JÜLICH
FORSCHUNGSZENTRUM

Gilbert Damping from First Principles

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INSPIRE Group Seminar

Outline

- Introduction
- The Landau-Lifshitz Gilbert Equation
- Calculation of the Gilbert damping
  - Breathing Fermi Surface model
  - Torque Correlation model
  - Dynamical susceptibility
- First principles calculations
  - Heusler alloys
  - Doped Permalloy
- Conclusion and Outlook

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Introduction

Some of the inherent limitations in **electronics** have sparked the research in other methods of information storage and transfer, such as **spintronics** and **magnonics**.

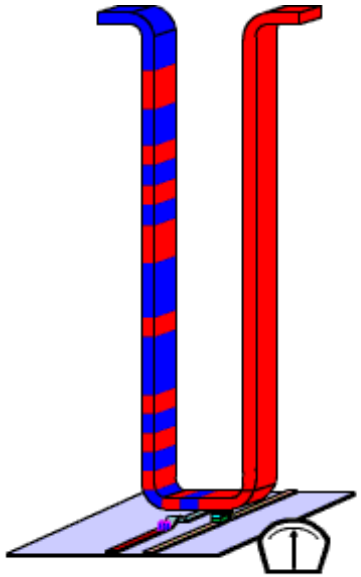
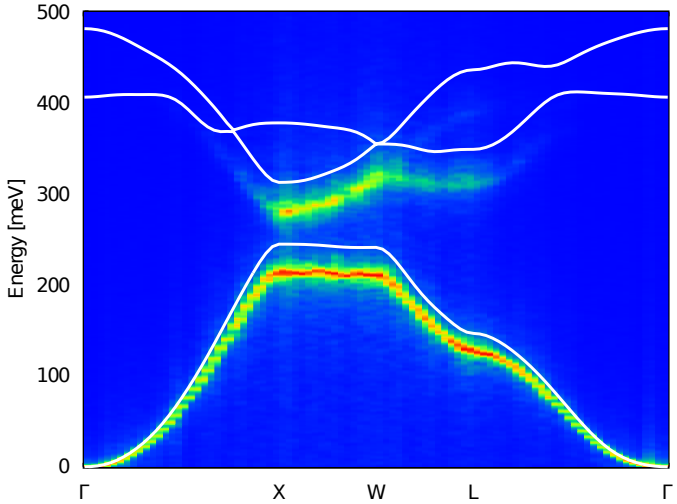


Image from http://researcher.watson.ibm.com/researcher/les/us-kproche/

Both these methods require a detailed knowledge of the **magnetization dynamics.**



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Magnetization dynamics

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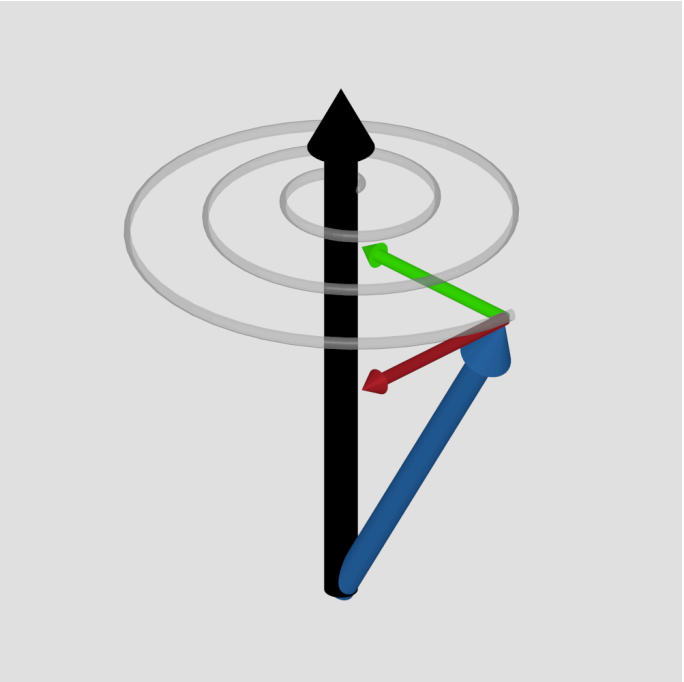
The Landau-Lifshitz Gilbert Equation

The equation of motion is the Landau-Lifshitz-Gilbert (LLG) equation

$$\frac{d\vec{M}}{dt} = -\frac{\gamma}{(1+\alpha^2)}\left[\vec{M}\times\vec{B}_{eff} + \frac{\alpha}{M}\vec{M}\times\left(\vec{M}\times\vec{B}_{eff}\right)\right]$$

Precession Damping

- The magnitude of the magnetization is kept constant.
- The magnetization is a 3D vector.
- α is the Gilbert damping.
- γ is the gyromagnetic ratio.
- $\vec{B}_{eff}$ is the effective field.



