JÜLICH FORSCHUNGSZENTRUM

Ab-initio study of the temperature dependent electron transport through magnetic nanostructures

11.03.2013 | DPG Regensburg

Roman Kováčik, Phivos Mavropoulos, Daniel Wortmann, and Stefan Blügel

Peter Grünberg Institut and Institute for Advanced Simulation

Introduction

Spincaloric transport

- coupling between *electrical, spin, and heat transport* in magnetic materials
- explaining mechanisms (e.g. spin-dependent Seebeck versus spin Seebeck effect)[1]
- extensive search for novel concepts in spintronics

Transport through nanostructures

- enhanced Peltier effect in subμm-sized metallic junctions (Co/Au, Fe/Au, Ni/Au)[2]
- giant Peltier coefficient proposed for quasi-1D nanowires (Konbu-phase)[3]

Outline

- electron transport through thin layers and nanowires considering non-collinear spin configurations
- effect of *temperature* (via *spin-disorder*) on resistance[4,5] . . .

  . . . *(spin-)Seebeck coefficient, thermal conductivity*

---

[1] see, e.g., Bauer et al.: Nature Mater. 11, 391 (2012)

[2] Fukushima et al.: Jpn. J. Appl. Phys. 44, L12 (2005)

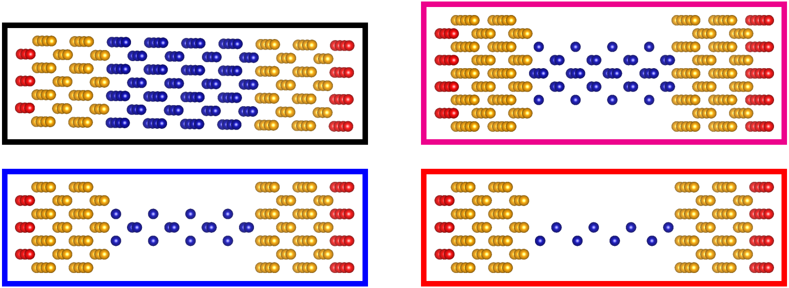
[3] Vu/Sato/Katayama-Yoshida: Appl. Phys. Express 4, 015203 (2011)

[4] Wysocki et al.: J. Appl. Phys. 101, 09G506 (2007)

[5] Kudrnovský et al.: PRB 86, 144423 (2012)

System setup and Methodology

System setup: **Cu**(semi-bulk)|**Cu**(4)|**Co**(8)|**Cu**(4)|**Cu**(semi-bulk), 2D-per.



Electronic structure: *KKR* Green function framework[6] (LDA, FP, $l_{\max} = 3$)

- exchange coupling parameters J_{ij} between magnetic atoms[7]

Monte Carlo: in-house program

- spin disordered configurations $\{\mathbf{S}_i(T)\}$

Electron transport: *Landauer-Büttiker* approach for ballistic transport in KKR[8]

using decimation technique to describe semi-infinite leads

---

[6] Papanikolaou et al.: J. Phys. Condens. Matter 14, 2799 (2002), also see: www.kkr-gf.org

[7] Liechtenstein et al.: J. Magn. Magn. Mater. 67, 65 (1987)

[8] Mavropoulos et al: PRB 69, 125104 (2004)

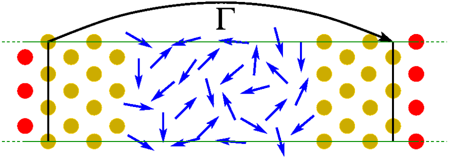
Conductance calculation

Electron transport:

$\approx 150 - 250$ sites

≈ 10 core-min. / conductance calc.

$\approx (20\,\varepsilon) \times (25\,T) \times$ up to $(800\,\{\mathbf{S}_i\})$



- *conductance matrix*[9] in spin space $\mathbf{\Gamma}(\varepsilon)$ as function of $\{\mathbf{S}_i\}$

  transport coefficients: $\mathbf{L}_n = -\int \mathbf{\Gamma}\,(\varepsilon)\,(\varepsilon - E_\mathrm{F})^n\,\partial_\varepsilon f(\varepsilon - E_\mathrm{F}, T)\,\mathrm{d}\varepsilon$
- conductance / area: $\mathbf{G}_\mathrm{A} = \mathbf{L}_0\,A^{-1}$

  resistance $\times$ area: $R^\mathrm{A} = \left(G_A^{\uparrow\uparrow} + G_A^{\downarrow\downarrow} + G_A^{\uparrow\downarrow} + G_A^{\downarrow\uparrow}\right)^{-1}$

  Seebeck coefficient, spin-Seebeck coefficient, thermal conductance

Spin-disorder resistivity benchmark for Co and Ni ($T \gg T_\mathrm{C}$)

