Ab initio theory of galvanomagnetic phenomena in random and non-random ferromagnets

I. Turek[1,2)]

1) Institute of Physics of Materials, Academy of Sciences, Brno, Czech Republic
2) Dept. of Condensed Matter Physics, Charles University, Prague, Czech Republic

In collaboration with:

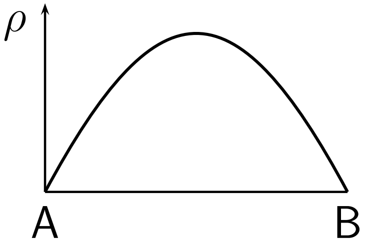
J. Kudrnovský, V. Drchal - Prague
K. Carva - Prague, Uppsala
O. Bengone - Strasbourg, Uppsala
T. Záležák - Brno
R. Sýkora - Prague

1. Introduction
2. Theoretical formulation
3. Results:
   a) residual resistivities of alloys
   b) anisotropic magnetoresistance (AMR)
   c) anomalous Hall effect (AHE)
   d) diluted magnetic semiconductors
   e) angular dependence of resistivities
4. Summary

1. Introduction

Transport properties of random systems

Residual resistivity $\rho(x)$ of $A_{1-x}B_x$ alloy



Nordheim rule (1931): $\rho(x) \sim x(1-x)$

Ferromagnets: two-current model

assumptions:

- collinear spin structures
- no spin-orbit coupling

$$\Rightarrow \quad \rho = \sigma^{-1}, \quad \sigma = \sigma^{\uparrow} + \sigma^{\downarrow}$$

Ferromagnets: two-current model

assumptions:

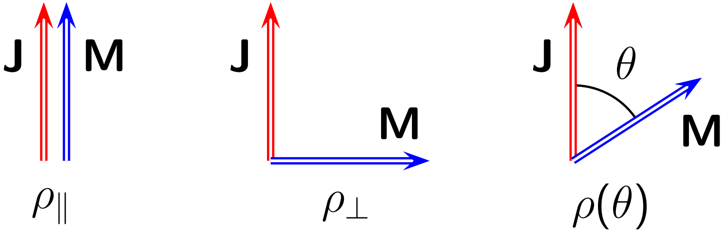
- collinear spin structures
- no spin-orbit coupling

$$\Rightarrow \quad \rho = \sigma^{-1}, \quad \sigma = \sigma^{\uparrow} + \sigma^{\downarrow}$$

consequences:

- ρ independent on magnetization direction
- conductivity tensor is symmetric
  (no Hall-like phenomena)

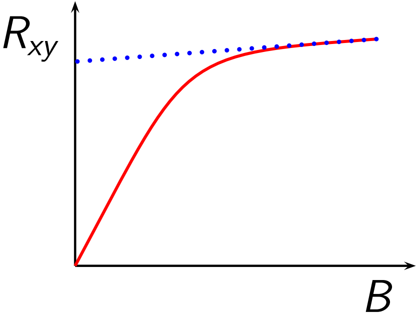
Anisotropic magnetoresistance (AMR)



AMR: $\Delta\rho = \rho_{\parallel} - \rho_{\perp}$ [W. Thomson (1857)]

$\rho(\theta) \; = \; a + b\cos^2\theta$ [W. Döring (1938)]

Anomalous Hall effect (AHE)



[E. Hall (1881)]

contributions to the AHE:

- intrinsic:
  band structure, exchange splitting,
  spin-orbit (SO) interaction
  $\Rightarrow$ *Berry curvature*

- extrinsic:
  scattering (impurities, phonons)
  $\Rightarrow$ *Green's functions*

[N. Nagaosa et al., RMP (2010)]

Conductivity tensor $\sigma^{\mu\nu}$

for cubic ferromagnets with magnetization along *z*-axis and with SO coupling:

$$\tilde{\sigma} = \begin{pmatrix} \sigma^{xx} & \sigma^{xy} & 0 \\ -\sigma^{xy} & \sigma^{xx} & 0 \\ 0 & 0 & \sigma^{zz} \end{pmatrix}$$

$\Rightarrow$ resistivity tensor $\tilde{\rho} = \tilde{\sigma}^{-1}$

$$\tilde{\rho} = \begin{pmatrix} \rho^{xx} & \rho^{xy} & 0 \\ -\rho^{xy} & \rho^{xx} & 0 \\ 0 & 0 & \rho^{zz} \end{pmatrix}$$

- isotropic resistivity: $\rho = (2\rho^{xx} + \rho^{zz})/3$
- AMR: $\Delta\rho = \rho^{zz} - \rho^{xx}$
- AHE: ρ^{xy}

Aims

- concentration trends of resistivities
- sensitivity to SO interaction
- systems with enhanced AMR
- AHE and its relation to the AMR
- angular dependence of resistivities

2. Ab initio theory of transport

- ground state from the DFT
- $T = 0$, impurity scattering
- Kubo linear response theory ($\omega = 0$) with non-interacting electrons:
  - dynamics from the KS-Hamiltonian
  - matrix elements from the KS-orbitals

Hamiltonian H, coordinate X^ν, $\eta \to 0^+$,

velocity operator: $V^\mu = -\mathrm{i}[X^\mu, H]$

Hamiltonian H, coordinate X^ν, $\eta \to 0^+$,

velocity operator: $V^\mu = -\mathrm{i}[X^\mu, H]$

$$\Rightarrow \quad \sigma^{\mu\nu} \; = \; \sum_{mn} V^\mu_{mn} X^\nu_{nm} \frac{f(E_m) - f(E_n)}{E_m - E_n + \mathrm{i}\eta}$$