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Gilbert damping

- Responsible for energy and angular momentum transfer from magnetic system to the lattice.
- In experiments both **extrinsic** and **intrinsic** contributions are present.
- In general a **tensor**, usually treated as a **constant**. In general **non-local**.
- Can depend of frequency. Usually Gilbert damping considered only for ferromagnetic precession.

Fähnle, M. *et al.* J. Phys. D: Appl. Phys. **41**, 164014 (2008)

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Calculation of the Gilbert damping

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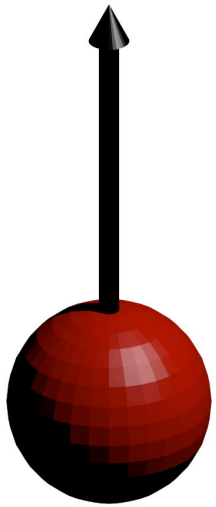
Breathing Fermi Surface model (BFS)

- Change in magnetization direction, $\delta\hat{m}$, due to SOC, changes population, f, and occupation numbers, n, of states around E_F.
- The change in population modifies the Fermi surface, making it “breathe”
- Lag in time between between the change in electrons and magnetic moments leads to damping.



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Breathing Fermi Surface model (BFS)

- The equilibrium single particle energies, ε, are kept.
- The change in occupation must result from electronic scattering.
- The scattering takes some time τ.
- τ is usually taken as a parameter.

$$n(j,\boldsymbol{k}) = f_{j,\boldsymbol{k}}(t) - \tau_{j,\boldsymbol{k}} \frac{d\, f_{\boldsymbol{i},\boldsymbol{k}}}{dt}$$

$$\alpha_{\mu\nu} = -\frac{\gamma}{|M|} \sum_{j,\boldsymbol{k}} \tau_{j,\boldsymbol{k}} \frac{\partial f_{j,\boldsymbol{k}}}{\partial \varepsilon_{j,\boldsymbol{k}}} \frac{\partial \varepsilon_{j,\boldsymbol{k}}}{\partial \delta \hat{m}_\mu}\bigg|_M \frac{\partial \varepsilon_{j,\boldsymbol{k}}}{\partial \delta \hat{m}_\nu}\bigg|_M$$

Kambersky, V. Czech. J. Phys. B **26**, 1366 (1976)

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Torque Correlation Model (TCM)

- The non-commutation of the Hamiltonian with the spin, due to SOC, generates a torque acting over the electrons.

- Uses the magnetic Torque operator $\mathrm{T}_\mu = \frac{\partial \mathcal{H}}{\partial \delta \hat{m}_\mu} = \beta B(\boldsymbol{r}) \sigma_\mu \cdot \delta \hat{m}_\mu$

- $$\alpha_{\mu\nu} = -\pi\hbar \sum_{i,j} \frac{\partial \delta \hat{m}_\mu}{\partial t} \frac{\partial \delta \hat{m}_\nu}{\partial t} \left\langle \psi_i \left| \frac{\partial \mathcal{H}}{\partial \delta \hat{m}_\mu} \right| \psi_j \right\rangle \left\langle \psi_j \left| \frac{\partial \mathcal{H}}{\partial \delta \hat{m}_\nu} \right| \psi_i \right\rangle$$

$$\delta(\epsilon_F - \epsilon_i)\delta(\epsilon_F - \epsilon_i)$$

- Dependence on scattering times can be eliminated.

