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Influence of spin-orbit coupling on the transport properties of spintronics materials

[1]H. Ebert, [1]S. Lowitzer, V. Popescu, [1]D. Ködderitzsch, [1]J. Minar , [1]S. Bornemann
[2]P.H. Dederichs, [2]R. Zeller
[3]H. Akai, [3] M. Ogura

[1]Univ. München, Germany Germany
[2]IFF Jülich, Germany
[3] Osaka University

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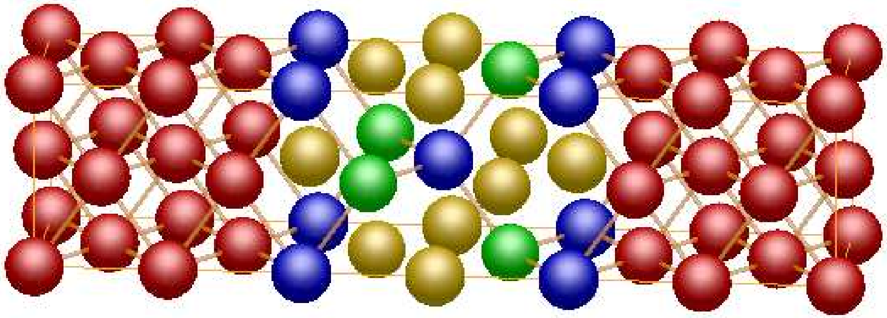
OUTLINE

- Introduction
  - electronic structure calculations
- Transport in trilayer systems
  - TMR
  - in/out of plane anisotropy TAMR
  - in plane TAMR
- Magnetotransport in bulk
  - formalism
  - Residual resistivity tensor
  - spin transport
- Summary

Green's function in 2D

FM/SC/FM-trilayers with perfect matching



Green's function (GF)

$$G^{\pm}(\vec{r},\vec{r}\,';E) = \lim_{\epsilon\to 0}\sum_{\lambda}\frac{\phi_\lambda(\vec{r})\;\phi_\lambda^{\times}(\vec{r})}{E-E_\lambda \pm i\epsilon} = G^{\pm}(\vec{r}_i+\vec{R}_i,\vec{r}\,'_j+\vec{R}_j,E)$$

tight-binding version of KKR-method

$$G^{+}(\vec{r},\vec{r}\,';E) \;=\; \frac{1}{A_{\mathrm{SBZ}}}\int_{\mathrm{SBZ}}\mathrm{d}^2k_{\|}\,\mathrm{e}^{\mathrm{i}\vec{k}_{\|}(\vec{\rho}_\nu-\vec{\rho}_{\nu'})}$$

$$\times\;\left[\sum_{\Lambda\Lambda'}R_\Lambda^{\nu}(\vec{r},E)\,G_{\Lambda\Lambda'}^{\nu\nu'}(\vec{k}_{\|},E)\,R_{\Lambda'}^{\nu'}(\vec{r}\,',E)\;-\;\mathrm{i}\,p\,\delta_{\nu\nu'}\sum_{\Lambda}R_\Lambda^{\nu}(\vec{r}_<,E)\,H_\Lambda^{\nu'}(\vec{r}_>,E)\right]$$

Accounting for Spin-Orbit Coupling (SOC)

Dirac Hamiltonian within LSDA
(Local Spin Density Approximation)

$$\widehat{H}_{\mathrm{D}} = c\vec{\alpha}\vec{p} + \beta mc^2 + V(\vec{r}) + \beta B(\vec{r})\sigma_{\mathrm{z}} \,, \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \; \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

$$= \left[\mathrm{i}\gamma_5 \sigma_r c \left(\frac{\partial}{\partial r} + \frac{1}{r}\left(1 - \beta\widehat{K}\right)\right) + V(r) + \beta\sigma_{\mathrm{z}} B(r) + (\beta - 1)\frac{c^2}{2} \right]$$

$$\widehat{K} = \widehat{\sigma}\,\widehat{L} + 1 \,, \quad \gamma_5 = \begin{pmatrix} 0 & -I_2 \\ -I_2 & 0 \end{pmatrix}, \; \sigma_r = \frac{1}{r}\vec{r}\cdot\vec{\sigma}$$

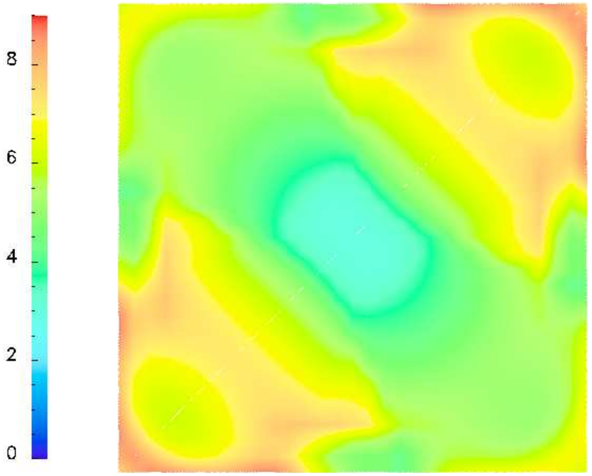
- four component Dirac formalism
- accounts for SOC and spin-polarisation on same level

Fe/GaAs/Fe – SOC-induced anisotropy

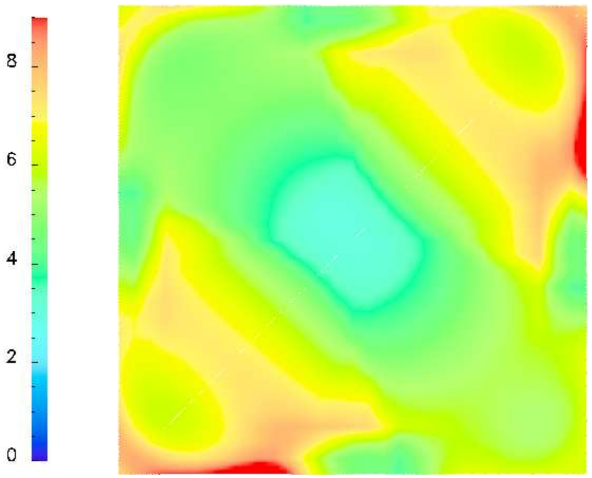
Bloch spectral functions $A(\vec{k}_{||}, E_F)$ – SC interface layer