Hamiltonian H, coordinate X^ν, $\eta \to 0^+$,

velocity operator: $V^\mu = -\mathrm{i}[X^\mu, H]$

$$\Rightarrow \quad \sigma^{\mu\nu} = \sum_{mn} V^\mu_{mn} X^\nu_{nm} \frac{f(E_m) - f(E_n)}{E_m - E_n + \mathrm{i}\eta}$$

$$= \int \mathrm{d}s \int \mathrm{d}t \, \frac{f(s) - f(t)}{s - t + \mathrm{i}\eta}$$

$$\times \operatorname{Tr}\{V^\mu \, \delta(t - H) \, X^\nu \, \delta(s - H)\}$$

Green's function: $G(z) = (z - H)^{-1}$,

$$G_\pm(s) \equiv G(s \pm \mathrm{i}0),$$

$$\delta(s - H) = \frac{\mathrm{i}}{2\pi}[G_+(s) - G_-(s)]$$

Green's function: $G(z) = (z - H)^{-1}$,

$$G_{\pm}(s) \equiv G(s \pm \mathrm{i}0),$$

$$\delta(s - H) = \frac{\mathrm{i}}{2\pi}[G_{+}(s) - G_{-}(s)]$$

$$\begin{aligned} \sigma^{\mu\nu} &= \frac{1}{2\pi} \int \mathrm{d}s\ f(s) \\ &\quad \times \mathrm{Tr}\,\{V^{\mu} G'_{+}(s) V^{\nu} [G_{+}(s) - G_{-}(s)] \\ &\quad - V^{\mu} [G_{+}(s) - G_{-}(s)] V^{\nu} G'_{-}(s)\} \end{aligned}$$

A. Bastin et al. (1971);

L. Smrčka and P. Středa (1977); P. Středa (1982)

A. Crépieux and P. Bruno, PRB (2001):

$$\sigma^{\mu\nu} = \sigma_1^{\mu\nu} + \sigma_2^{\mu\nu} + \sigma_3^{\mu\nu},$$

A. Crépieux and P. Bruno, PRB (2001):

$$\sigma^{\mu\nu} = \sigma_1^{\mu\nu} + \sigma_2^{\mu\nu} + \sigma_3^{\mu\nu},$$

$$\sigma_1^{\mu\nu} = \frac{1}{4\pi}\int \mathrm{d}s\ f'(s) \times \mathrm{Tr}\{V^\mu[G_+(s) - G_-(s)]V^\nu G_-(s) - V^\mu G_+(s)V^\nu[G_+(s) - G_-(s)]\},$$

A. Crépieux and P. Bruno, PRB (2001):

$$\sigma^{\mu\nu} = \sigma_1^{\mu\nu} + \sigma_2^{\mu\nu} + \sigma_3^{\mu\nu},$$

$$\begin{aligned}\sigma_1^{\mu\nu} &= \frac{1}{4\pi}\int \mathrm{d}s\ f'(s) \\ &\quad \times \mathrm{Tr}\{V^\mu[G_+(s) - G_-(s)]V^\nu G_-(s) \\ &\quad - V^\mu G_+(s) V^\nu [G_+(s) - G_-(s)]\},\end{aligned}$$

$$\begin{aligned}\sigma_2^{\mu\nu} &= \frac{\mathrm{i}}{4\pi}\int \mathrm{d}s\ f'(s)\ \mathrm{Tr}\{(X^\mu V^\nu - X^\nu V^\mu) \\ &\quad \times [G_+(s) - G_-(s)]\},\end{aligned}$$

$$\sigma_3^{\mu\nu} = \frac{1}{2\pi} \int \mathrm{d}s \; f(s) \times \mathrm{Tr}\left\{ [X^\nu, X^\mu] \, [G_+(s) - G_-(s)] \right\} .$$

$$\sigma_3^{\mu\nu} = \frac{1}{2\pi}\int \mathrm{d}s\ f(s) \times \mathrm{Tr}\left\{[X^\nu, X^\mu]\,[G_+(s) - G_-(s)]\right\}.$$

Kubo-Greenwood formula for the symmetric part of $\sigma^{\mu\nu}$:

$$\frac{\sigma^{\mu\nu} + \sigma^{\nu\mu}}{2} = \pi \int \mathrm{d}s\ f'(s) \times \mathrm{Tr}\{V^\mu\,\delta(s - H)\,V^\nu\,\delta(s - H)\}$$

Substitutionally disordered systems

- configuration averages $\langle Q \rangle \equiv \bar{Q}$:
  - treated within the coherent potential approximation (CPA)

Substitutionally disordered systems

- configuration averages $\langle Q \rangle \equiv \bar{Q}$:
  - treated within the coherent potential approximation (CPA)

- resolvent (Green's function): $\bar{G}(z) =$
  $= \left\langle (z - H)^{-1} \right\rangle = \left[z - \bar{H} - \Sigma(z) \right]^{-1}$

Substitutionally disordered systems

- configuration averages $\langle Q \rangle \equiv \bar{Q}$:
  - treated within the coherent potential approximation (CPA)
- resolvent (Green's function): $\bar{G}(z) =$
  $= \left\langle (z - H)^{-1} \right\rangle = \left[z - \bar{H} - \Sigma(z) \right]^{-1}$
- electronic structure: bands $\longrightarrow$
  $\longrightarrow$ Bloch spectral functions
  $$A(\mathbf{k}, E) \; \propto \; -\mathrm{Im}\, \bar{G}(\mathbf{k}, E + \mathrm{i}0)$$

