CALCULATION OF SPONTANEOUS RESISTANCE ANISOTROPY OF DISORDERED FERROMAGNETIC ALLOYS

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ABSTRACT

A first-principles theory of the electrical conductivity of disordered ferromagnetic alloys based on the Kubo-Greenwood formalism and the spin-polarised relativistic Korringa-Kohn-Rostoker coherent potential approximation (SPR-KKR-CPA) method is presented. Application to the alloy systems Fe–Ni, Co–Pd and Co–Pt yields results for the anisotropical residual resistivity which are in very satisfying agreement with experiment.

INTRODUCTION

There are a number of interesting phenomena related to impurity scattering in ferromagnetic alloys for which up to now no description from first-principles is available. One of these is the spontaneous magnetoresistance anisotropy (SMA) which occurs in principle in any ferromagnetic alloy and expresses the fact that the spontaneous magnetization reduces the symmetry of a crystalline system and leads to an electrical conductivity which depends on the relative orientation of the current and the magnetic field.

Quantitatively, both effects are expressed by means of the electrical resistivity (conductivity) tensor $\boldsymbol{\rho}$ ($\boldsymbol{\sigma}$) which for cubic systems with the magnetisation along the z-axis has the form[1]:

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

$\rho_\perp$ and $\rho_\parallel$ being the transverse and longitudinal resistivities. ρ_H is the Hall resistivity which shall not be considered in the present paper. The SMA is expressed by the ratio[1]:

$$\frac{\Delta\rho}{\bar{\rho}} = \left. \frac{\rho_\parallel(B) - \rho_\perp(B)}{\bar{\rho}(B)} \right|_{B\to 0} , \tag{2}$$

where $\bar{\rho} = \frac{1}{3}(2\rho_\perp + \rho_\parallel)$. All quantities are determined by extrapolation to a vanishing external magnetic field B.

To a great extent motivated by the technological importance of the SMA, there have been a large number of corresponding experimental investigations during the last four decades. Among the systems studied, Ni- and Co-based alloys received special attention because of the pronounced SMA found for many of them. In particular, the system Fe–Ni shows one of the largest SMA found so far for transition metal systems. The existing experimental SMA data at low temperatures of disordered, polycrystalline Fe–Ni alloys is summarised in Fig. 1.

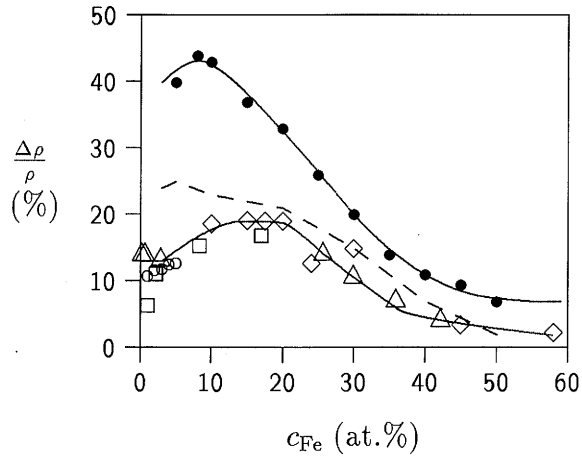

Figure 1: Spontaneous resistance anisotropy of Fe–Ni alloys. Open symbols: experimental values at low temperatures ($\square$[1], $\diamond$[2], $\triangle$[3,4], o[5]). Full circles: calculated values, broken line: calculated values corrected for extra isotropical scattering. Full lines serve as guides for the eye.

For isolated Fe impurities in Ni the residual resistivities $\rho_\perp$ and $\rho_{||}$ vary linearly with concentration (see below) and the SMA ratio $\Delta\rho/\bar{\rho}$ takes a constant value which is about 13%. As the impurities begin to interact for increasing Fe contents, the SMA ratio rises and reaches its maximum value for 10 to 20% iron. For even larger Fe contents the anisotropy rapidly decreases to very low values.

It was first noted by Smit[2] that the physical origin of the SMA is the spin-orbit interaction. Based on this central assumption several authors developed more and more sophisticated models to describe the SMA in the past[2,3]. However, all these approaches end up with the sd-picture of electronic conduction. This also applies to the most recent refinement by Malozemoff [6]. Moreover, all theories on SMA presented so far are based on the two-current model separating the total current into two distinct contributions coming from electrons of different spin orientation. Spin-orbit coupling gives rise to hybridisation of electronic states of different spin character and causes the SMA that way. The aim of the present work was to treat the SMA without assuming any simple electronic structure and without treating the spin-orbit interaction as small perturbation.

