

# Ab-initio calculations of the stiffness constants $D$ and $A_{\text{ex}}$ for permalloy doped with V, Gd, and Pt

Which factors *really* matter?

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# Outline

- ▶ Why to care? What to look for? How to do it?
- ▶ Trends of  $D$  and  $A_{\text{ex}}$  stiffness with concentration.  
Comparison with experiment
- ▶ Role of the polarizability of the dopant.
- ▶ Size of the regio that really matters:  
Simple *ansatz* for spin wave stiffness  $D$ .
- ▶ Conclusions.

# Doped permalloy

Doping:

promising way to modify the properties of (not only) magnetic materials.

Permalloy (Py):  $\text{Fe}_{19}\text{Ni}_{81}$

- ▶ fcc structure
- ▶ high magnetic permeability
- ▶ high and low electrical conductivity in the majority and minority spin channels

# Why to care about the stiffness?

Micromagnetics:

Continuum approximation, the angle of the magnetization changes slowly over atomic distances, spin vectors are replaced by a continuous function  $\mathbf{m}(\mathbf{r})$ .

$$E[\mathbf{m}] = \int_V d\mathbf{r} \left\{ A_{\text{ex}} \left[ \left( \frac{\partial \mathbf{m}}{\partial x} \right)^2 + \left( \frac{\partial \mathbf{m}}{\partial y} \right)^2 + \left( \frac{\partial \mathbf{m}}{\partial z} \right)^2 \right] + \dots \right\}$$

Exchange stiffness  $A_{\text{ex}}$ , spin wave stiffness  $D$ :

$$A_{\text{ex}} = \frac{D M_s}{2g\mu_B}$$

$M_s$  is saturation magnetization,  $g$  is Landé factor ( $g \approx 2$  for metals).

# What to look for

Understand better the mechanism how different dopants affect the spin wave and exchange stiffness.

Earlier suggestions:

**Polarizability** of the dopant will be an important factor.

This is *plausible* but is it also *correct*?

Look for a **simple model** that would enable a quick estimate how the stiffness will change upon a doping.

# Spin stiffness $D$ from exchange coupling constants (1)

By relying on the Heisenberg Hamiltonian

$$H = - \sum_{ij} J_{ij} \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j \quad ,$$

one arrives (for isotropic systems) to

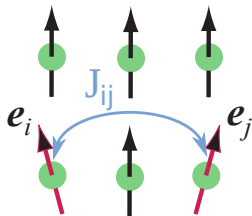
$$D = \sum_j \frac{2\mu_B}{3M} J_{0j} R_{0j}^2 \quad .$$

$R_{0j}$  is the interatomic distance.

Convergence issues solved by introducing the **damping parameter  $\eta$** :

$$D = \lim_{\eta \rightarrow 0} D(\eta) = \lim_{\eta \rightarrow 0} \sum_j \frac{2\mu_B}{3M} J_{0j} R_{0j}^2 \exp\left(-\eta \frac{R_{0j}}{a_0}\right) \quad .$$

$a_0$  is lattice parameter.



[Pajda *et al.* PRB **64**, 174402 (2001)]

## Spin stiffness $D$ from exchange coupling constants (2)

For alloys:

Atomic types labeled by  $\alpha$ , lattice sites labeled by  $j$ .

Concentration for a type  $\alpha$  is  $c_\alpha$  and magnetic moment  $\mu_\alpha$ .

Pairwise exchange coupling constant  $J_{0j}^{(\alpha\beta)}$  for atom of type  $\alpha$  at the origin and atom of type  $\beta$  at the site  $j$ .

$$D = \lim_{\eta \rightarrow 0} D(\eta),$$

$$D(\eta) = \sum_{\alpha} c_{\alpha} D_{\alpha}(\eta),$$

$$D_{\alpha}(\eta) = \sum_j \sum_{\beta} c_{\beta} \frac{2\mu_B}{3\sqrt{|\mu_{\alpha}|}|\mu_{\beta}|} J_{0j}^{(\alpha\beta)} R_{0j}^2 e^{-\eta \frac{R_{0j}}{R_{01}}}.$$

## Role of magnetic moments of the dopants

$$D = \lim_{\eta \rightarrow 0} \sum_{\alpha} c_{\alpha} \left[ \sum_j \sum_{\beta} c_{\beta} \frac{2\mu_B}{3\sqrt{|\mu_{\alpha}| |\mu_{\beta}|}} J_{0j}^{(\alpha\beta)} R_{0j}^2 e^{-\eta \frac{R_{0j}}{R_{01}}} \right].$$

Moments on **V** and **Pt** atoms are **induced**. When tilted, they follow magnetization direction of their neighbors.

Their participation can be *questioned*.

[Finite temperature: Polesya *et al.* PRB **82**, 214409 (2010)].

Our default: V and Pt moments **support** the orientations of moments at Fe and Ni but **do not contribute** to  $D$  directly.

The moments of **Gd** atoms are **intrinsic**: treat them in the same way as moments of Fe or Ni atoms.



# Computational method

Korringa-Kohn-Rostoker (KKR) Green function: SPRKKR.