Kuneš, J. And Kambersky, V. Phys. Rev. B **65**, 212411 (2002)
Brataas, A. *et al.* Phys. Rev. Lett. **101**, 037207 (2008)

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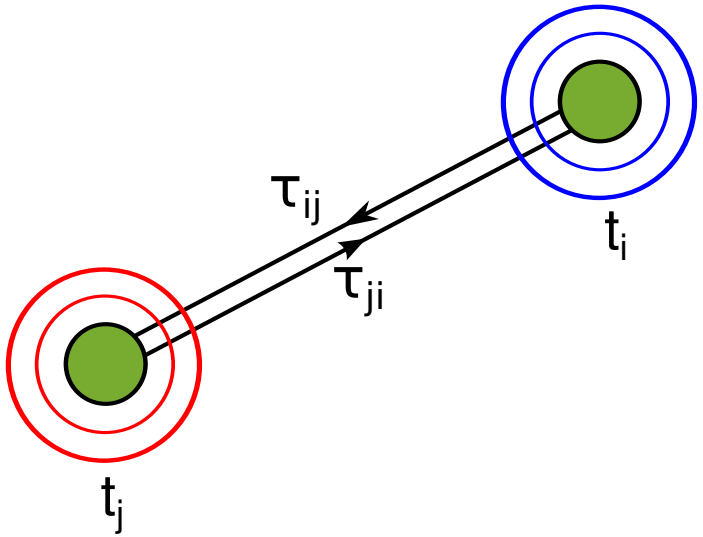
Torque Correlation Model (TCM)

- Temperature dependence can be included via CPA analogies.
- Vertex corrections can be included to improve the description.
- It can readily be expressed in the KKR formalism, to take into account the details of the scattering processes.



Sketch of the KKR treatment of the DFT problem. Making use of single site scattering matrices, t_i and the scattering path operators τ_{ij}

$$\alpha = \frac{g}{\pi |M|} \sum_n \underline{T}^{0\mu} \underline{\tau}^{0n} \underline{T}^{n\mu} \underline{\tau}^{n0}$$

Ebert, H. *et al.* Phys. Rev. Lett. **107**, 066603 (2011)
Ebert, H et al. Phys. Rev. B **91**, 165132 (2015)

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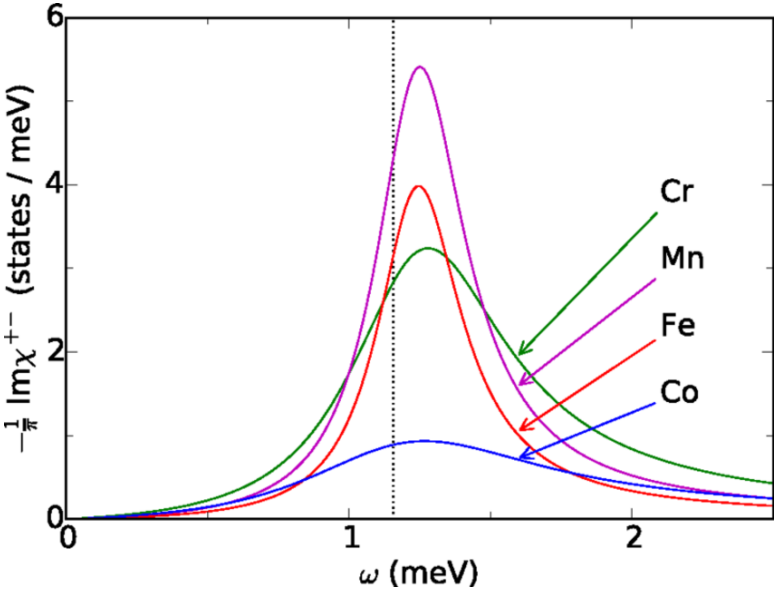
Dynamical susceptibility

- The dynamical susceptibility can be obtained via linear response TD-DFT.
- The response of the system to a magnetic field allows one to obtain the damping.
- It allows for multiple contributions not captured from other methods, such as spin pumping.



Imaginary part of the dynamical susceptibility for adatoms on Pt(111).

Schweflighaus, B. et al. Phys Rev B. ***93****, 035451 (2016)*

Louins, S. *et al.* Phys. Rev. B. **91**, 104420 (2015)

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First principle calculations