As-termination

- $\vec{M} \parallel (001)$

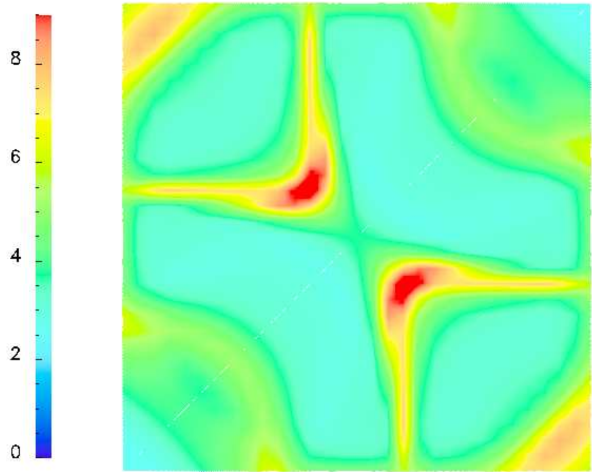


- $\vec{M} \parallel (110)$

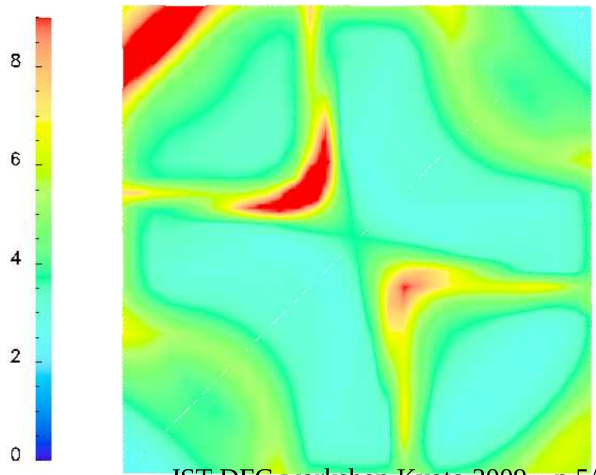


Ga-termination

- $\vec{M} \parallel (001)$

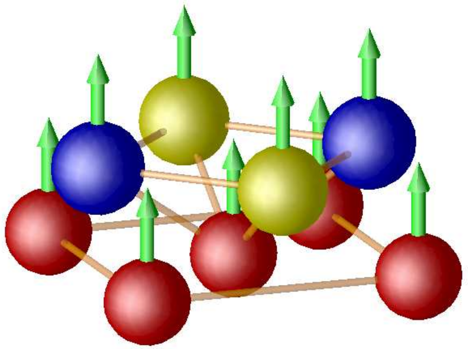


- $\vec{M} \parallel (110)$

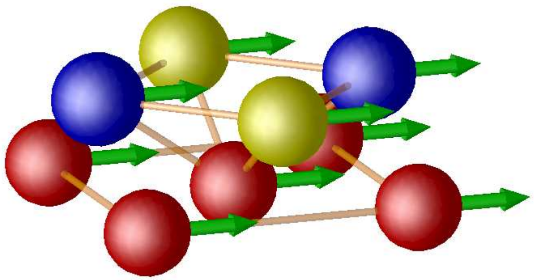


Symmetry breaking at the FM/SC-interface

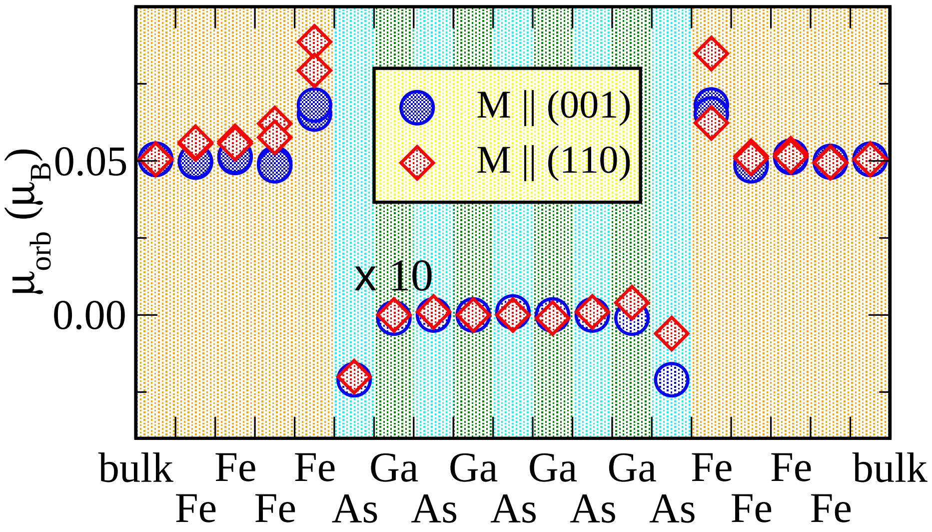
- $\vec{M} \parallel (001) - C_{2v}$

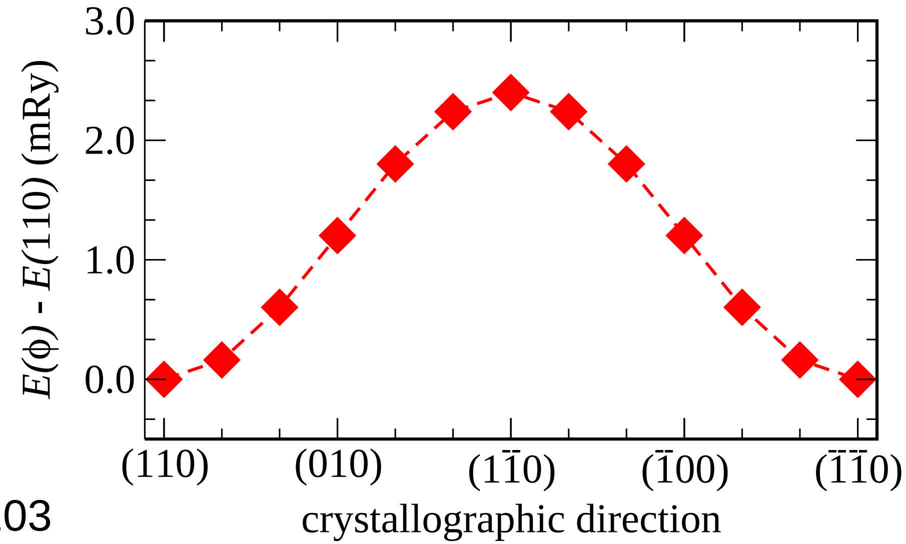


- $\vec{M} \parallel (110) - C_s$



- **Fe/9(GaAs)/Fe - μ_{orb} and MAE**





see also: Sjöstedt *et al.* 2002, PRL **89**, 267203

Košuth *et al.* 2005, EPL **72**, 816

Transport properties

Conductance - Landauer-Büttiker formalism

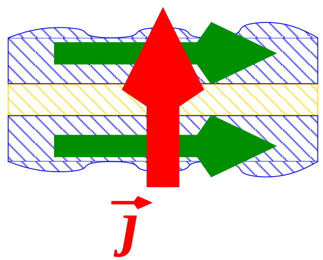
$$G = \frac{e^2}{h} \sum_{\vec{k}_\|} g(\vec{k}_\|)$$

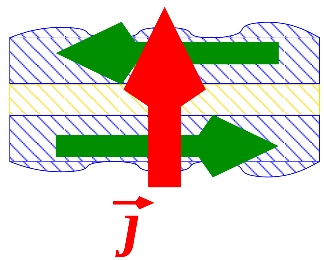
with $\vec{k}_\|$-resolved conductance:

$$\begin{aligned} g(\vec{k}_\|) &= \int_{A^{\mathrm{L}}_{\mathrm{WS}}} \mathrm{d}^2 r \int_{A^{\mathrm{R}}_{\mathrm{WS}}} \mathrm{d}^2 r' \, j_{\mathrm{z}}(\vec{r}) \, G(\vec{r}, \vec{r}\,'; \vec{k}_\|; E_{\mathrm{F}}) \, j_{\mathrm{z}}(\vec{r}\,') \, G^*(\vec{r}, \vec{r}\,'; \vec{k}_\|; E_{\mathrm{F}}) \\ j_{\mathrm{z}}(\vec{r}) &= \frac{c}{E_{\mathrm{F}} + mc^2} \left(-\mathrm{i}\hbar\nabla_{\mathrm{z}} + \frac{V}{c}\vec{\alpha}_{\mathrm{z}} - \mathrm{i}\frac{B}{c}\beta(\vec{\alpha} \times \vec{a}_{\mathrm{z}})_{\mathrm{z}} \right) \end{aligned}$$

”pessimistic” MR ratio

$$T = \frac{G^{\mathrm{P}} - G^{\mathrm{AP}}}{G^{\mathrm{P}}}$$





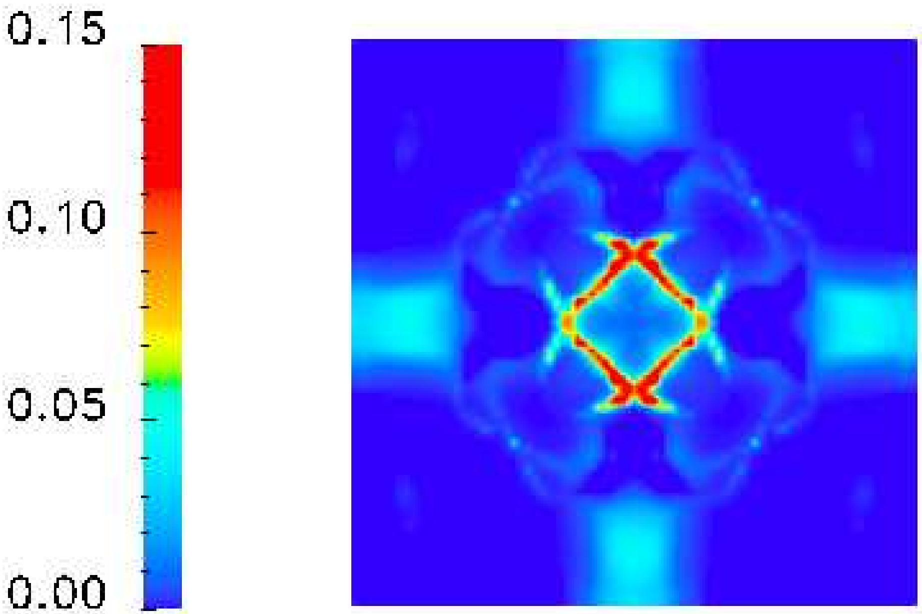
P / AP : parallel / antiparallel orientation of magnetisation KKR: Mavropoulos *et al.* (2004)