- $\mathrm{Tr}\,\langle V^\mu\, G(z_1)\, V^\nu\, G(z_2)\rangle \;=$

$$= \;\mathrm{Tr}\left\{\bar{V}^\mu\, \bar{G}(z_1)\, \bar{V}^\nu\, \bar{G}(z_2)\right\} \;+$$

$$+ \;\; \textit{vertex corrections}$$

- $\mathrm{Tr}\,\langle V^{\mu}\, G(z_1)\, V^{\nu}\, G(z_2)\rangle \;=$

  $= \;\mathrm{Tr}\left\{\bar{V}^{\mu}\,\bar{G}(z_1)\,\bar{V}^{\nu}\,\bar{G}(z_2)\right\} \;+$

  $+$ *vertex corrections*

- V^{μ} - velocity (current) operators:

  KKR method: $V^{\mu} = -\mathrm{i}\partial_{\mu} \quad (V^{\mu} = c\alpha^{\mu})$
  [W. H. Butler, PRB (1985)]

  TB-LMTO method: $V^{\mu} = -\mathrm{i}[X^{\mu}, H]$
  [I. Turek et al., PRB (2002)]

Formulation in the TB-LMTO method

$$H = C + \xi + \sqrt{\Delta}\, S^0 \left(1 - \gamma S^0\right)^{-1} \sqrt{\Delta}\,,$$

where C, Δ, γ, ξ - random, site-diagonal

Formulation in the TB-LMTO method

$$H = C + \xi + \sqrt{\Delta}\, S^0 \left(1 - \gamma S^0\right)^{-1} \sqrt{\Delta}\,,$$

where C, Δ, γ, ξ - random, site-diagonal

ξ - on-site SO-perturbation term:

$$\xi_{RLs,R'L's'} = \delta_{RR'}\, \delta_{\ell\ell'}\, \xi_{R\ell,ss'}\, \langle Ls | \mathbf{L} \cdot \mathbf{S} | L's' \rangle$$

R - sites, $L = (\ell, m)$ - orbitals, $s = \uparrow, \downarrow$ - spin

[I. Turek et al., Philos. Mag. (2008)]

Conductivity tensor in TB-LMTO method:

$$\sigma^{\mu\nu} \;\propto\; \mathrm{Tr}\left\langle v^{\mu}\left(g_{+}^{\alpha}-g_{-}^{\alpha}\right)v^{\nu}g_{-}^{\alpha} \right.$$
$$\left. -\; v^{\mu}g_{+}\,v^{\nu}\left(g_{+}^{\alpha}-g_{-}^{\alpha}\right)\right\rangle$$
$$+\;\mathrm{i}\,\mathrm{Tr}\left\{\left(X^{\mu}v^{\nu}-X^{\nu}v^{\mu}\right)\left\langle g_{+}^{\alpha}-g_{-}^{\alpha}\right\rangle\right\}$$

where:

$g_{\pm}^{\alpha} = g^{\alpha}(E_F \pm \mathrm{i}0)$ - auxiliary GF,

$v^{\mu} = -\mathrm{i}[X^{\mu}, S^{\alpha}]$ - non-random effective velocity operator

3. Results

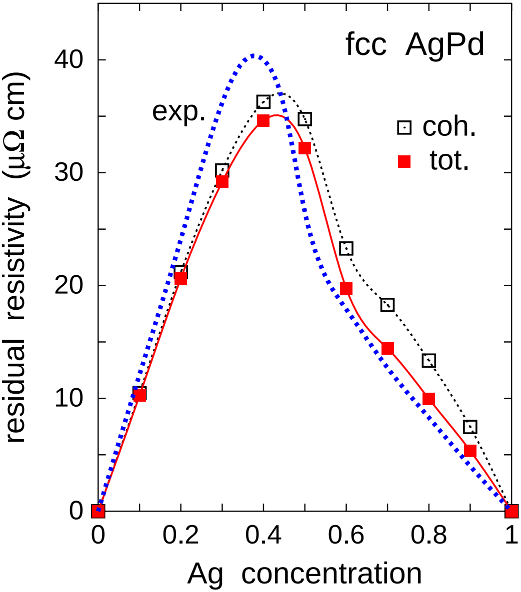
- TB-LMTO-CPA method,
  LSDA selfconsistency, *spd*-basis
- results in SRA and SRA+SO
- large numbers of **k**-points needed
  ($\gtrsim 10^8$ in full BZ); complex energy used
  ($E_F + \mathrm{i}\eta$, where $\eta = 10^{-5}$ Ry)
- CPA-vertex corrections included