THEORY

A straightforward and rigorous access to galvanomagnetic effects is supplied by the Kubo-Greenwood Eq. for the conductivity tensor $\boldsymbol{\sigma}$[7,8]:

$$\sigma_{\mu\nu} = \frac{\hbar}{\pi V_{\text{cryst}}} \text{Tr} \left\langle j_\mu \, \text{Im}G^+(E_\text{F}) \, j_\nu \, \text{Im}G^+(E_\text{F}) \right\rangle_{\text{conf.}} \tag{3}$$

Here $G^+(E_F)$, representing the electronic structure of the system, is the positive side limit of the single-particle Green function at the Fermi energy E_F, 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. By determining G^+ via the Korringa-Kohn-Rostoker method of bandstructure calculation in connection with the coherent-potential approximation (KKR–CPA), Eq. (3) can be evaluated in a most reliable way. The corresponding expressions for $\sigma_{\mu\nu}$ for paramagnetic systems and temperature T=0K have been derived by Butler[8] and have been applied with great success in their original non-relativistic form[9] as well as their corresponding fully relativistic form[10] to calculate the residual resistivity of various alloy systems.

To get access to the SMA in the limit T=0K Butler's approach was generalized by evaluating G^+ using the spin-polarized relativistic version of the KKR-CPA (SPR-KKR-CPA)[11]. This scheme, based on the Dirac-equation for a spin-dependent potential derived from local spin density functional theory, accounts on the same level – without using any parameters – for all relativistic effects as well as for the magnetic state. A natural consequence of this is that the symmetry reduction due to the simultaneous presence of spin-orbit interaction and magnetism – giving rise to the form of $\boldsymbol{\rho}$ in Eq. (1) – is automatically accounted for. Finally, one has to mention that using the SPR-KKR-CPA there is no need to rely on the two-current model anymore.

CALCULATIONS

Fe–Ni

As a first application of the presented approach the alloy system Fe-Ni in the fcc structure was studied. Assuming the magnetisation to point along the z-axis, the electronic structure for various compositions with $x_{Fe} \leq 50\%$ was calculated using the SPR-KKR-CPA with an angular momentum expansion up to $\ell_{\max} = 3$. For each concentration the tensor $\boldsymbol{\sigma}$ and its inverse $\boldsymbol{\rho}$ were determined on the basis of Eq. (3). The resulting longitudinal and transverse resistivities, $\rho_{\parallel}$ and $\rho_\perp$, resp., together with the average resistivity $\bar{\rho}$ are shown in Fig. 2.

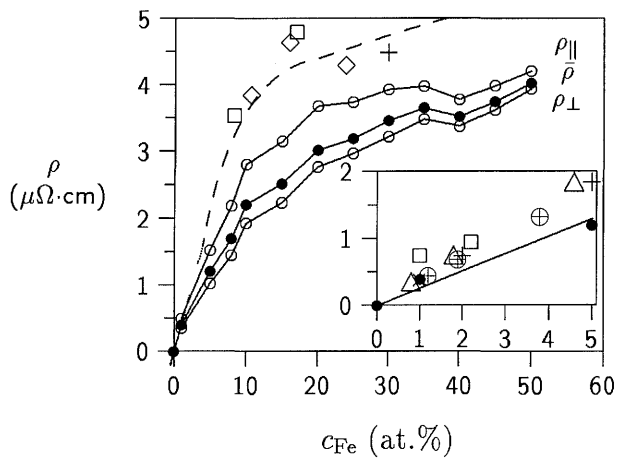

Figure 2: Calculated residual resistivities of Fe–Ni alloys: longitudinal ($\parallel$) and transverse ($\perp$) resistivity, average $\bar{\rho} = \frac{1}{3}(2\rho_\perp + \rho_{\parallel})$. Experimental low temperature resistivities $\bar{\rho}$ by various authors: $\square$[1], $\diamond$[2], $\times$[5], $\triangle$[13], $\oplus$[14], $+$[15]. Solid line connects calculated values. Dashed line is a guide for the experimental resistivities.

Comparison of $\bar{\rho}$ with experimental values reveals that the calculated resistivities are somewhat lower than the measured ones – especially for higher Fe contents. An important reason for the discrepancy might be that the CPA approach accounts only for chemical disorder but not for topological disorder as the source of the resistivity (see also below).

As one sees in Fig. 2, for all compositions we find $\rho_{||} > \rho_{\perp}$ corresponding to a positive anisotropy ratio. This is in full accordance with experimental findings for Fe-Ni. The SMA ratio calculated from $\rho_{\perp}$ and $\rho_{||}$ in Fig. 2 using Eq. (2) is shown in Fig. 1. The most prominent feature is the very pronounced decrease of $\Delta\rho/\bar{\rho}$ from about 40% for Ni-rich alloys to values of about 7% for 50% Fe. There is even slight evidence for a maximum value at 10% Fe. Obviously, this concentration dependence of the calculated SMA ratio is in rather satisfying agreement with experiment. However, the calculated SMA ratios are about twice as high as the measured ones and the maximum is less pronounced in the calculated curve. There are a number of reasons which could be responsible for the calculated SMA ratio to be much larger than found by experiment.