Transport properties of Fe/13(AsGa)/Fe

$\vec{k}_{||}$-resolved conductance – AP orientation

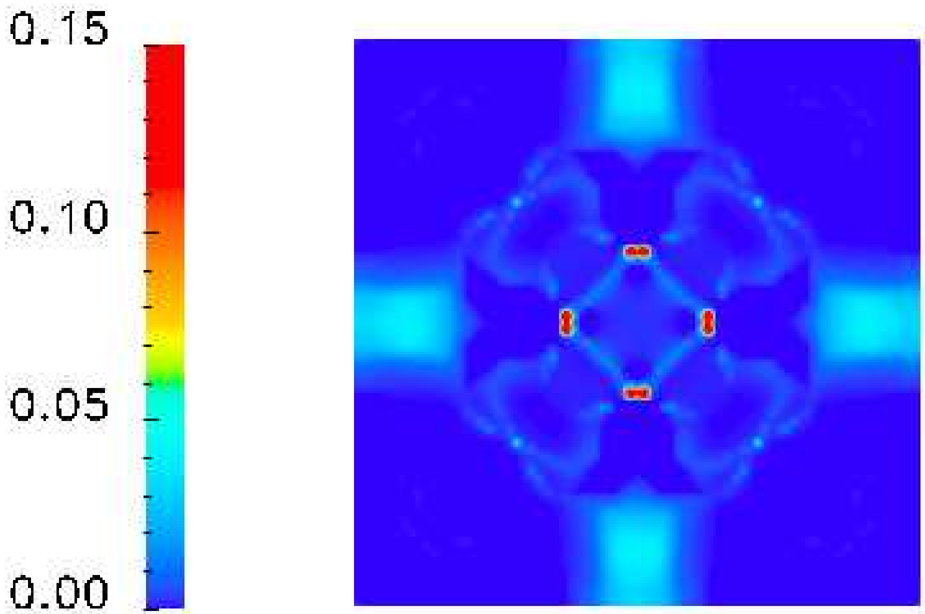
- effect of the spin-orbit coupling (SOC)

correct SOC



$$G^{\mathrm{AP}} = 0.0076\ e^2/h$$

SOC switched off



$$G^{\mathrm{AP}} = 0.0044\ e^2/h$$

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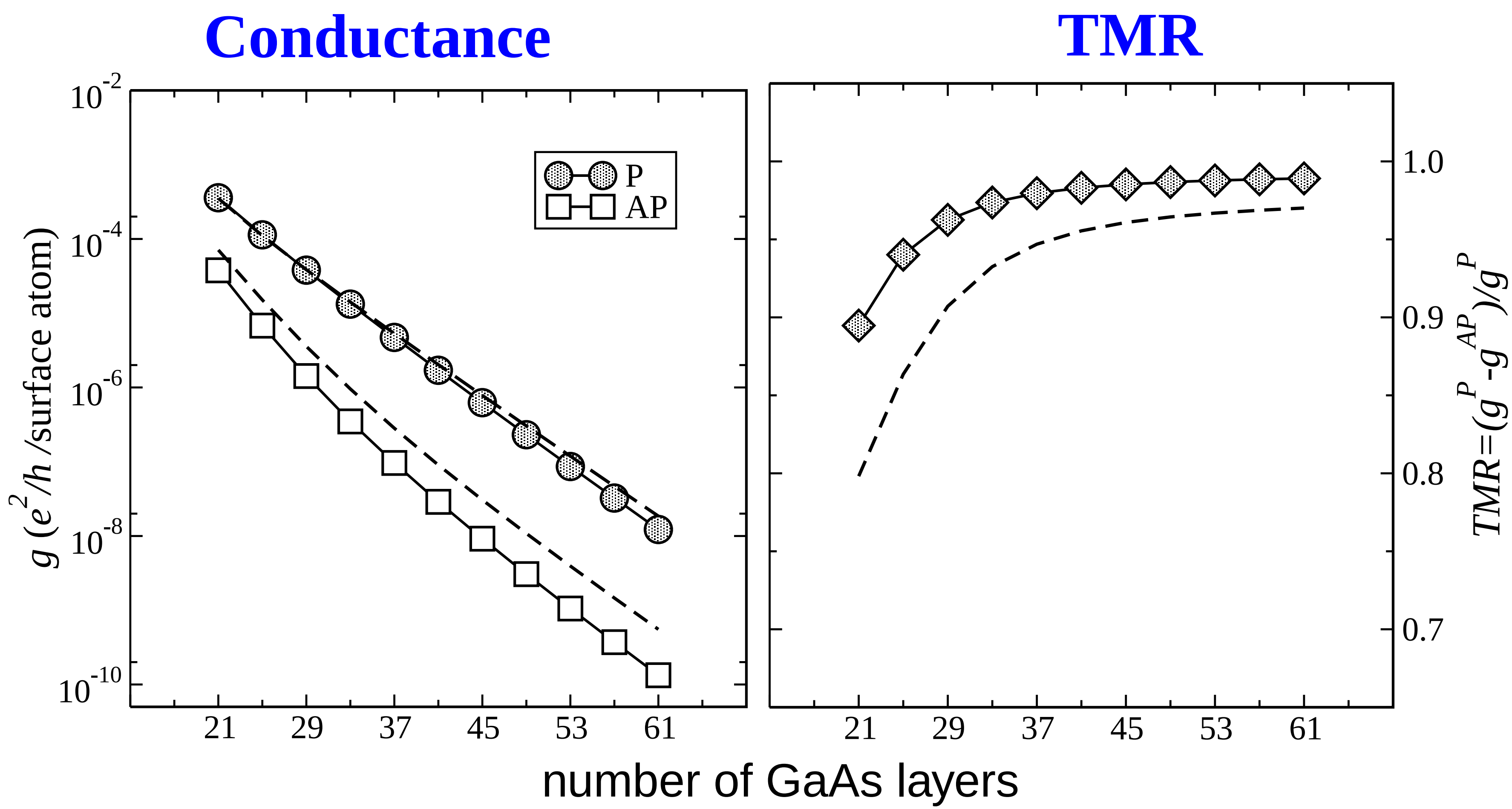
Tunneling Conductance for Fe/n(GaAs)/Fe

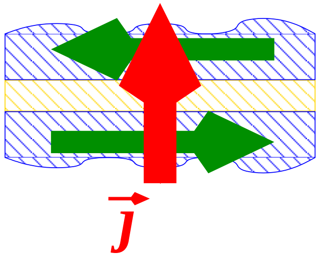


- Symbols: SOC suppressed for inner GaAs layers
- dashed lines: full SOC $\Rightarrow$ SOC increases g^{AP}

Dependence on orientation of $\vec{M}$

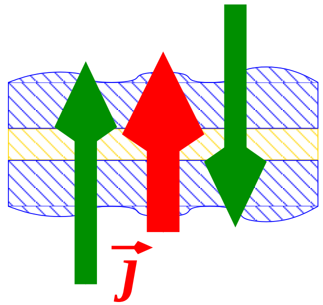
$\vec{M}$ along (110)