a) Residual resistivities

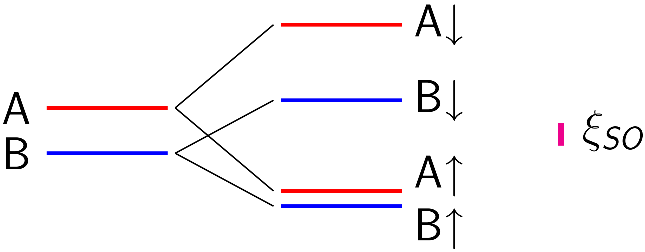
alloys: fcc AgPd (non-magnetic),

bcc FeCo, fcc NiFe, fcc NiCo

ρ of fcc AgPd alloy

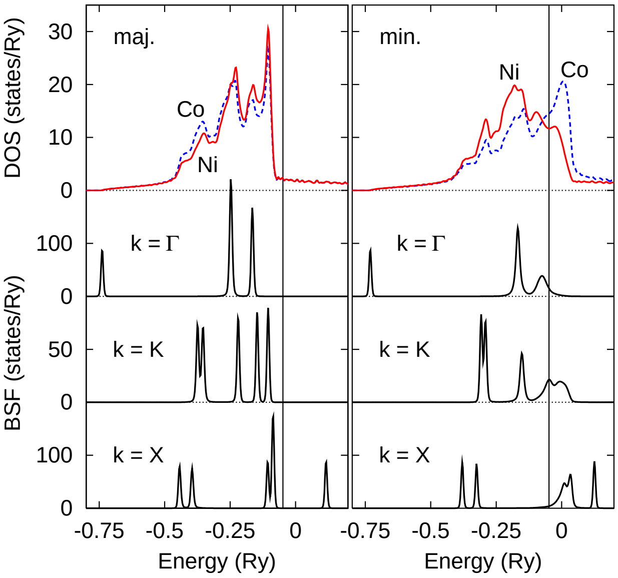


Spin-dependent disorder of *d*-levels in ferromagnetic binary alloys

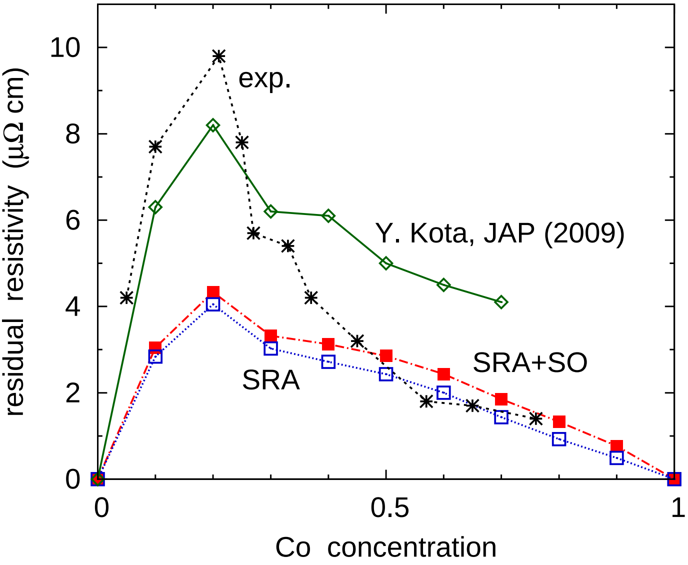


$$\begin{aligned} & \text{minority (spin-}\downarrow\text{) disorder} \gg \\ \gg\ & \text{majority (spin-}\uparrow\text{) disorder} \sim \\ \sim\ & \text{spin-orbit splitting} \end{aligned}$$

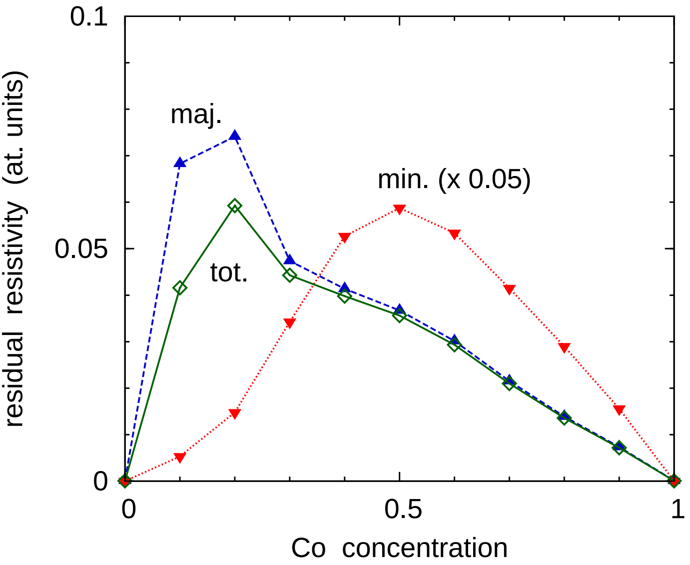
Spin-dependent disorder in fcc $Ni_{0.5}Co_{0.5}$



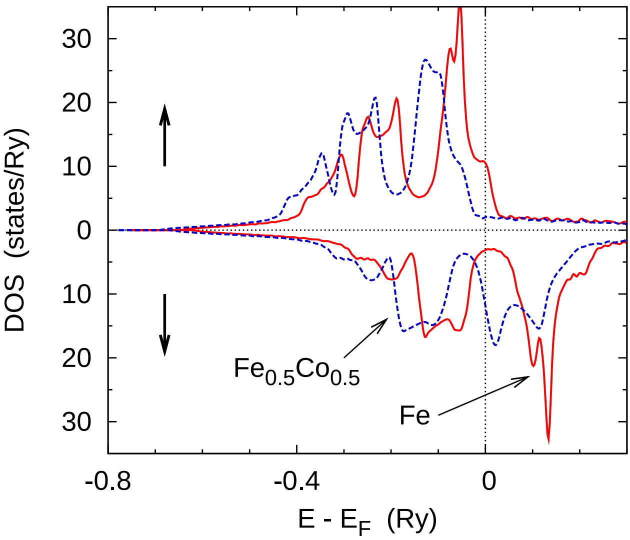
Residual resistivity of random bcc FeCo



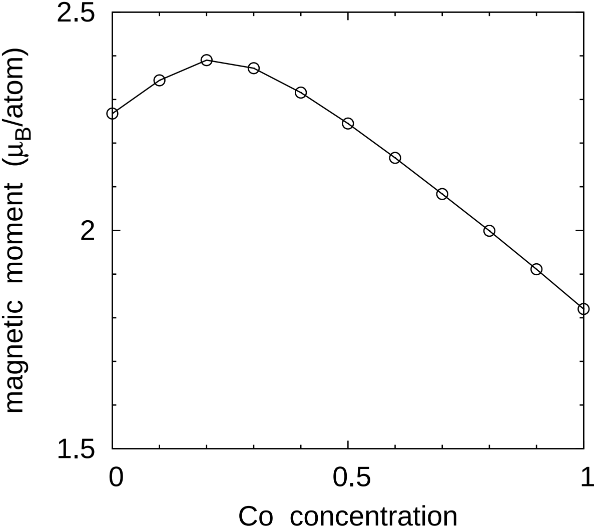
Spin-dependent resistivities of bcc FeCo



