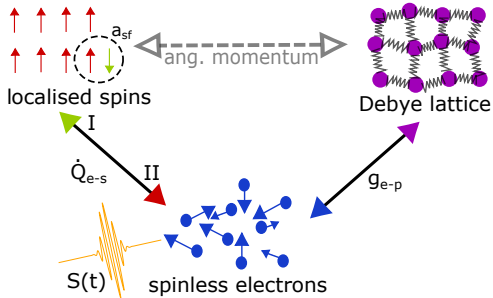


M3TM model concept



- decoupled systems of spinless electrons, phonons and localized spins in Mean field approximation (MFA)
- laser pulse heats electron system
- energy distribution to lattice and spins
(for FGT: no remagnetization so energy flow \dot{Q}_{es} (see next slide) unidirectional $e \rightarrow s$)
- spin flips (/magnon excitations) upon e-p scattering event from Elliott-Yafet spin mixing
- implicit angular momentum exchange between spins and lattice

M3TM equations

Dynamics of electronic, lattice and spin subsystems⁶

$$C_e \frac{dT_e}{dt} = g_{e-p}(T_p - T_e) + S_0 G(t, z) + \dot{Q}_{es}$$

$$C_p \frac{dT_p}{dt} = -g_{e-p}(T_p - T_e)$$

$$\frac{dm}{dt} = Rm \frac{T_p}{T_C} \left(1 - \frac{m}{B_S \left(\frac{J_m}{k_B T_e} \right)} \right)$$

$C_{e(p)}$ electron (phonon) heat capacity

g_{ep} electron phonon coupling

$\dot{Q}_{es} = Jmin/V_{at}$ energy exchange of spin-and electron system

$$R = 8 \frac{a_{sf} g_{ep} T_C V_{at}}{\mu_{at} k_B T_{Deb}^2}$$

magnetization rate parameter

a_{sf} spin flip probability upon e-p-scattering event

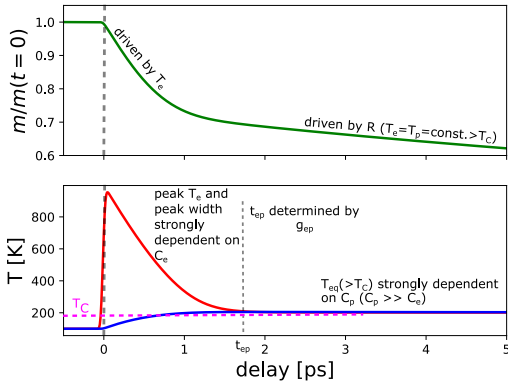
B_S Brillouin function for effective spin S

parameter impact

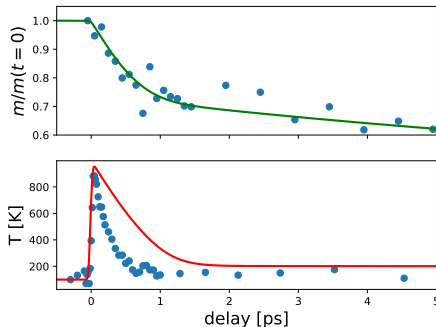
easy first attempt: take parameters used before for a very similar model

Model	symbol	meaning	estimate	unit
M3TM	$\mu_B t$	Atomic magnetic moment ^a	1.47×10^{-23}	Am ²
	γ	Electron heat capacity constant ^b	1561	Jm ⁻³ K ⁻²
	V_{at}	Atom spin density volume ^a	1.68×10^{-29}	m ³
	T_C	Curie temperature ^b	191	K
	σ	pulse width ^b	85	fs
	g_{ep}	Electron-phonon relaxation rate ^c	1.33×10^6	Jm ⁻³ K ⁻¹ ps ⁻¹
	C_p	phonon heat capacity ^c	6.28×10^6	Jm ⁻³ K ⁻¹
	E_D	Debye energy ^c	6.49×10^{-21}	J
	α_{ef}	Spin-flip probability	0.14	unity