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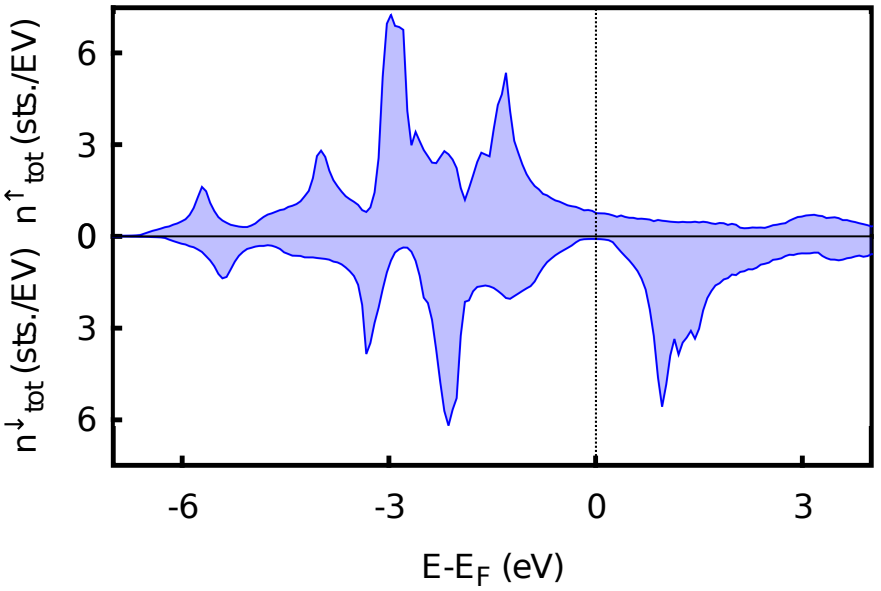
NiMnSb half-Heusler

- Potential candidates for spintronic/magnonic applications.
- Half-metallic nature can lead to
  - High *Tc* and spin stiffness *A*.
  - Low damping parameters.
- Alloying can be used to tailor properties, in particular the damping.



Density of states for NiMnSb. The gap in one of the spin channels showcases its half-metallic nature.

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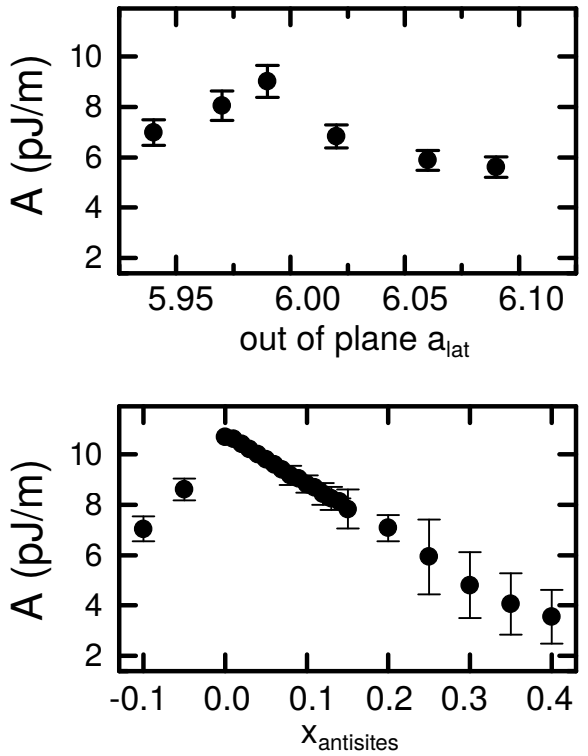
NiMnSb half-Heusler

- Exchange stiffness obtained from FMR experiments.
- Off-stochiometric $Ni_{1-x}Mn_{1+x}Sb$ half-Heusler.
- Experimental and theoretical trends agree well.
- The stiffness decreases due to AFM ordering of Mn moments in different sublattices.
- Error bars in theory due to supercell averages.



Exchange stiffness A for $Ni_{1-x}Mn_{1+x}Sb$. Negative values for x imply the introduction of Ni Mn antisites and positive values are related to Mn Ni antisite defects.

Dürrenfeld, P., *et al.* Phys. Rev. B. **92**, 214424 (2015)

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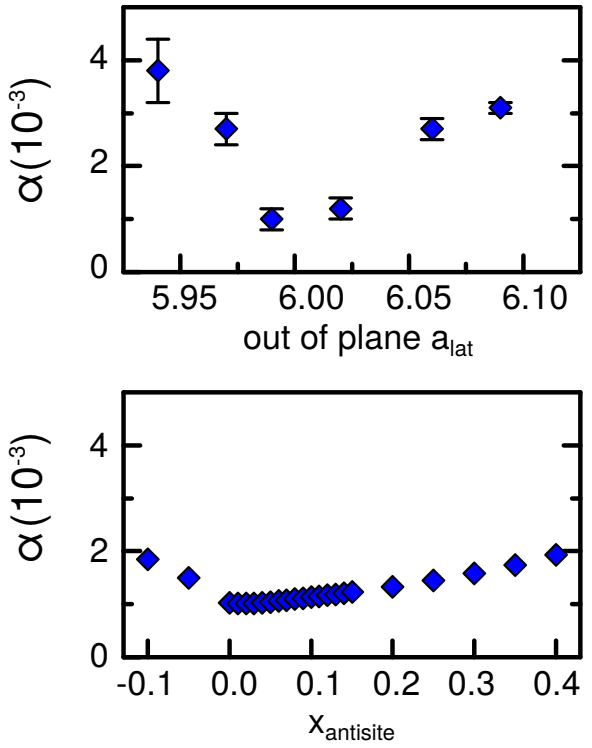
NiMnSb half-Heusler

