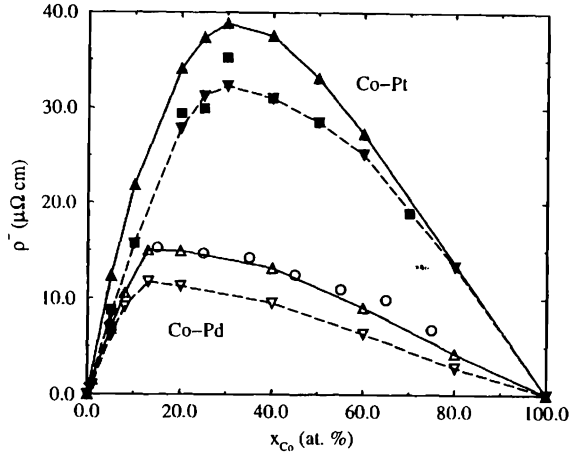

Figure 2: Residual isotropic resistivity $\bar{\rho}$ of disordered Co_xPd_{1-x} (open symbols) and Co_xPt_{1-x} (full symbols) alloys. Theoretical results obtained in a fully relativistic way and using the two-current model are given by up and down-pointing triangles, respectively. All other symbols represent experimental data taken from various sources [13, 14, 15, 16].

expected because of the higher spin-polarization at the Fermi level for Co_xPd_{1-x}.

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