FIRST-PRINCIPLES CALCULATION OF MAGNETIZATION RELAXATION WITH THERMAL DISORDER

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Landauer-Büttiker transmission formalism

Conductance $G = \frac{e^2}{h}\mathrm{Tr}\{tt^\dagger\}$

Scattering theory of magnetization relaxation [1]

The Gilbert damping in the Landau-Lifshitz-Gilbert equation

$$\frac{d\vec{M}}{dt} = -\gamma\vec{M}\times\vec{H}_{\mathrm{eff}} + \frac{\tilde{G}(\vec{M})}{\gamma M^2}\vec{M}\times\frac{d\vec{M}}{dt}$$

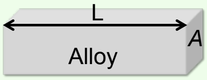
is evaluated using the scattering matrix S as

$$\tilde{G}_{ij} = \frac{\gamma^2\hbar}{4\pi}\mathrm{Re}\left\{\mathrm{Tr}\left[\frac{\partial S}{\partial m_i}\frac{\partial S^\dagger}{\partial m_j}\right]\right\} \text{ with } S(\mathbf{m}) = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

$\vec{\mathbf{m}}$ changes $S(\vec{\mathbf{m}})$ through *spin-orbit coupling*

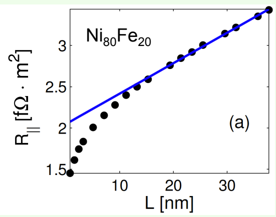
Scattering calculation for alloys

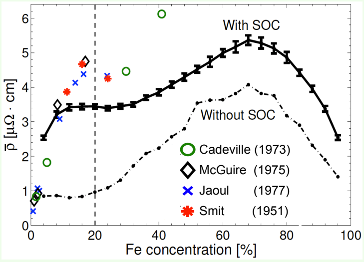
Scattering from *intrinsic chemical disorder*



fcc $Ni_{1-x}Fe_x$

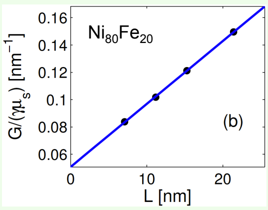
Resistance $R = \rho L$

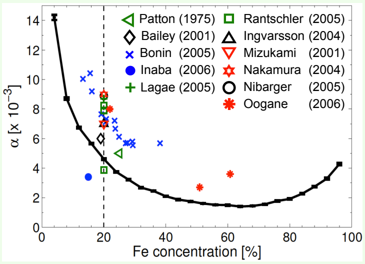




Gilbert damping parameter

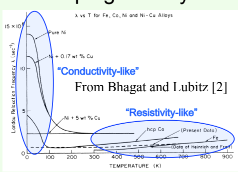
$$\alpha = \frac{\tilde{G}}{\gamma M} = \frac{\tilde{G}}{\gamma\mu_s L} \quad \mu_s = M/L$$





With intrinsic chemical disorder and SOC, scattering theory is capable of describing the resistivity and Gilbert damping of alloys.

! For clean metals, the resistivity increases with temperature, and non-monotonic Gilbert damping is experimentally observed as a function of temperature.

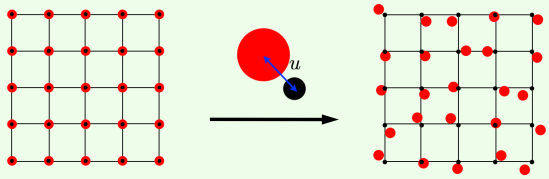


We need to introduce temperature dependent disorder.

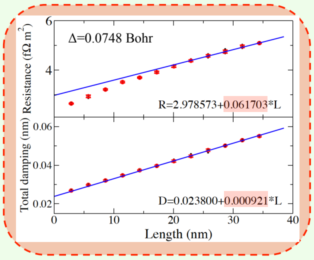
[1] A. Brataas, Y. Tserkovnyak, G.E.W. Bauer, Phys. Rev. Lett. **101**, 037207 (2008).
[2] S.M. Bhagat and P. Lubitz, Phys. Rev. B **10**, 179 (1974).
[3] K. Gilmore, Y.U. Idzerda, and M.D. Stiles, Phys. Rev. Lett. **99**, 027204 (2007).

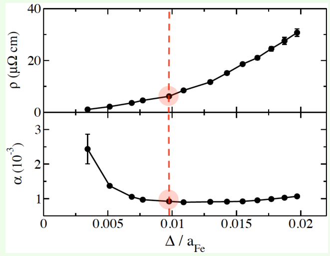
Thermal disorder in clean metals

We define *thermal disorder* by displacing atoms in the scattering region with a random Gaussian distribution characterized by the root-mean-square displacements $\Delta = \sqrt{\langle u^2\rangle}$.

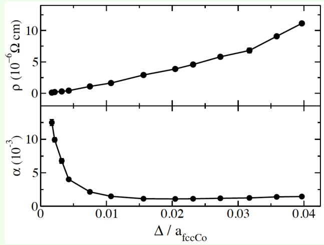


bcc Fe

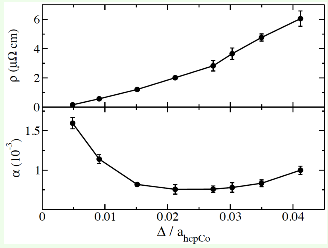




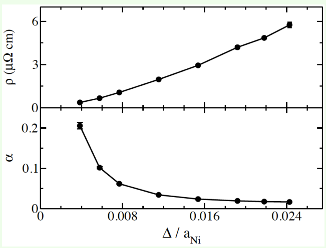
fcc Co



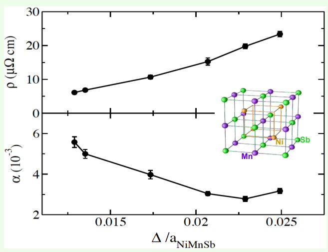
hcp Co



fcc Ni



Heusler alloy: NiMnSb



Minimum of $\tilde{G}$ (10^8 s^{-1})	bcc Fe (001)	hcp Co (0001)	fcc Ni (111)	NiMnSb (001)
Experiments [2]	8.8	9	29	3.94
Gilmore *et al.* [3]	5.4	3.7	21	–
This work	3.9	2.3	20	4.38

Future work:

1) map the displacements onto real temperatures using Debye model;
2) calculate phonon spectrum to get more realistic atomic distribution.

Conclusion: Within the framework of scattering theory, we calculate resistivity and Gilbert damping for permalloy with intrinsic chemical disorder, and obtain results in very good agreement with experiment. For clean metals, we introduce thermal disorder and obtain both conductivity-like and resistivity-like damping behaviour as observed in experiment. This method is also applicable to alloys.

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SEVENTH FRAMEWORK PROGRAMME

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