- AP orientation

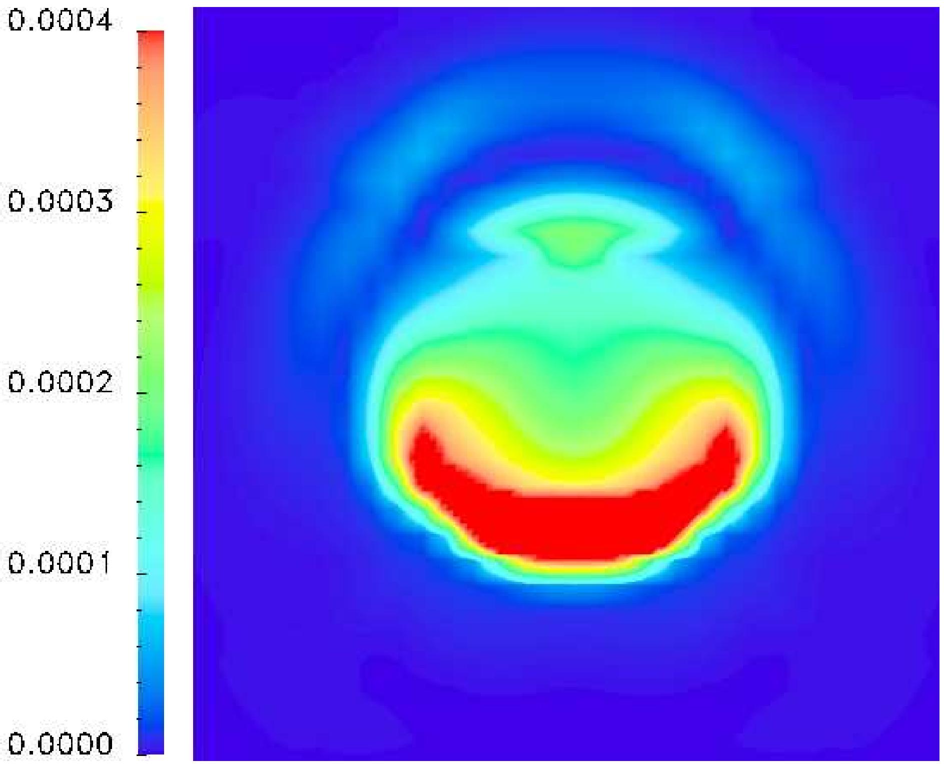


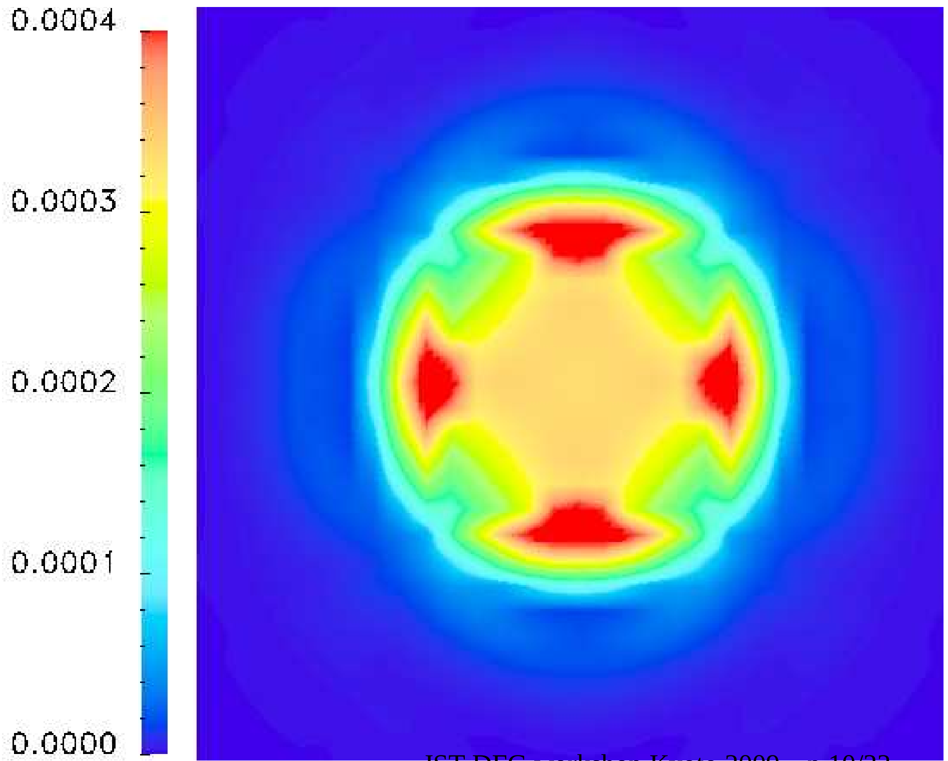
$\vec{M}$ along (001)

- AP orientation



$k_{\|}$-resolved conductance





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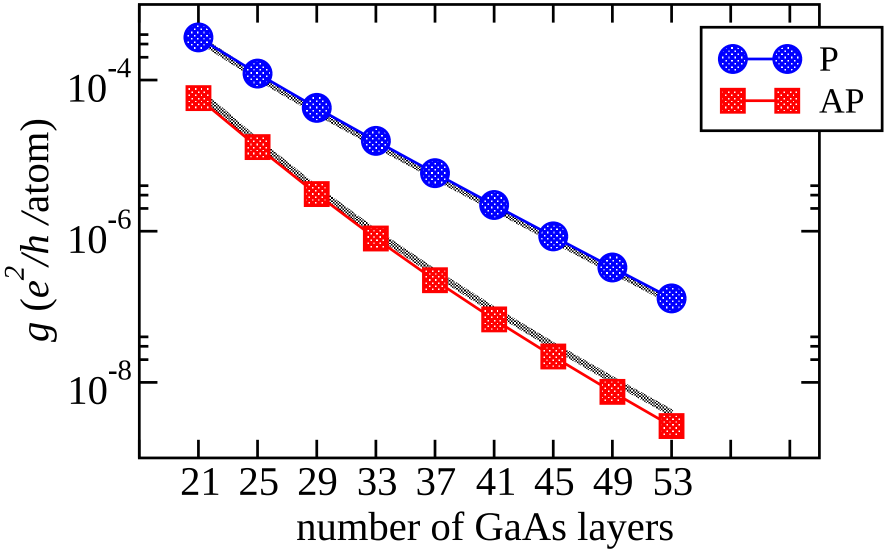
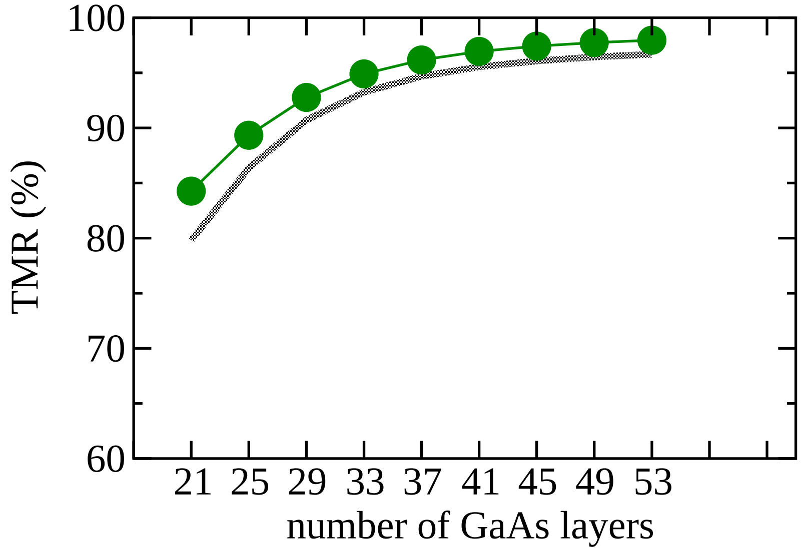
Dependence on orientation of $\vec{M}$

Conductance for $\vec{M} \parallel (110)$ and (001)

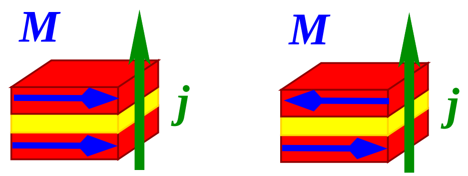
- conductance for P/AP alignment



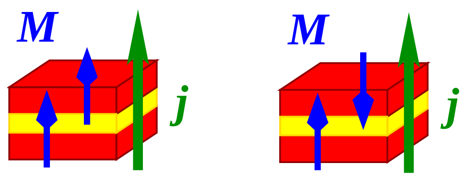
- TMR = $(G^{\mathrm{P}} - G^{\mathrm{AP}})/G^{\mathrm{P}}$



