Transport and dynamical properties of permalloy domain walls from first-principles

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Motivation: Current-induced domain wall motion

The magnetization dynamics of a domain wall (DW) in the presence of a spin-polarized electric current **j** is described by the generalized Landau-Lifshitz-Gilbert equation:

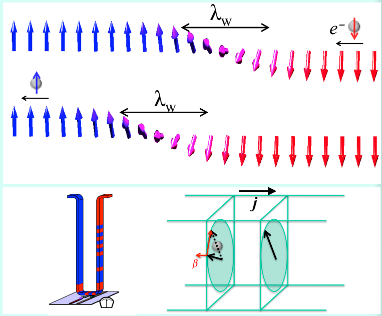
$$\frac{d\mathbf{m}}{dt} = -\gamma \mathbf{m}\times\mathbf{H}_{\mathrm{eff}} + \alpha\mathbf{m}\times\frac{d\mathbf{m}}{dt} - (1-\beta\mathbf{m}\times)(\mathbf{v}_s\cdot\nabla)\mathbf{m}$$

$$\mathbf{v}_s = \hbar\gamma P\mathbf{j}/2eM_s$$

P : current polarization

M_s: saturation magnetization

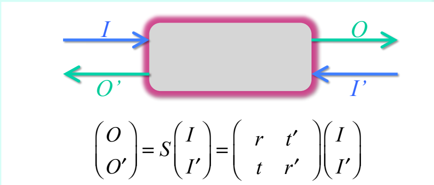
- *α* and *β* determine the magnetization dynamics of DWs: the current-induced DW velocity is ~ *β*/*α*
- The physical origin and numerical value of *β* are still under debate: for $Ni_{80}Fe_{20}$ DWs, measured values of *β* range between 0.01 and 0.13.



Methods: First-principles spin transport

α and *β* are evaluated using a scattering matrix $S(r_w)$ [1] calculated from first-principles [2]

$$\alpha = \frac{\hbar\gamma\lambda_w}{8\pi A M_s}\mathrm{Tr}\left(\frac{\partial S}{\partial r_w}\frac{\partial S^\dagger}{\partial r_w}\right) \qquad \beta = \frac{\lambda_w}{2P}\frac{\mathrm{Im}\left[\mathrm{Tr}\left(\frac{\partial S}{\partial r_w}S^\dagger\hat{\tau}_z\right)\right]}{\mathrm{Tr}(tt^\dagger)} \qquad G = \frac{e^2}{h}\mathrm{Tr}\{tt^\dagger\}$$



$$\begin{pmatrix} O \\ O' \end{pmatrix} = S\begin{pmatrix} I \\ I' \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}\begin{pmatrix} I \\ I' \end{pmatrix}$$

- Landauer-Büttiker scattering formalism implemented with TB-LMTO
- "Wave function matching" scheme to calculate scattering matrix
- Self-consistent ASA potentials based on LSDA of density-functional theory and CPA
- Spin-orbit coupling, non-collinearity and disorder on an equal footing
- 8300 atoms in scattering region, 96x96 k-points for a 5x5 lateral supercell

[1] K.M.D. Hals, A.K. Nguyen, A. Brataas, Phys. Rev. Lett. **102**, 256601 (2009).

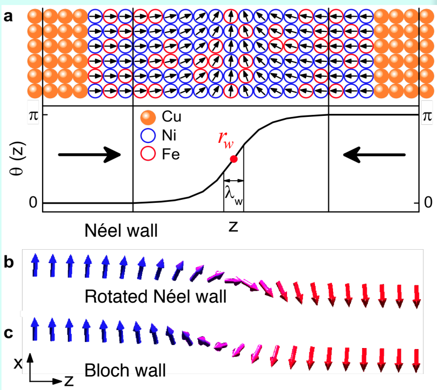
[2] K. Xia, M. Zwierzycki, M. Talanana, P.J. Kelly and G.E.W. Bauer, Phys. Rev. B **73**, 064420 (2006).

Modeling: 3 types of DWs

a) Neel wall: $\mathbf{m} = \left[\mathrm{sech}\frac{z-r_w}{\lambda_w},\ 0,\ -\tanh\frac{z-r_w}{\lambda_w}\right]$;

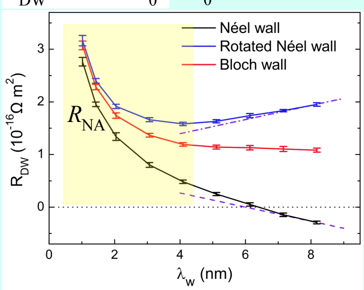
b) Rotated Neel wall: $\mathbf{m} = \left[-\tanh\frac{z-r_w}{\lambda_w},\ 0,\ \mathrm{sech}\frac{z-r_w}{\lambda_w}\right]$;

c) Bloch wall: $\mathbf{m} = \left[-\tanh\frac{z-r_w}{\lambda_w},\ \mathrm{sech}\frac{z-r_w}{\lambda_w},\ 0\right]$.



Domain-wall resistance R_{DW}:

$R_{DW} = G^{-1} - G_0^{-1}$ $\quad G_0$: without a DW.



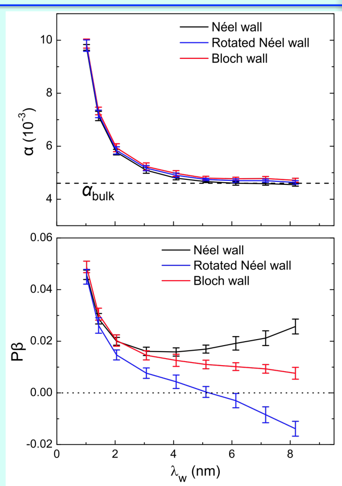
$$R_{DW} = R_{NA} + R_I + R_{AMR}$$

R_I: intrinsic DW resistance

$$R_{AMR}^{RN} = -R_{AMR}^{N} = 2\lambda_w(\rho_{//} - \rho_\perp)$$

Gilbert damping parameter *α* and out-of-plane spin torque parameter *β*:

- *α* is identical for all three types of DW because the disorder scattering is strong;
- In the adiabatic limit, DW scattering has little effect on the Gilbert damping;
- Rapidly-varying magnetization dominates the non-adiabatic behaviour of *α* and *β* in narrow DWs;
- In the adiabatic limit, *β* is NOT a constant, but a function of DW width and type. It is determined by the spin density accumulation in the DW due to spin-orbit coupling.



Conclusion: We report the results of first-principles calculations of the resistance, the effective Gilbert damping and the out-of-plane spin torque of $Ni_{80}Fe_{20}$ DWs. The rapid variation of magnetization in narrow DWs yields non-adiabatic contributions to R_{DW}, *α* and *β* that decrease with the DW width. In the adiabatic limit, the spin-orbit coupling mediated reflection of incident electrons at the DW determines R_{DW} and *β*. Surprisingly, the adiabatic *β* varies with the DW width and type. Our results should provide valuable guidance for further experimental investigations.

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