- Gilbert damping experimentally measured via FMR.
- Theoretical calculations match well with experiments.
- Theoretical damping is smaller than the measured values.
  - Extrinsic effects.
  - Approximations in the models.
- Temperature effects taken via an alloy analogy



Gilbert damping, α, for $Ni_{1-x}Mn_{1+x}Sb$. Negative values for x imply the introduction of Ni Mn antisites and positive values are related to Mn Ni antisite defects.

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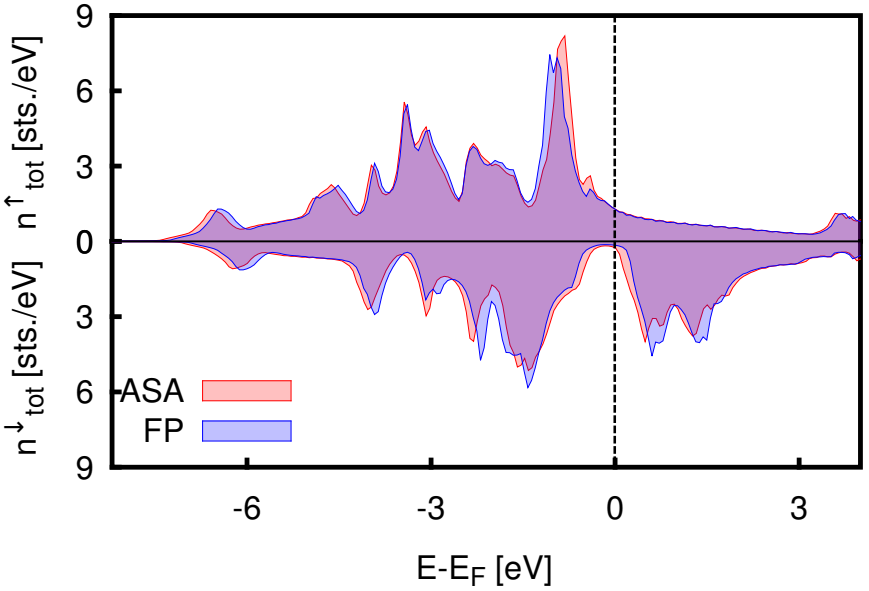
Full Heusler Co_2MnZ, Co_2FeZ and Mn_2VZ

- Effect of Z=(Al, Si, Ga, Ge) on magnetic properties.
- Under several approximations the materials are half-metallic.
- They are predicted to have small damping.
- A systematic study using different approximations was performed.



Density of states for Co_2MnSi in LSDA, when the potential is taken in ASA or a Full Potential approach.

Chico, J., *et al.* Phys. Rev. B. **93**, 214439 (2016)