Scalar-relativistic, atomic sphere approximation (ASA), coherent potential approximation (CPA).

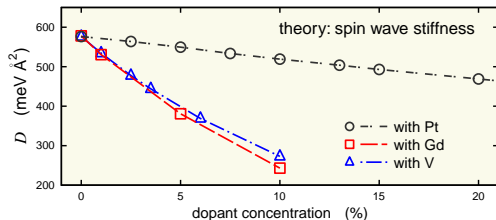
**Gd atoms:** electronic structure via the open core formalism ( $f$  electrons treated as tightly bound core electrons, their number kept fixed during the self-consistency loop).

Spoiler: it does not really matter. . .

$J_{0j}^{(\alpha\beta)}$  constants via the prescription of Liechtenstein *et al.*

Taking the limit  $\lim_{\eta \rightarrow 0} D(\eta)$  delicate but manageable.

# Spin wave stiffness and exchange stiffness

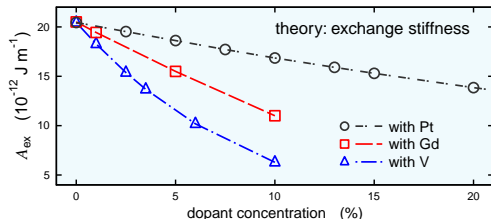


For spin wave stiffness  $D$  trends for V and Gd dopants are similar.

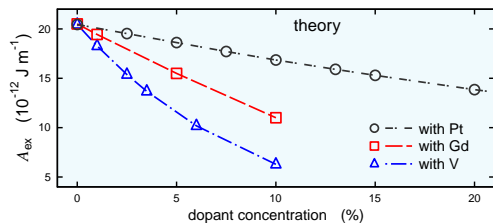
For exchange stiffness  $A_{\text{ex}}$  trend for V and Gd dopants differ because the magnetization differs:

$$A_{\text{ex}} = DM_s / (2g\mu_B)$$

Moments of V are small and antiparallel to moments of the host, moment of Gd are large and parallel to moments of the host.



# Exchange stiffness: theory and experiment



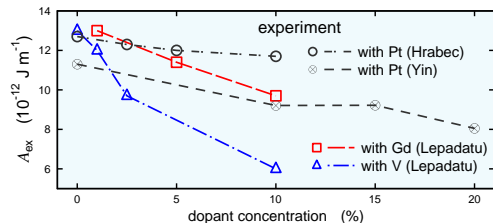
Trends of  $A_{\text{ex}}$  with dopant concentration reproduced.

Differences in absolute values:

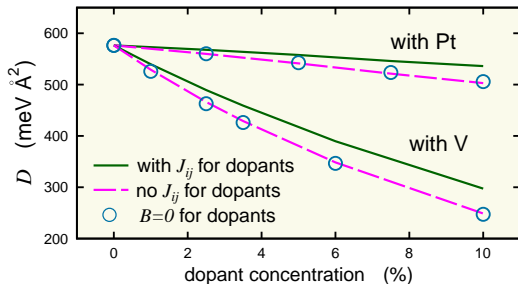
Partly due to the temperature effect.

Partly due to problems in describing magnetism Ni via  $J_{ij}$ 's.

(Similar difference found earlier for undoped Py, larger difference found for Ni.)



# Role of the polarizability of the dopant



*Full lines:*  $J_{ij}^{(\alpha\beta)}$ 's for V or Pt in the same way as for Fe and Ni.

*Dashed lines:*  $J_{ij}^{(\alpha\beta)}$ 's for V or Pt completely ignored.

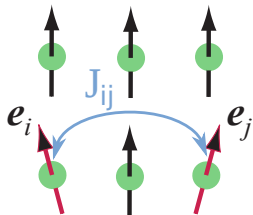
*Circles:* exchange field  $B$  for the dopant atoms suppressed.

Polarizability of the dopants **does not have a significant influence** on the spin wave stiffness  $D$  of doped permalloy.

# Size of the region that *really* matters (1)

Recall the basic equation for  $D$ :

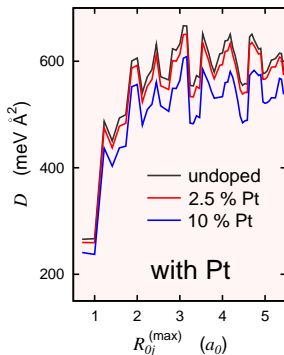
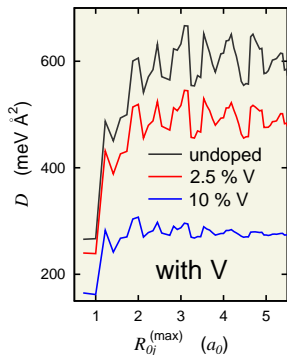
$$D = \sum_j \frac{2\mu_B}{3M} J_{0j} R_{0j}^2 .$$



How far do we have to go with the sum over the sites  $\sum_j$  ?

What is the largest inter-atomic distance  $R_{0j}$  that has to be taken into account?