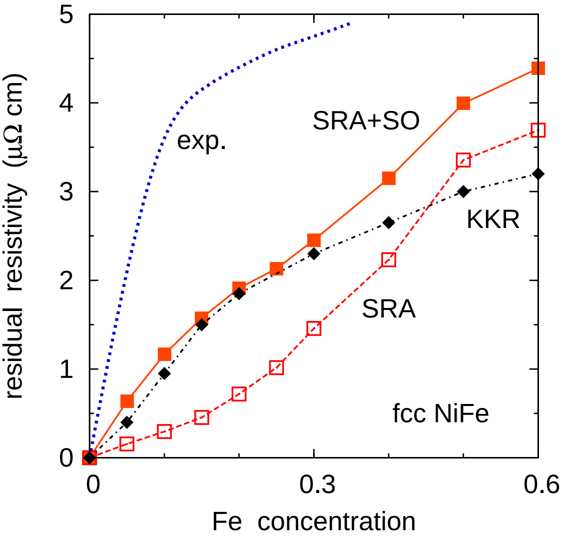
DOS of bcc Fe and of random $Fe_{0.5}Co_{0.5}$



Alloy magnetization of random bcc FeCo

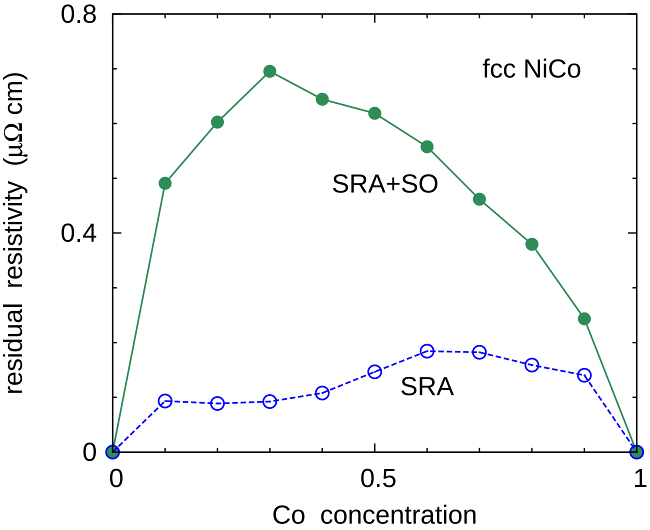


ρ of fcc
NiFe alloy

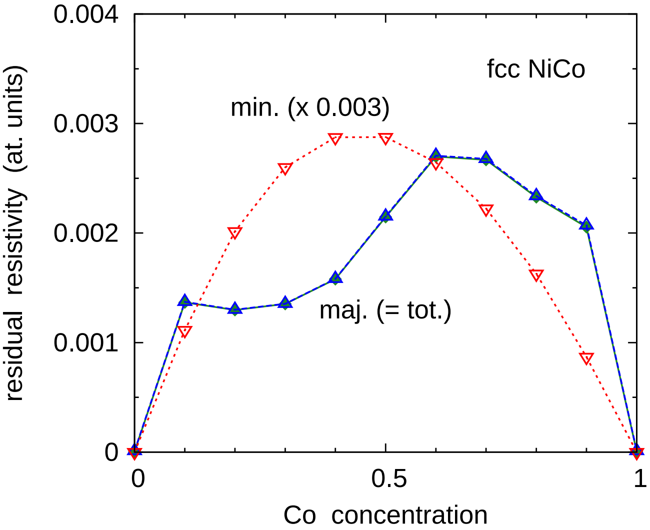


[KKR: J. Banhart et al., PRB (1997)]

Resistivity of fcc NiCo: effect of SOC



Spin-dependent resistivities of NiCo alloys



b) Anisotropic magnetoresistance

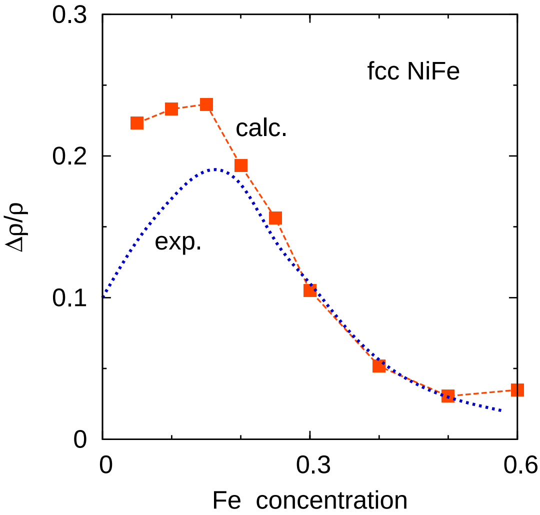
fcc Ni-based alloys:

- $Ni_{1-x}Co_x$ $[\Delta Z(x) = x]$
- $Ni_{1-x}Fe_x$ $[\Delta Z(x) = 2x]$
- $Ni_{1-x}Mn_x$ $[\Delta Z(x) = 3x]$
- $Ni_{1-x}Fe_x(*)$ $[\Delta Z(x) = 2x]$
  - with suppressed spin-$\uparrow$ disorder