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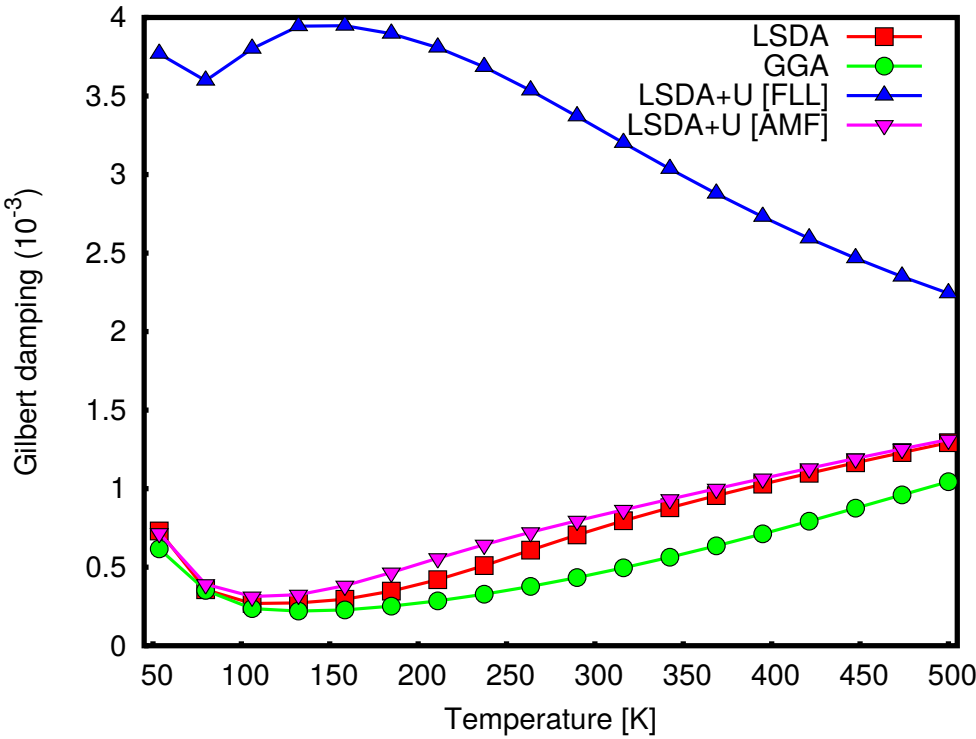
Temperature dependence

- The damping shows the expected conductivity-like behaviour at low temperatures and resistivity like at high temperatures.
- LDA+U with double counting in the fully localized limit result in unexpected behaviour.
  - This is due to the lost of HM in this approach.



Temperature dependence of the damping fotrCo_2MnSi

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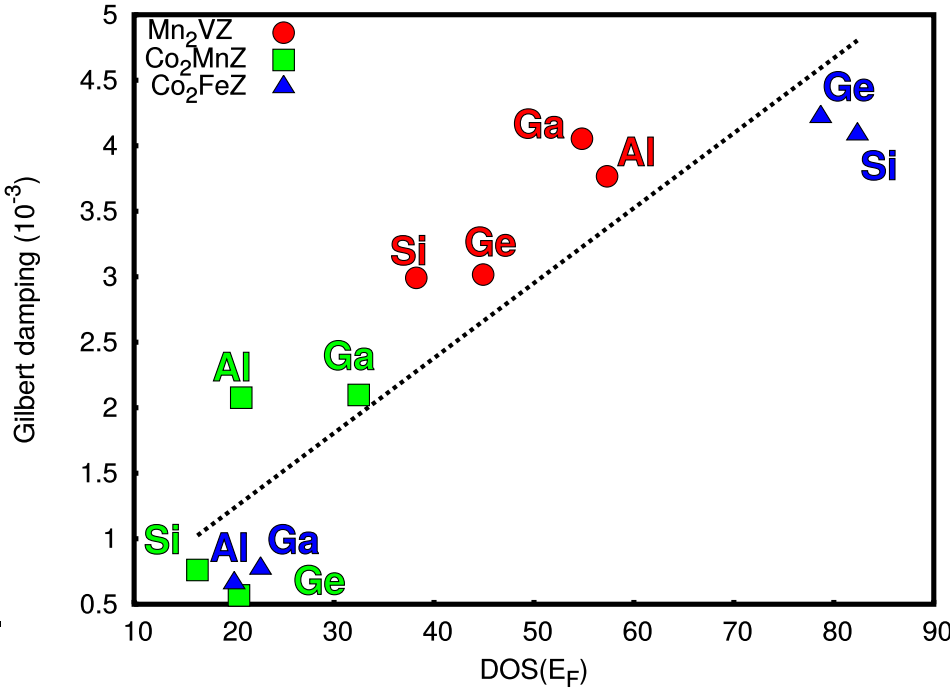
Influence of the DOS at the Fermi level

- Gilbert damping is correlated to the DOS.
- Overall values are smaller than experiments.
- Obtained values match with previous calculations.
- Loss of half-metallicity leads to higher damping than expected, e.g. $Co_2Fe(Ge,Si)$.



Correlation between the DOS at the E_F and the Gilbert damping When ASA and LSDA are considered.