- symbols for $\vec{M} \parallel (110)$



lines for $\vec{M} \parallel (001)$

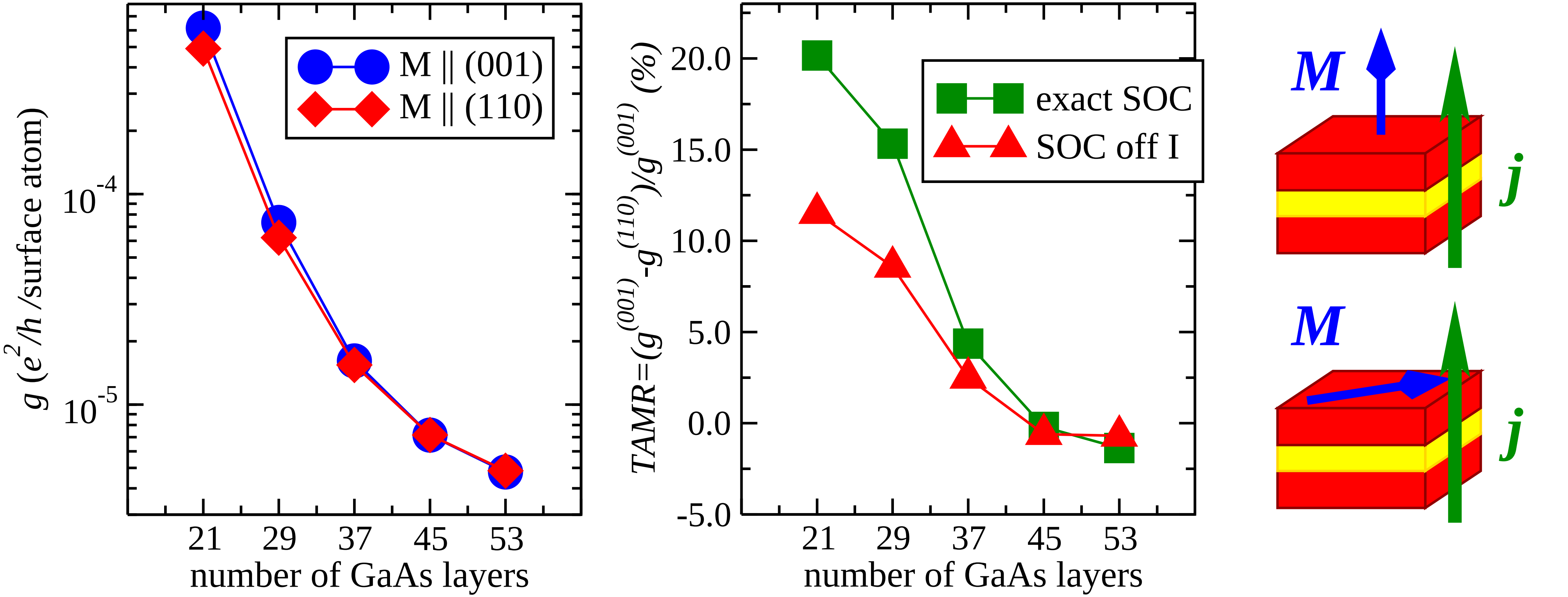


- difference of G largest for AP configuration

Fe/GaAs/Fe – TAMR calculations

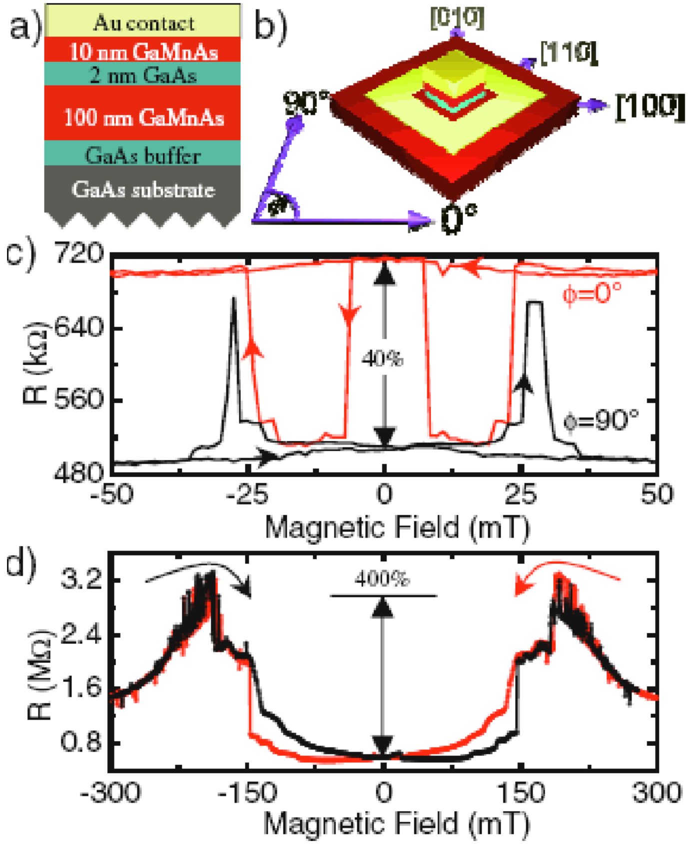
Fe/n(GaAs)/Fe tunnelling junction – Ga-termination

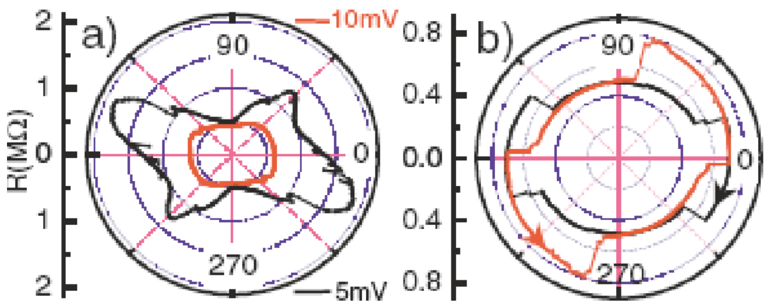
- conductance
- TAMR



- strong TAMR effect for thin spacer
- suppressing SOC at the interface reduces the TAMR by ≈50%
- TAMR ≈ 6 × larger than for As termination

Tunneling Anisotropic Magneto-Resistance





Gould *et al.* 2004, PRL **93**, 117203
Rüster *et al.* 2005, PRL **94**, 027203

- **spin-valve** behaviour with only one (or two coupled) magnetic layer
- depending on ϕ width and sign change (**unlike** TMR)
- at saturation, the sample is a sensor of the **absolute direction** of $\vec{H}$
- modelling conductance g
  - $g \propto$ 'tunnelling' DOS
  - ΔDOS$\equiv$DOS(M$\|$x) $-$ DOS(M$\|$y)
- **spin-orbit coupling (SOC)** induced anisotropy

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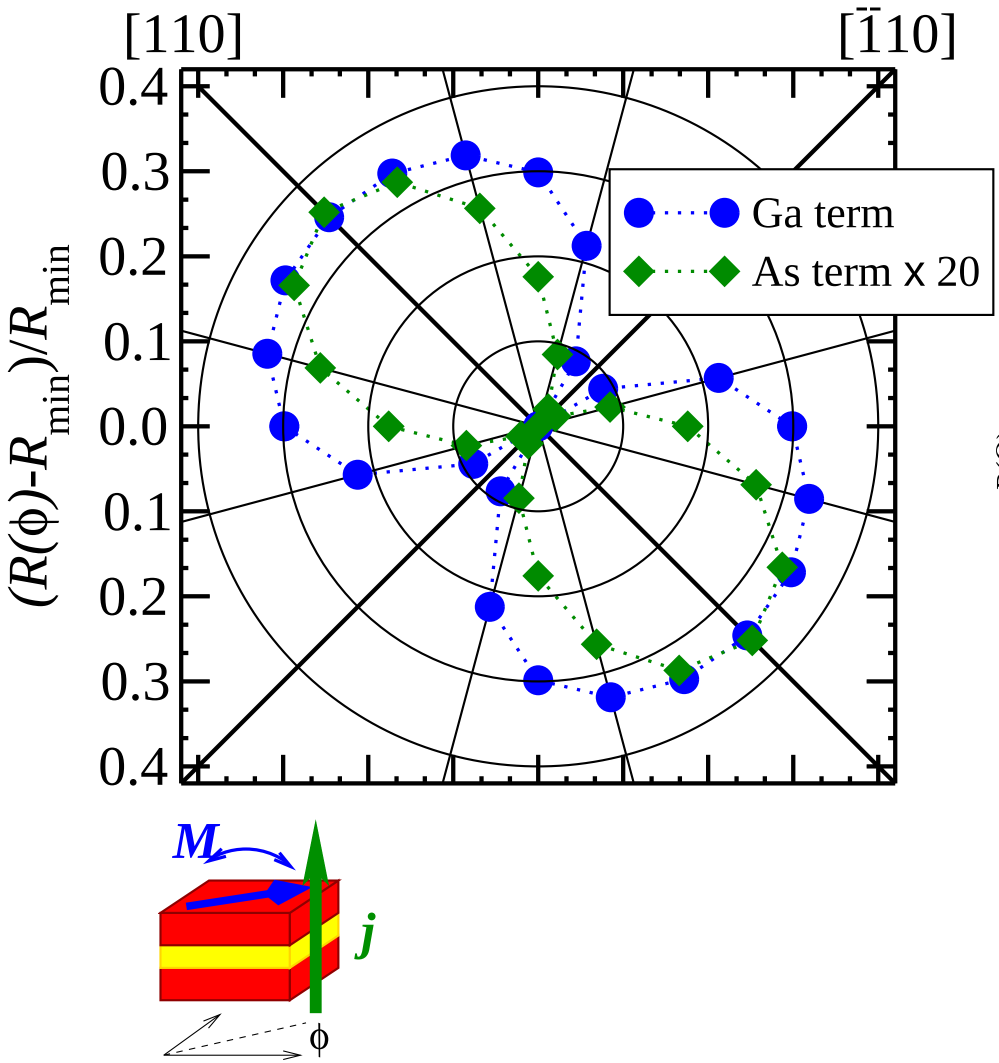
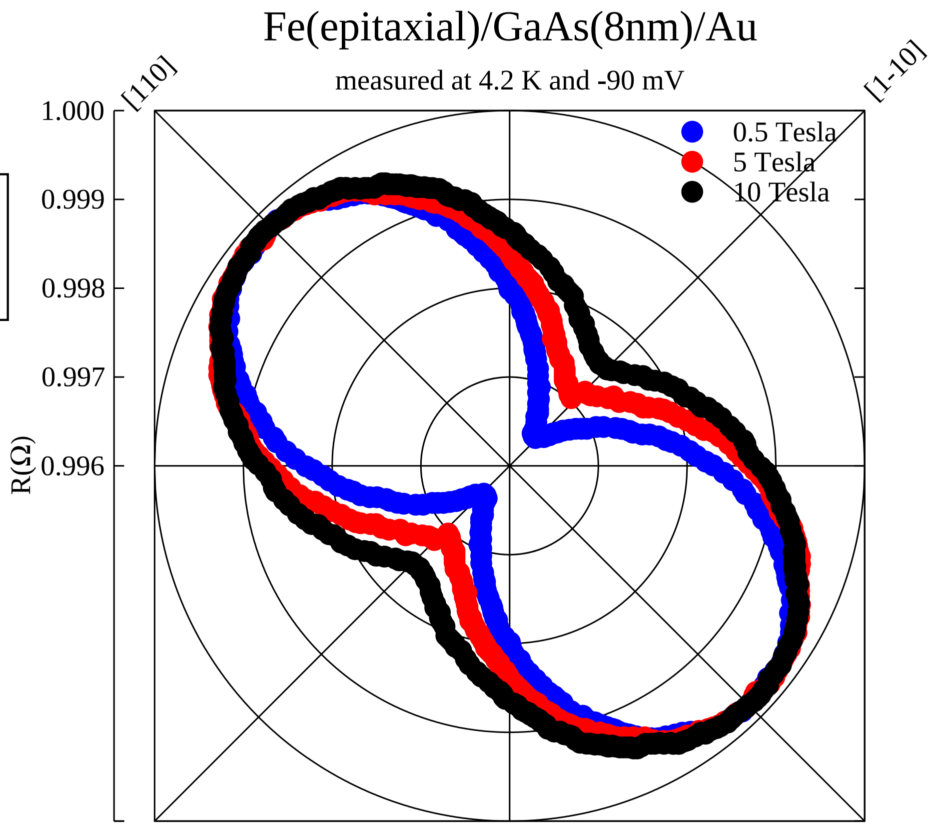
Fe/29(GaAs)/Au – in-plane TAMR