AMR ratio

($\equiv \Delta\rho/\rho$)

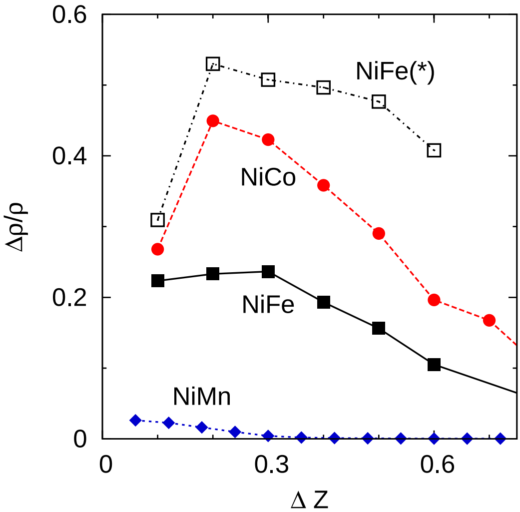
of NiFe



[KKR: J. Banhart,

EPL (1995); S. Khmelevskyi, PRB (2003)]

AMR of Ni-based alloys



large AMR due to tiny spin-↑ disorder

c) Anomalous Hall effect

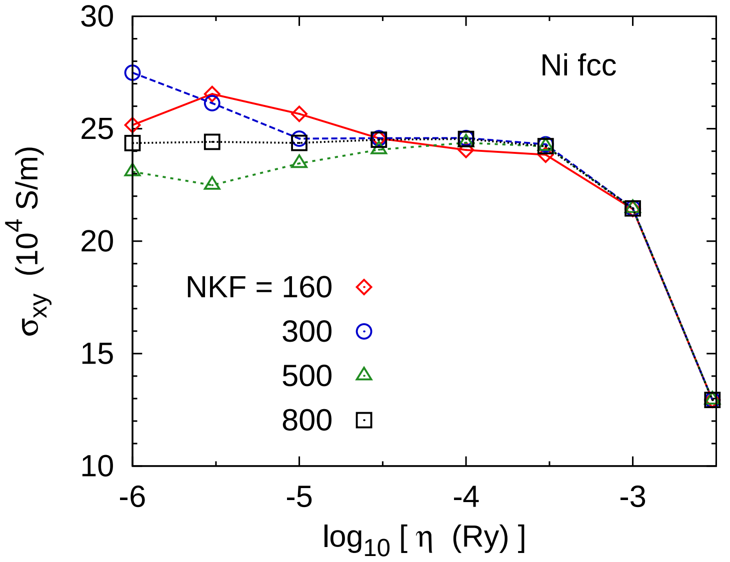
σ^{xy} (kS/m) of pure metals:

metal	calculated	exp.
Fe bcc (001)	-55 / -75^p	-103
Co fcc (001)	-34 / -25^q	
Ni fcc (001)	243 /	
Ni fcc (111)	230 / 227^r	65

p) Y. Yao, PRL (2004)

q) E. Roman, PRL (2009)

r) X. Wang, PRB (2007)



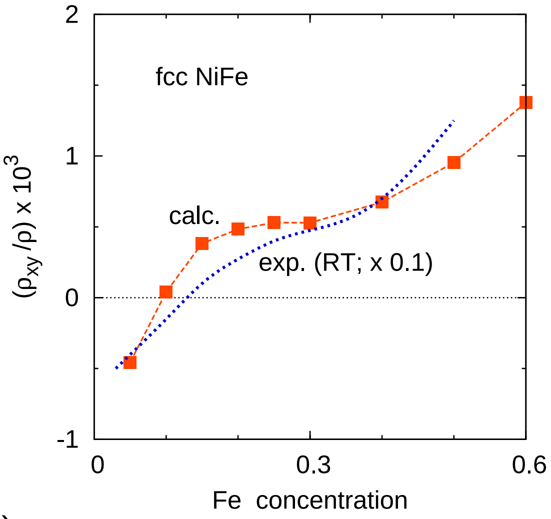
Ni fcc
NKF = 160
300
500
800
30
25
20
15
10
-6
-5
-4
-3
σ_{xy} (10^4 S/m)
$\log_{10}$ [η (Ry)]

AHE for fcc Ni-based alloys:

- $Ni_{1-x}Co_x$ $[\Delta Z(x) = x]$
- $Ni_{1-x}Fe_x$ $[\Delta Z(x) = 2x]$
- $Ni_{1-x}Mn_x$ $[\Delta Z(x) = 3x]$
- $Ni_{1-x}Fe_x(*)$ $[\Delta Z(x) = 2x]$
- $Ni_{1-x}Co_x(*)$ $[\Delta Z(x) = x]$
  - treated in VCA: $Z_{eff}(x) = 28 - x$

AHE of fcc NiFe

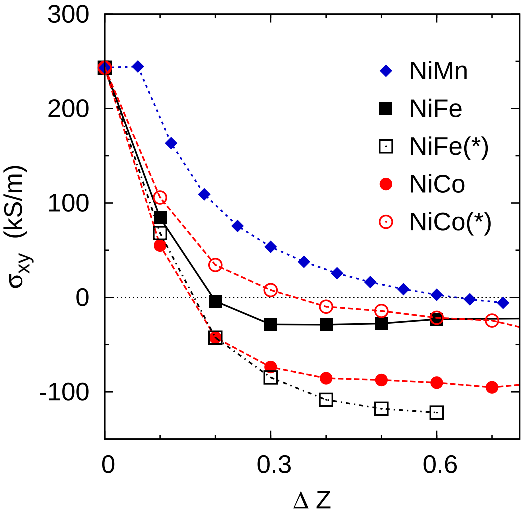
(ρ^{xy}/ρ - Hall angle)