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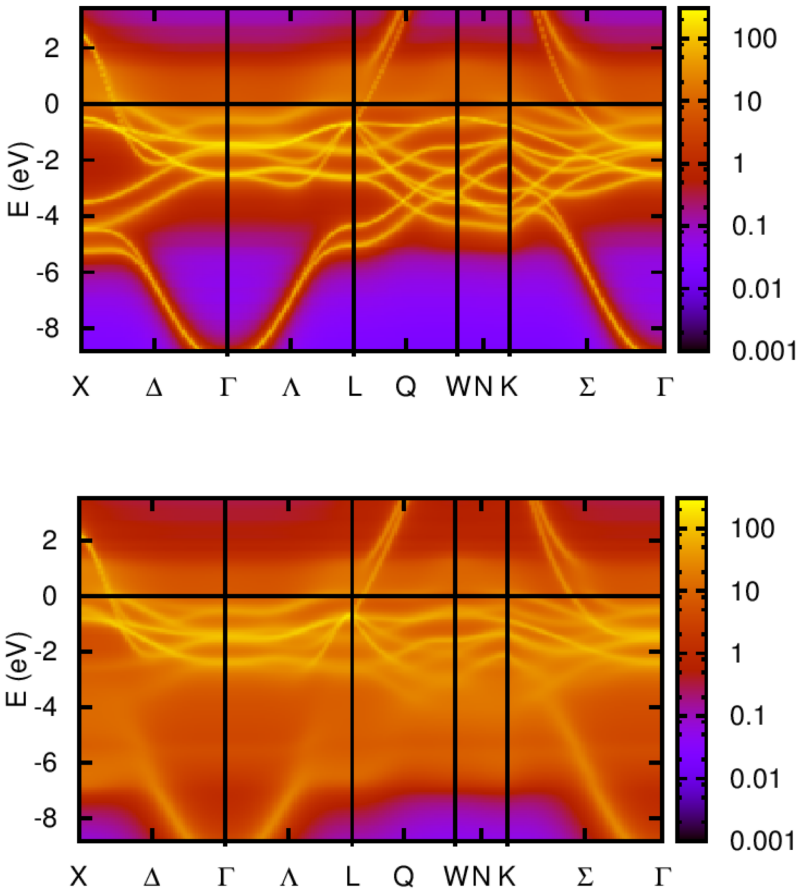
Doped Permalloy

- Magnetic compound in the fcc structure $Ni_{0.80}Fe_{0.20}$.
- Widely used in experiments and industrial applications.
- Small damping. Small anisotropy.
- *4d* and *5d* elements can be doped in small concentrations.
  - Damping.
  - Saturation magnetization.
  - Exchange stiffness.



Bloch spectral function of pure Py and doped with 20% of Pt impurities.

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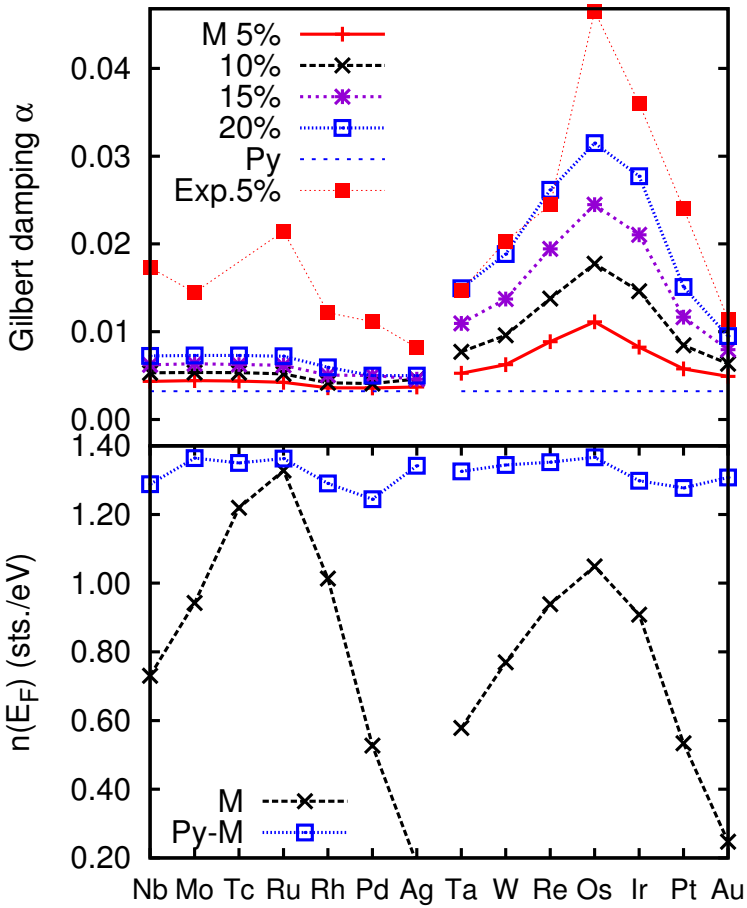
Doped Permalloy