- **theory**
- **experiment**





Moser *et al.*, Univ. of Regensburg

Phys. Rev. Lett. **99** 056601 (2007)

- qualitative (but not quantitative) agreement between theory and experiment

Full conductivity tensor σ

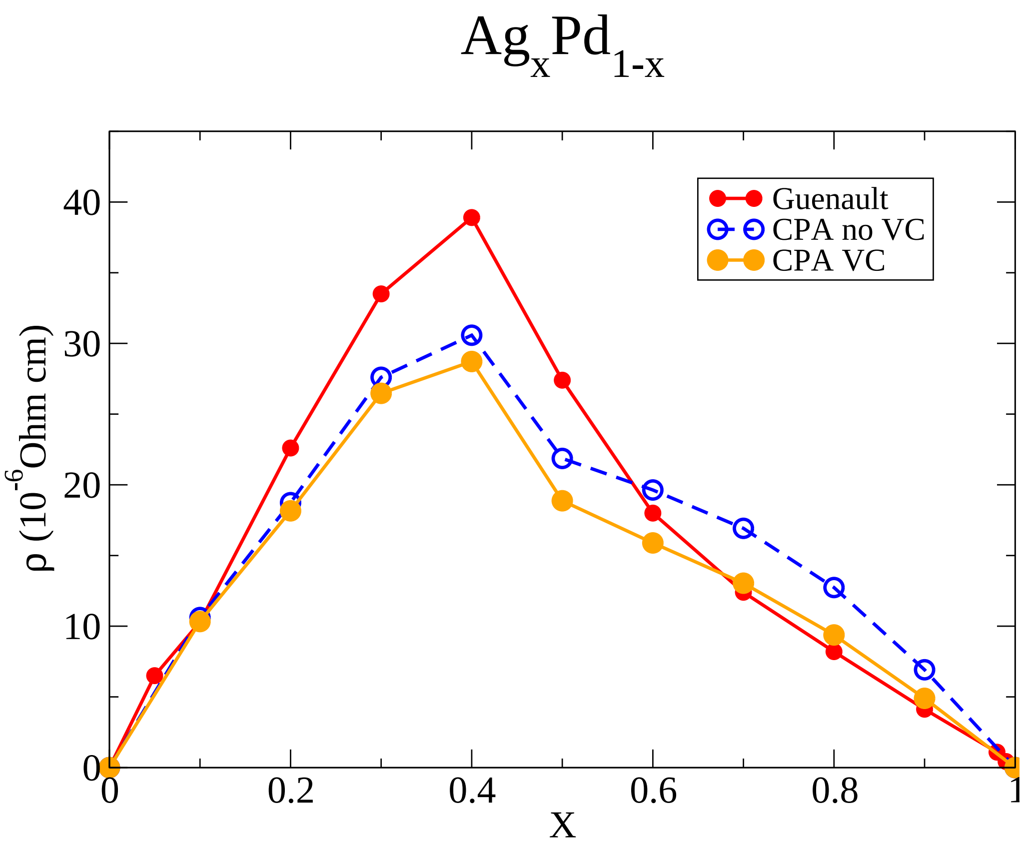
Středa, Smirčka, JPF (1975,1977)

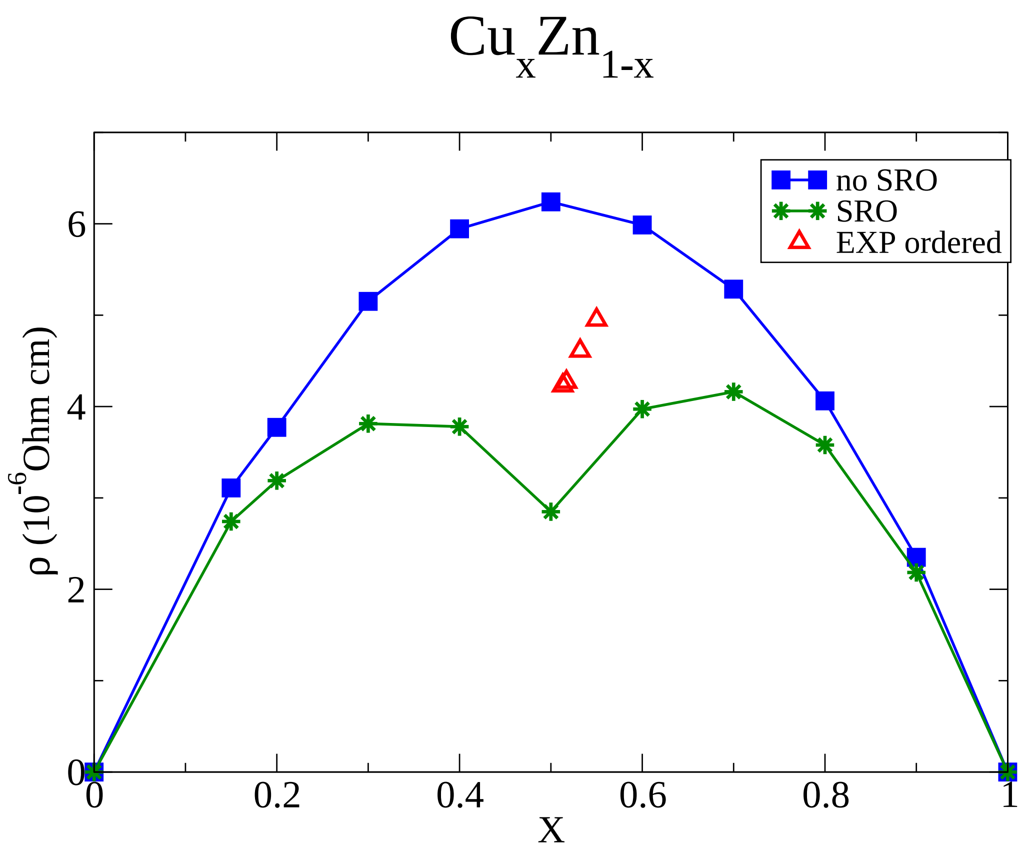
$$\sigma_{\mu\nu} = -\frac{\hbar}{2\pi V}\int_{-\infty}^{+\infty} dE\, f(E)\, \text{Tr}\left\langle \hat{j}_\mu \frac{dG^+}{dE}\hat{j}_\nu(G^+ - G^-) - \hat{j}_\mu(G^+ - G^-)\hat{j}_\nu\frac{dG^-}{dE}\right\rangle$$

Crépieux, Bruno, PRB (2001), ($T = 0$)

$$\begin{aligned}\sigma_{\mu\nu} &= \frac{\hbar}{4\pi V}\text{Tr}\left\langle \hat{j}_\mu(G^+ - G^-)\hat{j}_\nu G^- - \hat{j}_\mu G^+\hat{j}_\nu(G^+ - G^-)\right\rangle \\ &+ \frac{e}{4i\pi V}\text{Tr}\left\langle (G^+ - G^-)(r_\mu\hat{j}_\nu - r_\nu\hat{j}_\mu)\right\rangle\end{aligned}$$

Residual resistivity of non-magnetic alloys





Experiment:

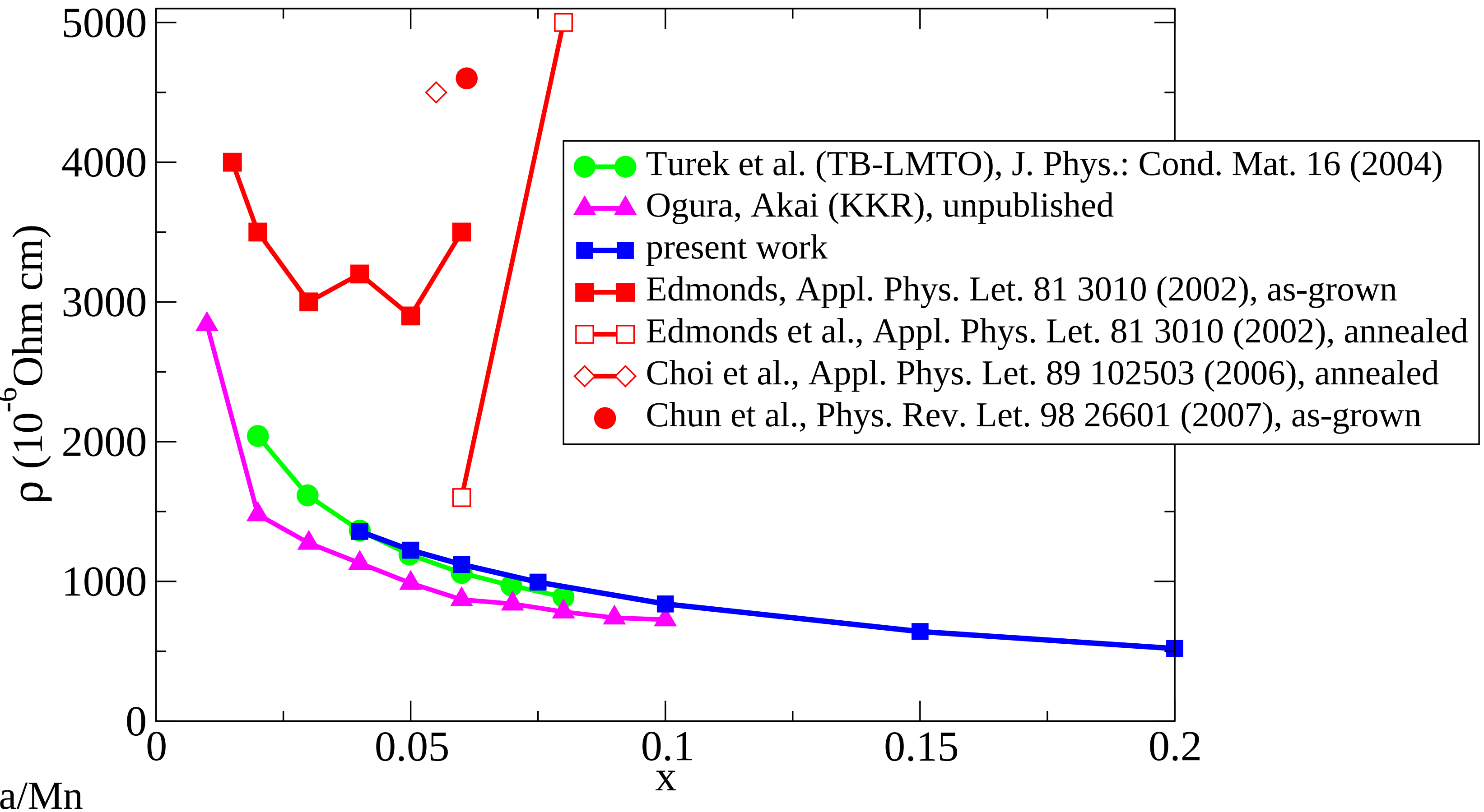
Guénault, Phil. Mag. 30, 641, 1974

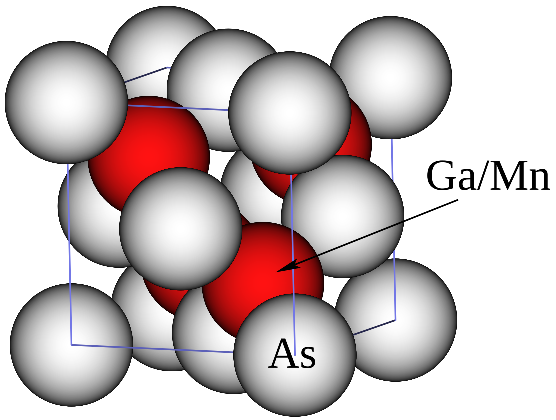
W. Webb, Phys. Rev. 55, 297, 1938

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

Residual resistivity

comparison with experiment

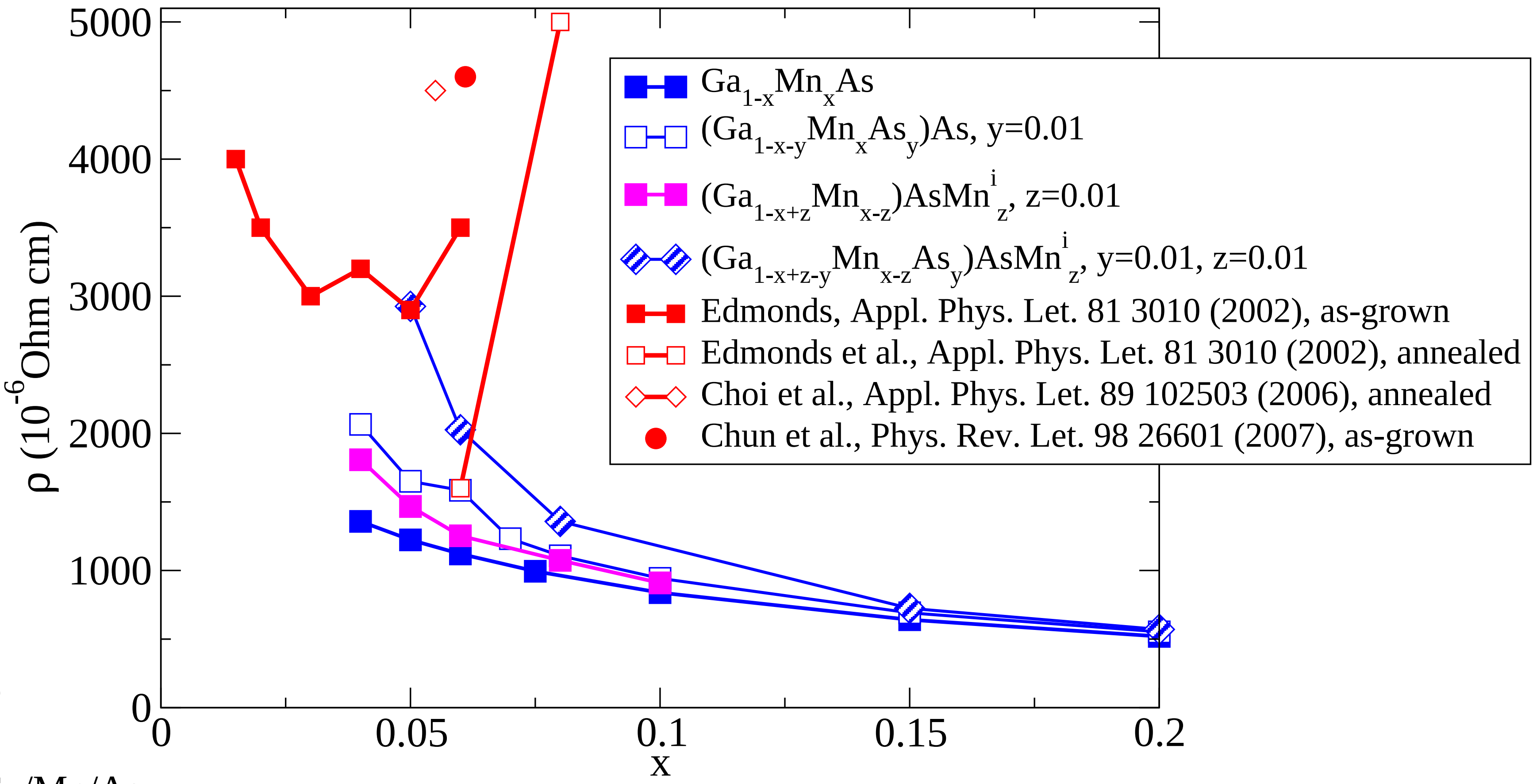


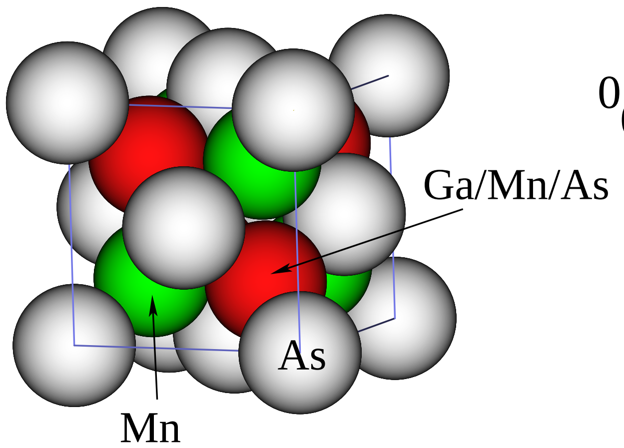


$(Ga_{1-x+z-y}Mn_{x-z}As_y)AsMn^i_z$

Residual Resistivity

influence of antisite and interstitial occupation





Galvano-magnetic effects

Cubic ferromagnet $\vec{M} \parallel \vec{z}$

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

Isotropic resistance $\bar{\rho} = \frac{1}{3}(2\rho_{\|} + \rho_{\perp})$

Anomalous magneto-resistance $AMR = \frac{\rho_{\|} - \rho_{\perp}}{\bar{\rho}}$

spontaneous Hall effect ρ_{xy}

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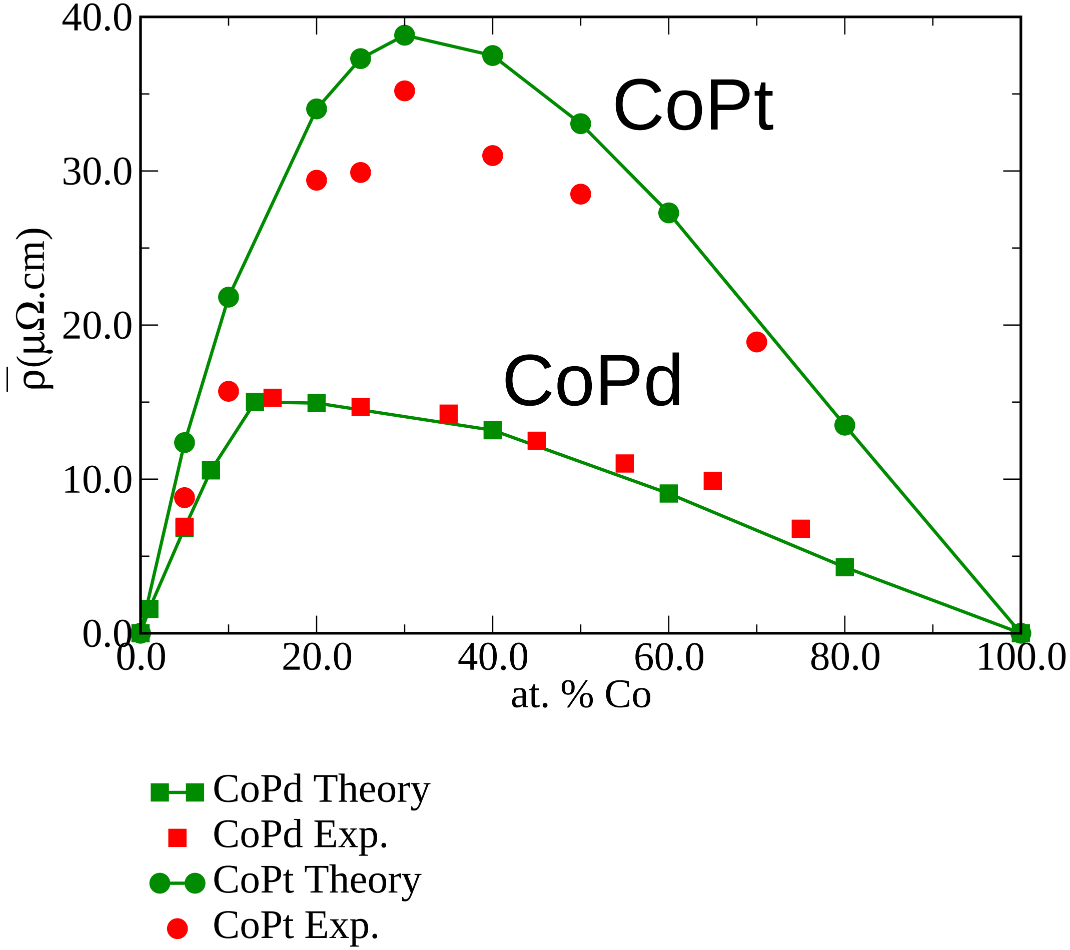
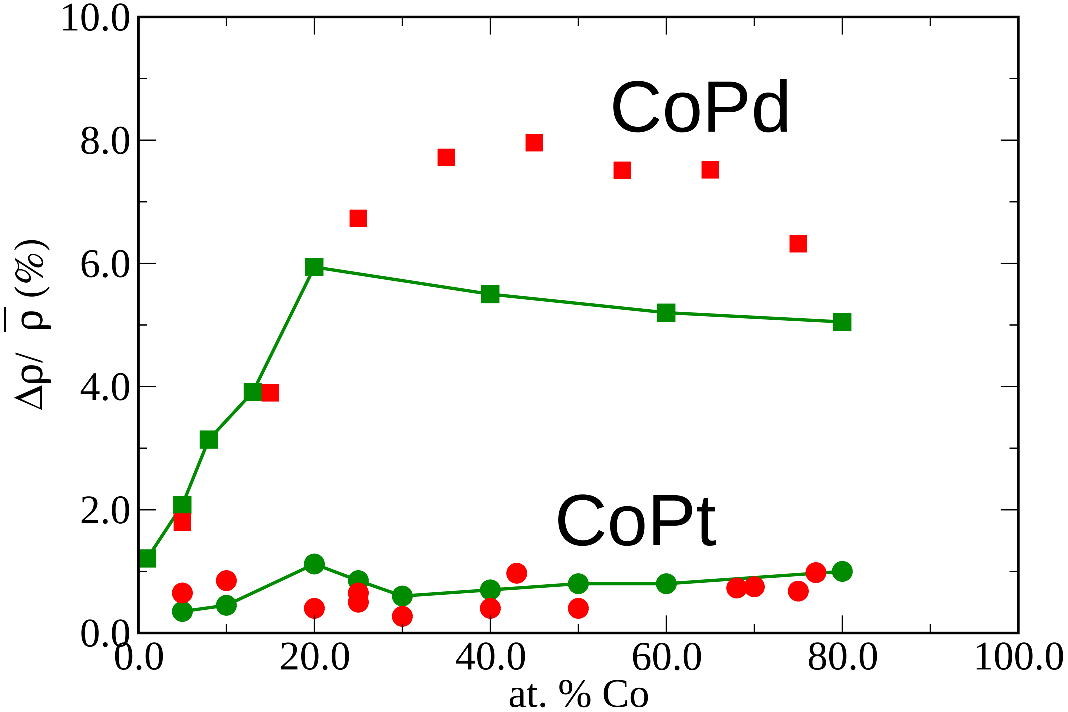
Resistivity tensor of $\mathrm{Co}_x\mathrm{Pd}_{1-x}$ and $\mathrm{Co}_x\mathrm{Pt}_{1-x}$

Isotropic resistivity $\overline{\rho}$

Anomalous Magneto-Resistivity $\frac{\Delta\rho}{\overline{\rho}}$