## Size of the region that *really* matters (2)



$$D = \sum_j \frac{2\mu_B}{3M} J_{0j} R_{0j}^2$$

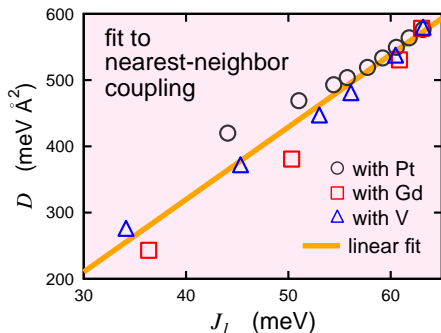
Dependence of  $D$  on the maximum distance  $R_{0j}^{(\max)}$  included in the sum over sites.

**Significant** variations of the spin wave stiffness constant  $D$  only within **few nearest shells**.

Afterwards,  $D$  just oscillates around the mean value.

Including large distances  $R_{0j}$  is thus necessary just for technical reasons.

# Stiffness and nearest-neighbors exchange coupling (1)



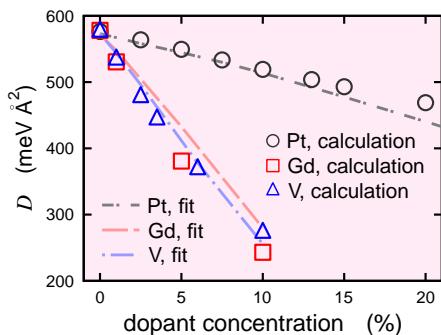
Define *effective coupling* originating from the nearest neighbors only:

$$J_1 = \sum_{\alpha} c_{\alpha} 12 \sum_{\beta} c_{\beta} J_{01}^{(\alpha\beta)}$$

Linear fit:  $D = 109.4 J_1 - 118$

**Universal** fit, for various concentrations and **different dopant atoms**.

## Stiffness and nearest-neighbors exchange coupling (2)



For each dopant concentration:  
(i) evaluate effective nearest-neighbor coupling  $J_1$ ,  
(ii) from this  $J_1$  evaluate  $D$  via the fit

$$D = 109.4 J_1 - 118 .$$

*Trend* of the spin wave stiffness  $D$  with the dopant concentration is, to a decisive degree, determined just by the **coupling among the nearest neighbors**.



# Conclusion

- ▶ Calculated exchange stiffness constant  $A_{\text{ex}}$  decreases with increasing dopant concentration, **in agreement with experiment.**
  - ▶ The influence of V-doping and of Gd-doping on the spin wave stiffness  $D$  is very similar. The difference in the trends for the exchange stiffness  $A_{\text{ex}}$  comes from the differences in the magnetization  $M_S$ .
- ▶ **Polarizability** of the dopant is **not** an important factor for the spin wave stiffness  $D$  (unlike what was conjectured before).
- ▶ The **trends** of the spin wave stiffness  $D$  when the dopant concentration is varied can be discussed by considering the influence of the atoms in the **first coordination shell.**

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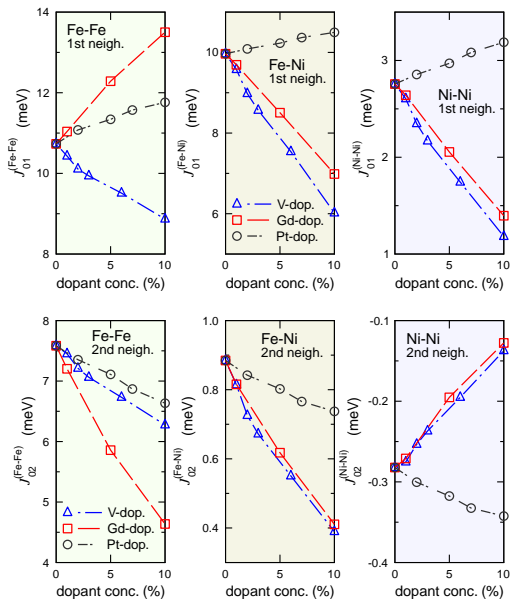


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# Exchange coupling constants



## GGA and open-core results for Gd dopants

conc. (%)	open-core potential		GGA potential	
	$M_s$ ( $\mu_B/\text{cell}$ )	$D$ ( $\text{meV \AA}^2$ )	$M_s$ ( $\mu_B/\text{cell}$ )	$D$ ( $\text{meV \AA}^2$ )
1.0	1.067	531	1.066	532
5.0	1.244	381	1.239	387
10.0	1.477	243	1.463	250

Magnetic moments per unit cell  $M_s$  and spin waves stiffness constant  $D$  for Gd-doped Py obtained by taking the potential from the open-core calculations and from the GGA-based band structure calculations.

# Technical details of the calculations

$62 \times 62 \times 62$  **k**-points in full BZ.

Angular momentum expansion of the Green function up to  $l_{\max} = 3$ .

Interatomic distances up to  $20.5 a_0$  ( $a_0$  is the interatoms distance).  
Comprises about 136000 atoms.

Numerically reliable  $D(\eta)$  values obtained for  $\eta$  from 0.2 to 1.

Extrapolation to  $\eta = 0$  using fifth-degree polynomial.