J. Smit (1955):

change of sign of AHE $\Leftrightarrow$ *enhanced AMR ?*

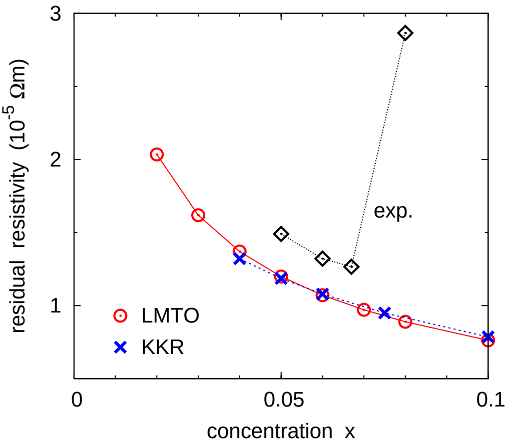
σ^{xy} for Ni-based alloys



change of sign of AHE due to *d*-band filling

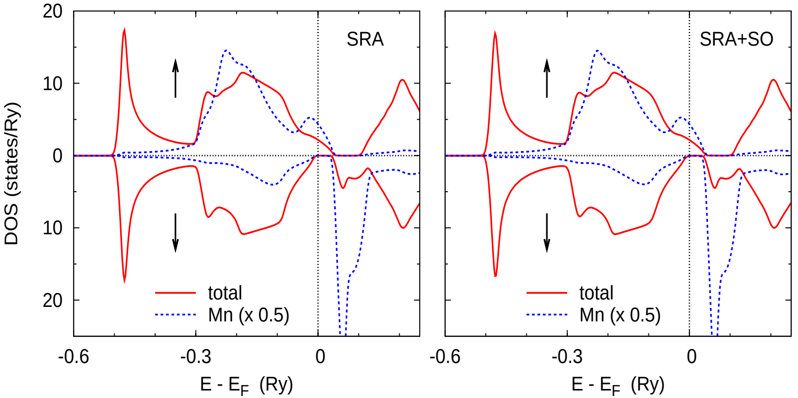
d) Diluted magnetic semiconductors

$\rho(x)$ for $(Ga_{1-x}Mn_x)As$ in SRA



[K. Sato et al., RMP (2010)]

DOS of Mn-doped GaAs (5% Mn)



(Ga,Mn)As with 5% Mn: spin polarization of DOS at E_F

DOS$\downarrow$ = 2.0% of DOS$\uparrow$

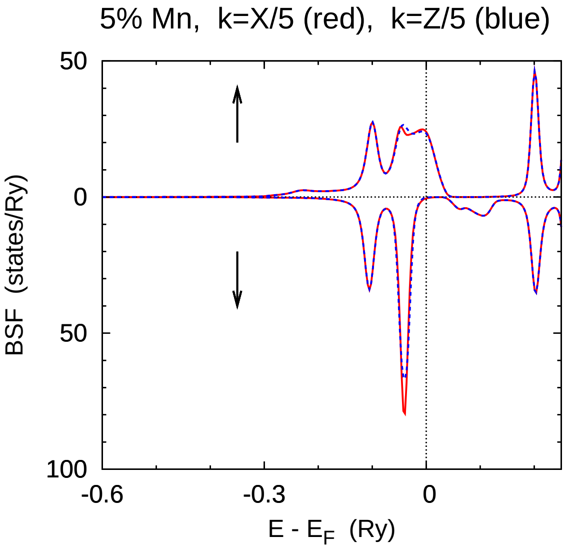
KKR: DOS$\downarrow$ = 4.2% of DOS$\uparrow$
[Ph. Mavropoulos et al., PRB (2004)]

(Ga,Mn)As with 5% Mn

- sensitivity to SO interaction

	SRA	SRA+SO
Mn moment (μ_B)	3.698	3.705
resistivity ($\mu\Omega$ cm)	1194	1175

Anisotropy of BSF of Mn-doped GaAs



AMR in $(Ga_{1-x}Mn_x)As$

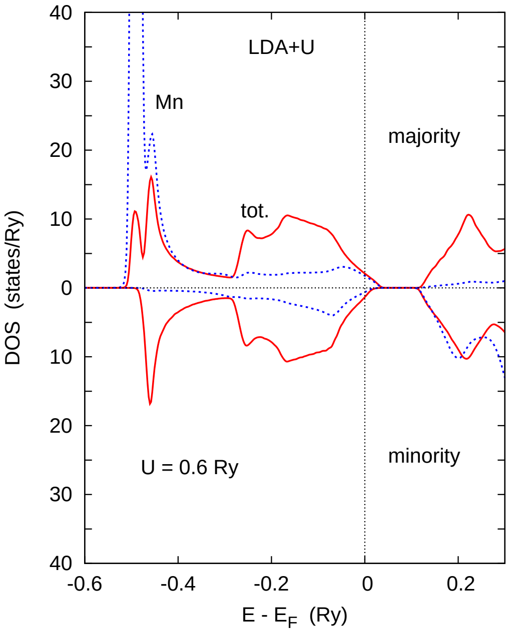
$\Delta\rho/\rho$	$x = 0.02$	$x = 0.05$
LSDA	-0.20%	-0.06%
LDA+U[a]	-6.75%	-2.70%
exp.	-7%	-3%

[a] $U = 0.25$ Ry (for Mn d orbitals)

correlation effects shift Mn $d\uparrow$ level deeper below E_F $\Rightarrow$ reduced broadening of electron states $\Rightarrow$ SO effects more pronounced