A possible source for the deviation are isotropic contributions to the electrical resistivity which are not included in the calculation and which merely enhance $\bar{\rho}$ but not $\Delta\rho$. That such contributions are present is strongly suggested by the results for $\bar{\rho}$ in Fig. 2. Scattering at grain boundaries, short-range order, clusters etc. could enhance the isotropical resistivity without increasing $\Delta\rho$ because this extra scattering is independent of the magnetisation and adds the same ρ_{extra} to $\rho_{||}$ and to $\rho_{\perp}$ thus not changing $\Delta\rho = \rho_{||} - \rho_{\perp}$. In order to get an idea of how this extra scattering might influence the SMA ratio $\Delta\rho/\bar{\rho}$ was calculated using experimental values for $\bar{\rho}$ instead of the smaller calculated values. The result, shown in Fig. 1 as a dashed line, lies much closer to the experimental curve than the uncorrected calculated values.

Analysis of the matrix element of the current operator in Eq. 3 allows one to investigate the role of spin-flip scattering processes for SMA. Within non-relativistic theory these may not occur because the current operator $j_{\mu} = -i\hbar(e/m)\nabla_{\mu}$ does not couple to the spin degree of freedom. This differs from the relativistic case where j_{μ} is given by $ec\alpha_{\mu}$ with α_{μ} one of the Dirac matrices. This operator can be transformed to a form having as a leading term one that is proportional to the non-relativistic j_{μ} and two additional terms involving α_{μ} and allowing for spin-flip processes[12]. The matrix elements for the ∇_{μ}-related term were found to be at least 100 times larger than for the corresponding two other terms. Thus, spin-flip processes have – at least for 3d-systems – practically no influence on the SMA. This confirms the generally used assumption that spin-orbit interaction causes SMA primarily by hybridisation of states of different spin character.

Co–Pd and Co–Pt

The calculational procedure applied to Fe–Ni was used to determine the spontaneous resistance anisotropy for the two ferromagnetic alloys Co–Pd and Co–Pt. For Co–Pd this calculation was carried out for maximum angular momenta of $\ell_{\text{max}} = 2$ and $\ell_{\text{max}} = 3$ in two different calculations. It was found that the omission of f-states causes a too high resistivity but hardly influences the anisotropy ratio. Fig. 3 shows results for Cu–Pd based on $\ell_{\text{max}} = 3$ (averaged resistivities $\bar{\rho}$ shown). As one can see, the agreement between experimental and calculated resistivities is excellent. No deviation of the magnitude found for Fe–Ni is encountered.

The anisotropy ratios calculated from the transverse and longitudinal resistivities are shown in Fig. 4 for the two alloy systems Co–Pd and Co–Pt. The calculation on the latter system was based on a maximum ℓ of 2. As one sees, the anisotropy is much larger

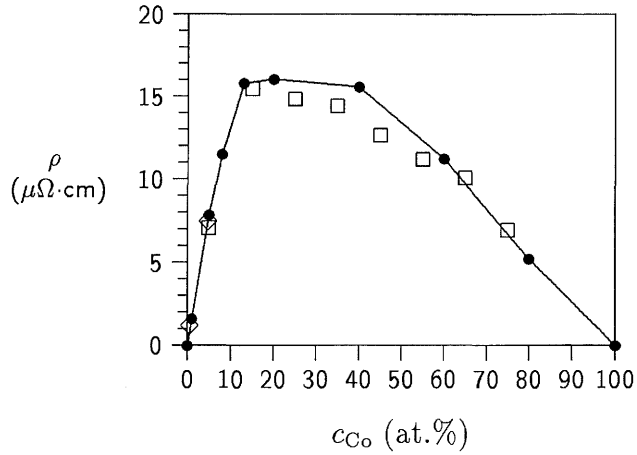

Figure 3: Residual resistivity of disordered Co–Pd alloys. Full circles: calculated, boxes: experimental values[16].

for Co–Pd than for Co–Pt, both for the calculated and for the measured values. The agreement between theory and experiment is again impressive. The good agreement for the resistivities seems to correspond with a good agreement for the anisotropies, thus supporting the supposition of the preceding section that extra isotropical scattering might be responsible for the deviations observed for Fe–Ni.

