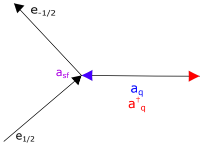


Short presentation on M3TM implementation

Theodor Griepe
Freie Universität Berlin

Meeting with Martin Weinelt, Dominic Lawrence, Unai

Outline

Microscopic Three temperature Model

experiment and simulation

Results

- UFD in Nickel, Iron, Cobalt
- Gadolinium

Outlook

- s-d-model
- Multilayer-implementation

T- and M-Dynamics for $S = \frac{1}{2}$

Dynamics of electronic, lattice and spin subsystems[1,2]

$$C_\mathrm{e}\frac{dT_\mathrm{e}}{dt} = g_{\mathrm{e-p}}(T_\mathrm{p} - T_\mathrm{e}) + S(z,t) + \frac{dQ_{se}}{dt}$$

$$C_\mathrm{p}\frac{dT_\mathrm{p}}{dt} = -g_{\mathrm{e-p}}(T_\mathrm{p} - T_\mathrm{e})$$

$$\frac{dm}{dt} = R\frac{T_\mathrm{p}}{T_C}\left(1 - \frac{m}{B_{1/2}\left(\frac{Jm}{k_B T_e}\right)}\right)$$

$$\mathrm{R} = a_{sf} 8 g_{ep} k_B T_C^2 V_{at}/(\mu_{at} E_D^2)$$

$$\frac{dQ_{se}}{dt} = Jm\frac{dm}{dt}$$

*Ab initio parameters

[1] Koopmans et al., nature materials, 2009
[2] Zahn et al., arXiv:2008.04611, 2020

M-Dynamics for arbitrary spin

material	S_{eff} [3]
Nickel	$\frac{1}{2}$
Iron	2
Cobalt	$\frac{3}{2}$

Arbitrary Spin Rate Equations [4]

$$\frac{dm}{dt} = -\frac{1}{S}\sum_{ms=-S}^{ms=+S} m_s \frac{df_{m_s}}{dt}$$

$$\frac{df_{m_s}}{dt} = -(W^{+}_{m_s} + W^{-}_{m_s})f_{m_s} + W^{+}_{m_{s-1}} f_{m_{s-1}} + W^{-}_{m_{s+1}} f_{m_{s+1}}$$

$$W^{\pm}_{m_s} = R\frac{Jm}{4Sk_BT_c}\frac{T_p}{T_c}\frac{e^{\mp\frac{Jm}{2Sk_BT_e}}}{\sinh(\frac{Jm}{2Sk_BT_e})}(S(S+1) - m_s(m_s \pm 1))$$

[3] Köbler et al., Condensed matter, 2003

[4] Beens et al., Phys. Rev. B, 2019

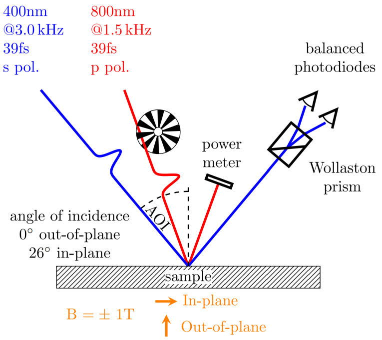
Critique of M3TM

- spin flip probability found by Koopmans very high
- Carva et al.[5] computed Elliott-Yafet $P_s^{b^2}$ and P_s, confirm discrepancy

Sample	$\mathbf{P_s{}^{b^2}}$	$\mathbf{P_s}$	Koopmans	simulated
Nickel	$0.07-0.12$	$0.04-0.09$	$0.17-0.2$	$0.05-0.067$
Cobalt	$0.06-0.11$	$0.01-0.022$	$0.135-0.165$	$0.04-0.05$
Iron	$0.07-0.14$	$0.04-0.07$		$0.03-0.05$

[5] Carva et al., Phys. Rev. B, 2013

Experimental setup



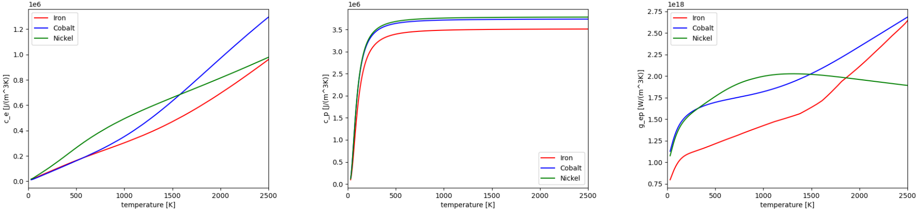
- Ni, Fe, Co thin films ($d = 15$ nm)
- magnetron sputtered on glass wafers, capped with 2 nm Ta
- MOKE technique with pump and probe pulse of FWHM$=$ 39 fs
- magnetization measured under same conditions for several pump fluences