Spin conductivity tensor

$$\Sigma_{\mu\nu} = -\frac{\hbar}{2\pi V}\int_{-\infty}^{+\infty} dE\, f(E)\, \mathrm{Tr}\left\langle \vec{J}_\mu \frac{dG^+}{dE}\hat{j}_\nu (G^+ - G^-) - \vec{J}_\mu (G^+ - G^-)\hat{j}_\nu \frac{dG^-}{dE}\right\rangle$$

$\vec{J}_\mu$ spin current operator for direction μ

j_ν electrical current operator for direction ν ($\vec{j} = ec\vec{\alpha}$)

Naive definition $J^z_\mu = \sigma_z\, j_\mu / e$

Introduce auxilary current that fulfills continuity equation

$$J^z_\mu = \frac{d}{dt}(\sigma_z\, r_\mu) = \sigma_z\, j_\mu / e + \left(\frac{d}{dt}\,\sigma_z\right) r_\mu$$

$\frac{d}{dt}\,\sigma_z$ spin-flip events due to SOC or non-collinear magnetism

Semi-relativistic: Niu (2005) and several others

Relativistic: Gyorffy, Szunyogh (2008)

Summary

- Fully relativistiv description of transport within
  - Landauer-Büttiker
  - Kubo-Greenwood (and extensions)
- Role of SOC
  - influence on conductance G
  - in/out of plane anisotropy of TMR
  - in plane anisotropy of TMR-TAMR
  - source for bulk galvano-magnetotransport
- Formal basis for corresponding spin transport calculations