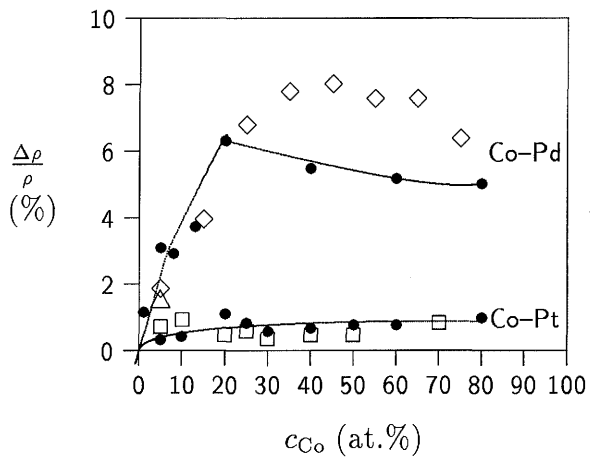

Figure 4: Spontaneous resistance anisotropy of Co-Pd and Co–Pt alloys. Full circles: calculated values, open symbols: experimental values[16,17].

Non-relativistic calculations

The relativistic calculations include all effects of spin-orbit interaction and spin-polarisation and therefore lead to a very satisfactory description of the anisotropy phenomena discussed. In order to show that it is indeed essential to carry out the calculations relativistically, non-relativistic calculations were made for the alloys $Fe_{20}Ni_{80}$, $Co_{20}Pd_{80}$ and $Co_{20}Pt_{80}$. A separate resistivity calculation was carried out for each of the two potentials $V^{\uparrow}$ and $V^{\downarrow}$. For the single spin-channel the alloy was treated as paramagnetic system, but the common Fermi energy of the two spin-bands was used. The result were two resistivities $\rho^{\uparrow}$ and $\rho^{\downarrow}$ for each spin direction. The total non-relativistic resistivity is determined by $(\rho^{nr})^{-1} = (\rho^{\uparrow})^{-1} + (\rho^{\downarrow})^{-1}$ and compared to the result obtained by the relativistic calculation (ρ^{rel}) in table 1.

Table 1: Results of non-relativistic resistivity calculations for various alloys.

Alloy	$\rho^{\uparrow}$	$\rho^{\downarrow}$	$\rho^{\downarrow}/\rho^{\uparrow}$	ρ^{nr}	ρ^{rel}	ρ^{rel}/ρ^{nr}
$Fe_{20}Ni_{80}$	0.8	94	117	0.79	3	3.8
$Co_{20}Pd_{80}$	10.6	71	6.6	9.4	16	1.7
$Co_{20}Pt_{80}$	36	46	1.3	20.4	27	1.3

Two observations are obvious: firstly, the non-relativistic resistivities of the two spin channels can be quite different. The highest ratio $\rho^{\downarrow}/\rho^{\uparrow}$ corresponds to the largest SMA (Fe–Ni), whereas the low ratio for Co–Pt reflects a small SMA. This behaviour is compatible with the models based on the two-current model[3]. Secondly, the relativistic resistivity is much higher that the non-relativistic one for all the alloys. Most of this difference is probably due to spin-orbit effects which this way are shown to be of unexpected importance.

CONCLUSIONS

In conclusion the fully relativistic spin-polarised KKR–CPA in conjunction with the Kubo-Greenwood theory for electrical conduction allowed for the first rigorous and parameter-free calculation of the anisotropical spontaneous resistivity in disordered ferromagnetic alloys. Application to the systems Fe-Ni, Co–Pd and Co–Pt led to a very satisfying agreement with experiment. Comparison with non-relativistic results shows that a relativistic treatment is essential for such systems.

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REFERENCES

1. T.R. McGuire and R.I. Potter, IEEE Trans. Mag. 11:1018 (1975)
2. J. Smit, Physica 16:612 (1951)
3. I.A. Campbell, A. Fert and O. Jaoul, J. Phys. C3:S95 (1970)
4. I.A. Campbell, J. Phys. F4:L181 (1974)
5. J.W.F. Dorleijn, Philips Res. Repts. 31:287 (1976)
6. A.P. Malozemoff, Phys. Rev. B34:1853 (1986)
7. D. A. Greenwood, Proc. Phys. Soc. London, 71:585 (1958)
8. W.H. Butler, Phys. Rev. B31:3260 (1985)
9. J.C. Swihart, W.H. Butler, G.M. Stocks, D.M. Nicholson and R.C. Ward, Phys. Rev. Lett. 57:1181 (1986)
10. J. Banhart, H. Ebert, J. Voitländer and P. Weinberger, Phys. Rev. B50:2104 (1994)
11. H. Ebert, B. Drittler and and H. Akai, J. Magn. Magn. Mater. 104-107:733 (1992)
12. G.-Y. Guo and H. Ebert, Phys. Rev. B50:1037 (1994)
13. T. Farrell and D. Greig, J. Phys. F1:1359 (1968)
14. F.C. Schwerer and J.W. Conroy, J. Phys. F1:877 (1971)
15. M.C. Cadeville and B. Loegel, J. Phys. F3:L115 (1973)
16. S.U. Jen, Phys. Rev. 45:9819 (1992)
17. S.U. Jen, T.P. Chen and B.L. Chao, Phys. Rev. 48:12789 (1993)

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