Borchert et al., arXiv:2008.12612, 2020

simulation details

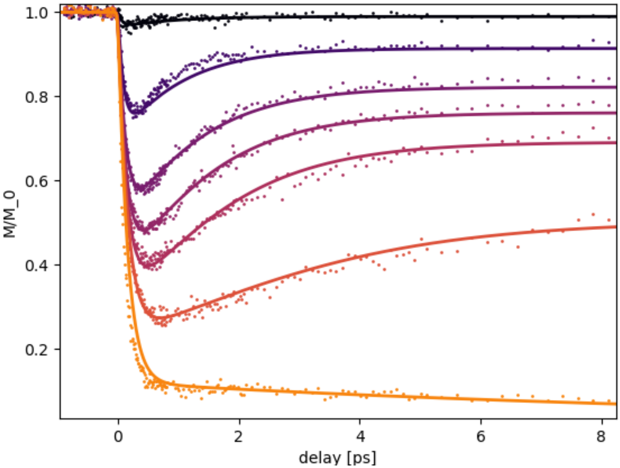
- sample treated single unit cell with uniform magnetization
- only nearest neighbor interaction
- exchange splitting $J = 3k_B T_C \frac{S}{S+1}$
- time resolution $dt = 0.1$ fs
- initial temperature $T_0 = 293K$
- **free parameters** $P_0,\ a_{sf}$

Ab initio parameters



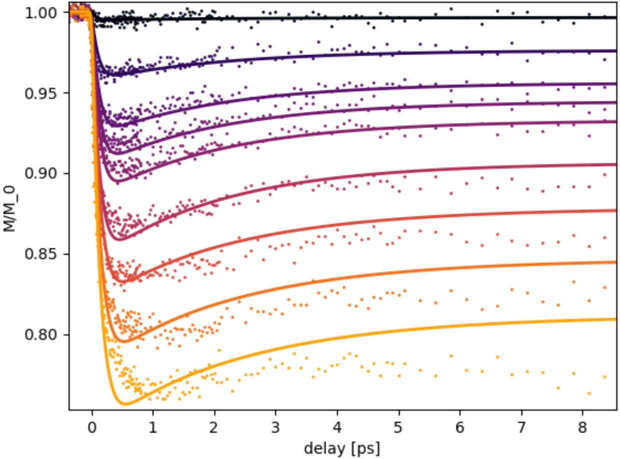
Zahn et al., arXiv:2008.04611, 2020

Nickel



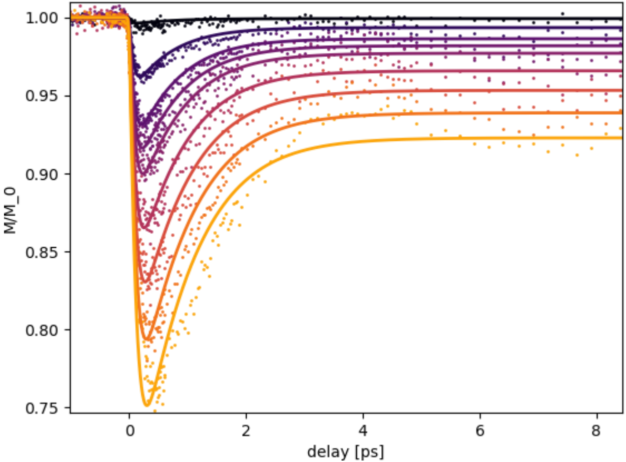
Sample	$P_s b^2$	P_s	Koopmans	simulated
Nickel	0.07 – 0.12	0.04 – 0.09	0.17 – 0.2	0.05 – 0.06
Cobalt	0.06 – 0.11	0.01 – 0.022	0.135 – 0.165	0.04 – 0.05
Iron	0.07 – 0.14	0.04 – 0.07		0.03 – 0.035