- $\rho_\mathrm{Co} = 50\,\mu\Omega\,\mathrm{cm}$, $\rho_\mathrm{Ni} = 15\,\mu\Omega\,\mathrm{cm}$, expt.[10]
- $\rho_\mathrm{Co} = 53\,\mu\Omega\,\mathrm{cm}$, $\rho_\mathrm{Ni} = 26\,\mu\Omega\,\mathrm{cm}$, present work

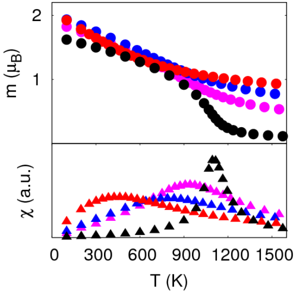
[9] see, e.g., Yavorsky/Mertig: PRB 74, 174402 (2006)

[10] Weiss/Marotta: JPCS 9, 302 (1959)

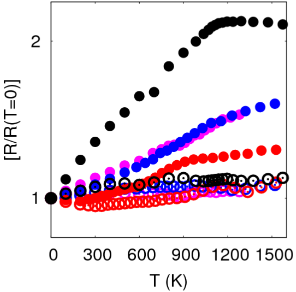
Spin-disorder resistance (SDR)

[with SD: ● ● ● ●, without SD: ○ ○ ○ ○]

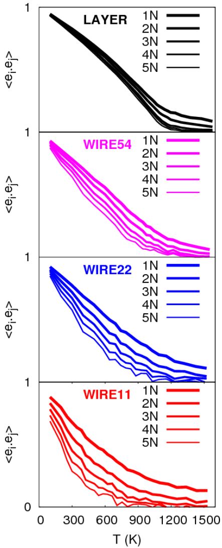
Monte Carlo



SDR relative to $T = 0$ *K*



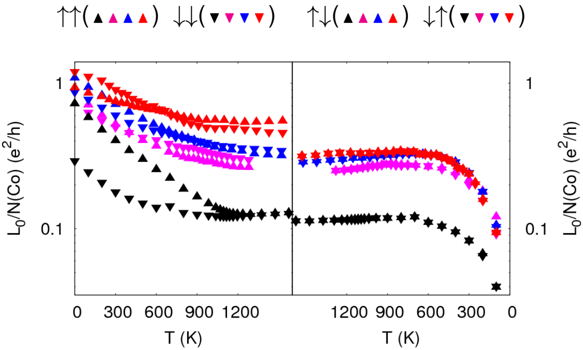
spatial correlation



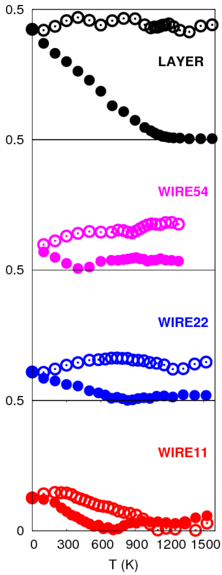
- LAYER shows loss of short-range order at $T \approx 1100$ K; wires behave like a macro-spin
- suppressed SDR for the wires, strongest for WIRE11
- kink in SDR(T) correlates with onset of long-range order loss in [001] direction

Electrical conductance

[with SD: ● ● ● ●, without SD: ○ ○ ○ ○]



current polarization



- wires show slightly increased conductance per Co cross section, conductance decrease due to spin-disorder is strongly suppressed for the wires
- at high T, spin-preserving conductance significantly higher than spin-mixing conductance for WIRE11
- current polarization $(G^{\uparrow} - G^{\downarrow})/(G^{\uparrow} + G^{\downarrow})$ drops considerably due to the spin-disorder

Thermopower

[with SD: ● ● ● ●, without SD: ○ ○ ○ ○]

Seebeck coefficient:

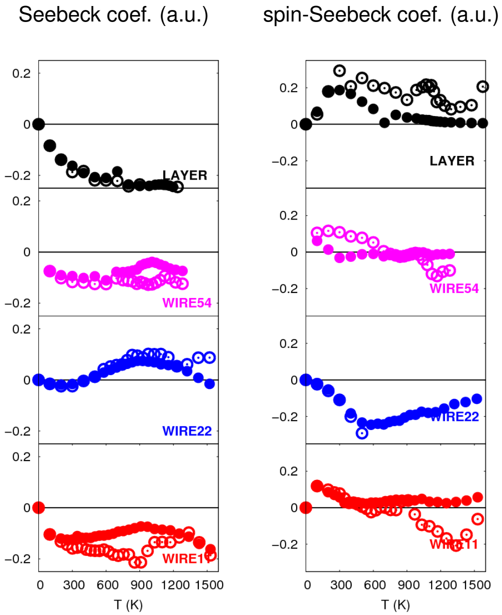
$$S_c = -\frac{\sum_{ss'} L_1^{ss'}}{eT \sum_{ss'} L_0^{ss'}}$$