- DOS at *EF* correlates with changes in damping across the series.
- Doping with 4*d* elements results in smaller damping than with 5*d*s.
  - This is due to the effect of SOC.
- Higher concentrations of defect also increase the damping.

Calculated Gilbert damping for T = 10K. Exp. data at T = 300K.



Total (blue) and impurity (black) density of states at the Fermi level E_f for 10% impurities in Py.

Pan, F. *et al.* Phys. Rev. B. **94**, 214410 (2016)

Rantschler, J.O. *et al.* J. Appl. Phys. **101,** 033911 (2007)

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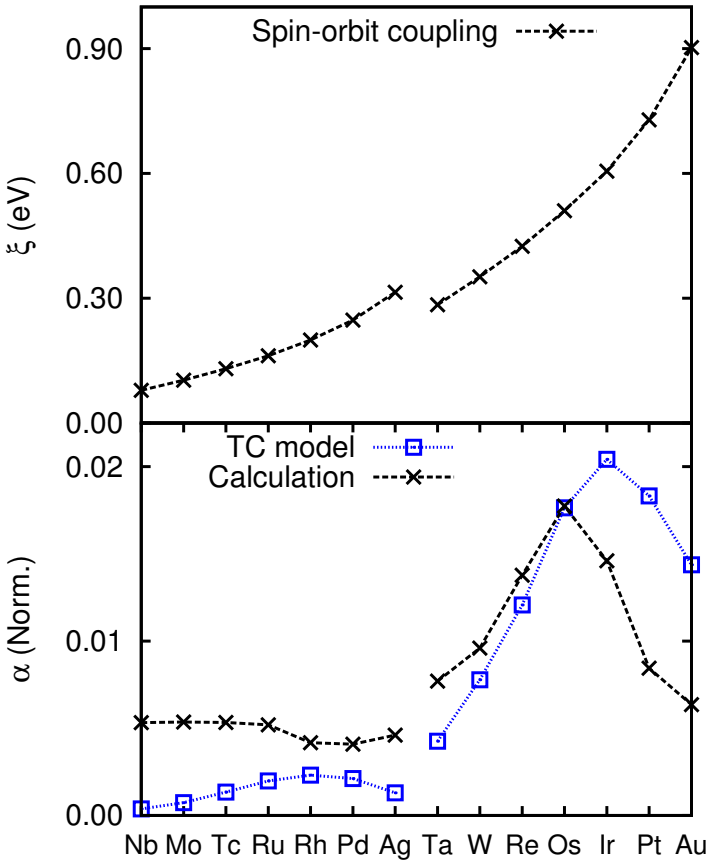
Doped Permalloy

- SOC parameter, ξ, increases across the series.
- One can compare with the TCM model result.

$$\alpha = \frac{1}{\gamma M_s}\left(\frac{\gamma}{2}\right)^2 n(E_F)\xi^2 \frac{(g-2)^2}{\tau}$$

- The simplified TCM calculation corresponds well with the calculations.

Strength of SOC of d-electrons of the impurity atoms.



Comparison between DFT calculations and the TCM for the system with 10% of impurity concentration.

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Conclusions

- The TCM model can be used to calculate the intrinsic Gilbert damping, yielding values in good agreement with experiments.
- As expected from the BFS and TCM models the DOS at the E_F and SOC play a large role in the value of the damping.
- Temperature effects can also play a large role in the behaviour of the damping.
- Hesuler alloys and Permalloy are materials which can exhibit very low damping parameters, which can be tuned via doping.

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Outlook

- The divergence of the damping at low temperature, i.e. low scattering rates, might not be correct. *J. Phys. Condens. Matter. 28, 086004 (2016)*
- Similar approaches can be used to calculate the non-adiabatic parameter. *Phys. Rev. B 79, 104416 (2000)*
- Effects of the non-locality and tensorial nature of this objects in the dynamics of magnetic textures.

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Acknowledgments

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Thank you for your attention!
Questions?

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