Iron



Sample	$P_s b^2$	P_s	Koopmans	simulated
Nickel	0.07 – 0.12	0.04 – 0.09	0.17 – 0.2	0.05 – 0.06
Iron	0.07 – 0.14	0.04 – 0.07		0.03 – 0.035
Cobalt	0.06 – 0.11	0.01 – 0.022	0.135 – 0.165	0.04 – 0.05

Cobalt

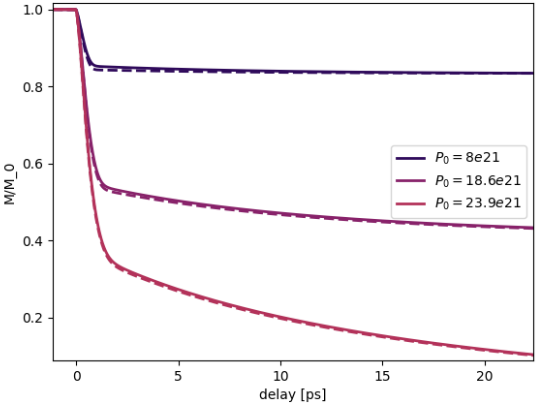


Sample	$P_s b^2$	P_s	Koopmans	simulated
Nickel	0.07 – 0.12	0.04 – 0.09	0.17 – 0.2	0.05 – 0.06
Iron	0.07 – 0.14	0.04 – 0.07		0.03 – 0.035
Cobalt	0.06 – 0.11	0.01 – 0.022	0.135 – 0.165	0.04 – 0.05

Pump Powers

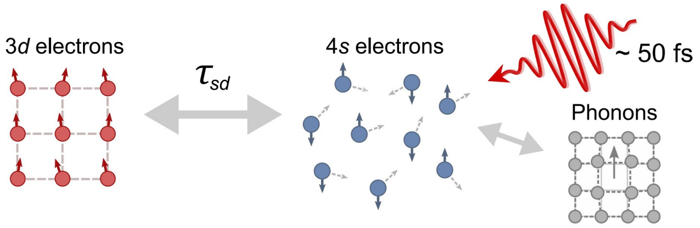
fluence [$\frac{mJ}{cm^2}$]	P_0 [$10^{21}\,\frac{W}{m^3}$] Nickel	P_0 [$10^{21}\,\frac{W}{m^3}$] Iron	P_0 [$10^{21}\,\frac{W}{m^3}$] Cobalt
0.5	1.68	1.33	1.33
3	10.08	8	8
5	16.8	13.3	13.3
6	20.3	16	16
7	23.7	18.6	18.6
9	30.5	23.9	23.9
11	38.5	29	29
13		34.2	34.2
15		39.4	39.4

Gadolinium



C_p	1.51e6 [$\frac{J}{m^3K}$]
γ_e	225 [$\frac{J}{m^3K^2}$]
g_{ep}	2.5e17 [$\frac{W}{m^3K}$]
T_C	293 [K]
T_0	50 K
R	0.184e12 [s^{-1}]
S_{eff}	3.5
μ_{at}	7.5 [μ_B]

P_0 is given in units of $\frac{W}{m^3K}$, solid lines represent regular M3TM



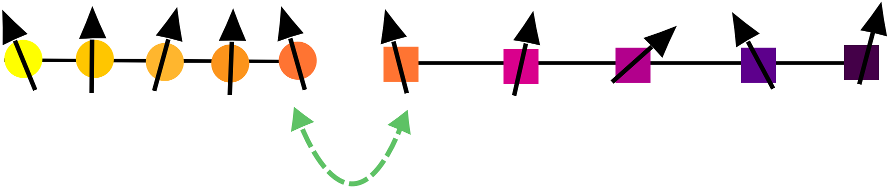
Magnetic rate equations [6]

$$\frac{dm_d}{dt} = \frac{1}{\tau_{sd}}\left(m_d - \frac{\mu_s}{2k_BT_C}\right)\left[1 - m_d \coth\left(\frac{2m_dk_BT_C - \mu_s}{2k_BT_e}\right)\right]$$

$$\frac{d\mu_s}{dt} = -\frac{\mu_s}{\tau_s} + \left(\frac{D_\uparrow + D_\downarrow}{2D_\uparrow D_\downarrow} - \frac{J_{sd}}{2}\right)\frac{dm_d}{dt}$$

[6] Beens et al., arXiv:2005.03905, 2020

Implementation of bilayers



coupling through
itenerant electrons
or
exchange interaction