- strong spin-disorder effect observed in WIRE11, WIRE54
- WIRE22 shows sign reversal

spin-Seebeck coefficient:

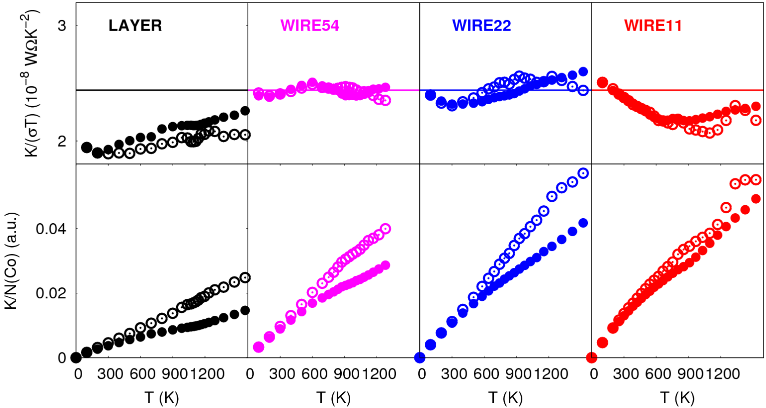
$$S_s = -\frac{L_1^{\uparrow\uparrow} + L_1^{\uparrow\downarrow} - L_1^{\downarrow\downarrow} - L_1^{\downarrow\uparrow}}{eT \sum_{ss'} L_0^{ss'}}$$

- WIRE22 shows large S_s due to opposite sign of $S^{\uparrow}$ and $S^{\downarrow}$



Thermal conductance

[with SD: ● ● ● ●, without SD: ○ ○ ○ ○]



- thermal conductance $K_A = \left[\sum_{ss'} L_2^{ss'} - \left(\sum_{ss'} L_1^{ss'}\right)^2 / \sum_{ss'} L_0^{ss'}\right] / (T\,A)$ is strongly suppressed by spin-disorder except for the WIRE11
- no large deviation from Wiedemann–Franz law is observed $[K/(\sigma T) = 2.44 \times 10^{-8}\, \mathrm{W}\,\Omega\, K^{-2}]$

Summary

- implementation of calculation of G, K, S within KKR GF framework for magnetic systems with spin-disorder based on MC simulation
- effect of spin-disorder on G, K, S in Co thin layer and nanowires between Cu leads

Outlook

- effect of magnetic layer thickness / nanowire length
- half-metallic FM CrTe nanostructures in insulating ZnTe matrix between Ag leads

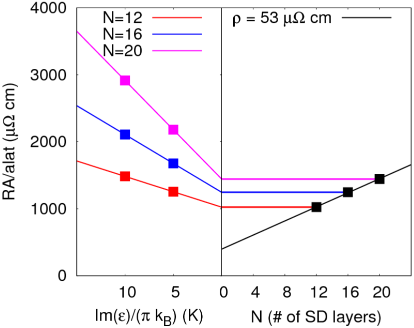
Thanks to

- DFG Priority Program “Spin Caloric Transpor” (SPP 1538), for support
- Forschungszentrum Jülich, for computational resources
- you, for your attention !

Spin-disorder resistivity in Co and Ni ($T \gg T_C$)

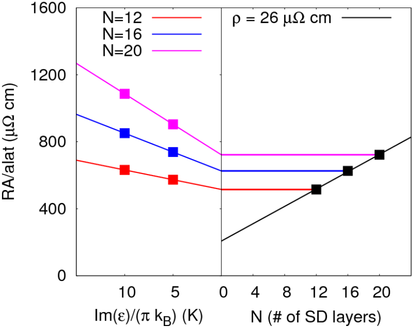
- $p3\times3$ [001]-oriented fcc supercell FM(4)/FM(N-disordered)/FM(4)
  expt. lattice constant
- spin configurations generated for $T = 10000\,\mathrm{K}$
  spatial correlation $\langle \mathbf{e}_i \cdot \mathbf{e}_j \rangle$ between nearest neighbors $i, j \to 0$

Cobalt (1.65 μ_B)



expt.[11]: $\rho = 50\,\mu\Omega\,\mathrm{cm}$

Nickel (0.63 μ_B)



expt.[11]: $\rho = 15\,\mu\Omega\,\mathrm{cm}$

[11] Weiss/Marotta: JPCS 9, 302 (1959)