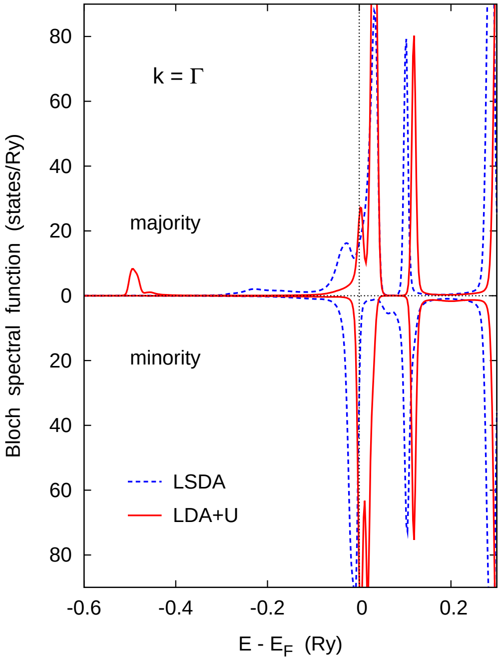
(Ga,Mn)As:
DOS
for 5% Mn

(in LDA+U,
$U = 0.6$ Ry)

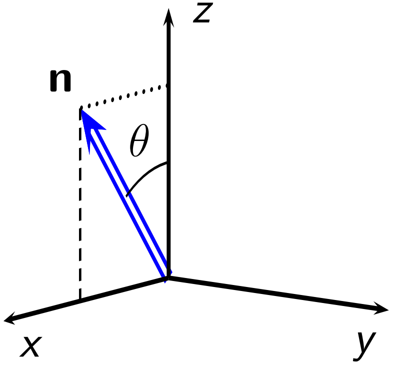


(Ga,Mn)As: BSF ($\mathbf{k} = \Gamma$) for 5% Mn

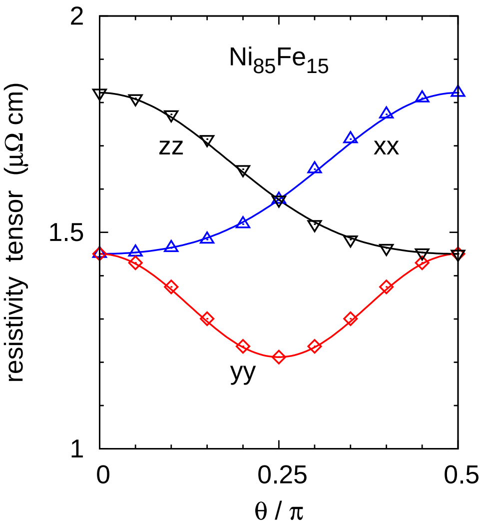
(in LSDA and LDA+U, $U = 0.6$ Ry)



e) Angular dependence of resistivities



$\rho^{\mu\mu}(\theta)$ for
fcc $Ni_{85}Fe_{15}$



[KKR: $\rho^{zz}(\theta)$ - S. Khmelevskyi, PRB (2003)]

Phenomenological angular dependence

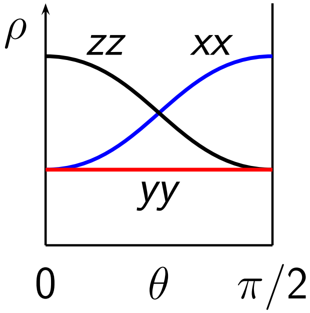
[W. Döring, Ann. Phys. 32 (1938) 259]

$$\begin{aligned}
\rho^{xx}(\theta) &= a_0 + a_1 \sin^2\theta + a_2 \sin^4\theta, \\
\rho^{yy}(\theta) &= a_0 + a_3 \sin^2\theta \cos^2\theta, \\
\rho^{zz}(\theta) &= a_0 + a_1 \cos^2\theta + a_2 \cos^4\theta.
\end{aligned}$$

Perturbative treatment of AMR

in 2nd order of perturbation expansion:

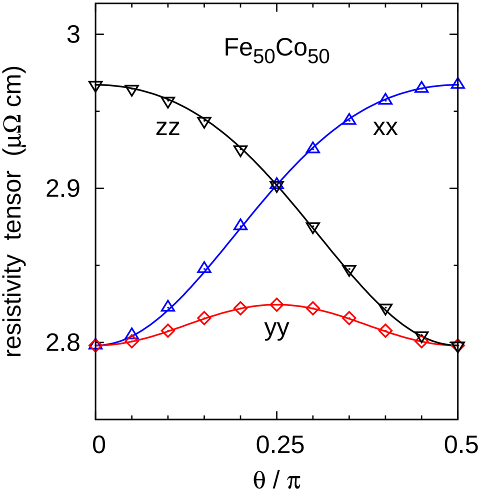
$$
\begin{aligned}
\sigma^{xx} &= b_0 + b_1 \sin^2\theta, \\
\sigma^{yy} &= b_0, \\
\sigma^{zz} &= b_0 + b_1 \cos^2\theta.
\end{aligned}
$$



θ-variation of ρ^{yy}

('transverse' AMR) $\Leftrightarrow$ strong effect of SOC

$\rho^{\mu\mu}(\theta)$ for bcc $Fe_{50}Co_{50}$



4. Summary

- enhanced AMR in Ni-based alloys due to small disorder in majority spin channel; analogy also in Mn-doped GaAs
- change of sign of AHE in Ni-based alloys ascribed to *d*-band filling
- strong influence of SO interaction: residual resistivity, 'transverse' AMR