Lichtenberg et al., arXiv:2206.01452v1

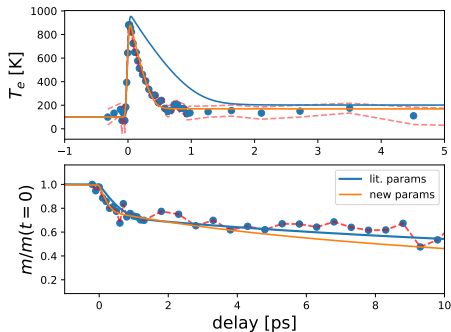


Fitting with literature parameters



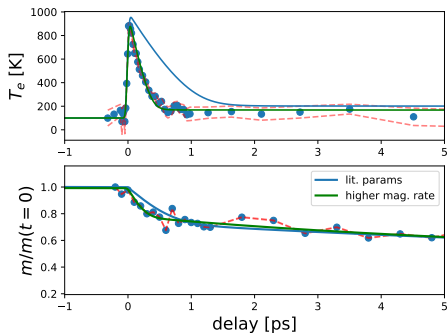
- parameters used to fit magnetization dynamics in paper cited above
- good fit of mag dynamics
- electron dynamics ≈ 3 times slower than in experiment
- equilibrium temperature too high in simulations

first try of fit adjustment



- increase c_p by a factor of 1.5 to adjust equilibrium magnetization
- increase g_{ep} by a factor of 3 to speed up electron dynamics
- decrease spin flip probability by a factor of 3 to stabilize magnetization dynamics
- → **electron dynamics well reproduced**
- **magnetization rate after e-p-equilibration seems to fast**
- **next try: increase a_{sf} at the cost of pump power to match the magnetization behaviour for $t > \tau_{ep}$**

Fitting irrespective of absorbed energies



- both T_e and m are nicely reproduced
- lattice dynamics data important to validate use of g_{ep} , c_p
- instead of rate parameter, also c_e can be changed to adapt peak of T_e and magnetization rate
- investigation for multiple fluences important (I'd like to talk again about the initial conditions and repetition rate/effective starting temperature)

New fits respecting absorbed energies

- treating experimental absorbed

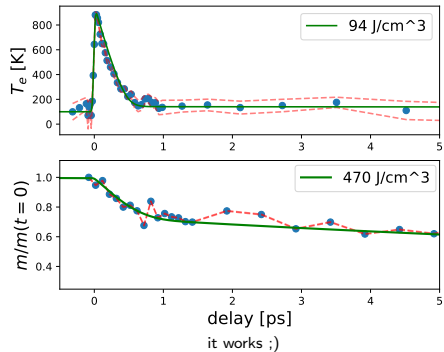
energies:

- XMCD/UED signals recorded in transmission, so average absorbed energy density can be directly used for monolayer simulations
- ARPES signal detected from hot surface of the sample, so that simulated absorbed energy adjusted by
- $E_{sim} = E_{exp} N / (\sum_{i=0}^N \exp(-\frac{idz}{\lambda}))$
- dz is unit cell thickness, λ is penetration depth of laser pulse, for $N = 1$: $E_{sim} = E_{exp}$

Absorbed energy density [$\frac{J}{cm^3}$]	measurement
98	ARPES
250-380	UED
490	XMCD

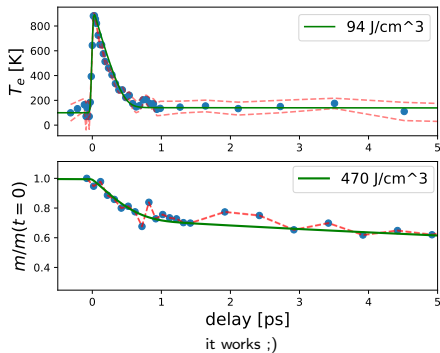
New fits respecting absorbed energies

- fix absorbed energy for ARPES signal, then adjust C_e , g_{eP} and C_p to fit data
- increase pump power by factor of 5 and hope that adjusting spin-flip probability a_{sf} (mag. rate parameter R) fits XMCD signal



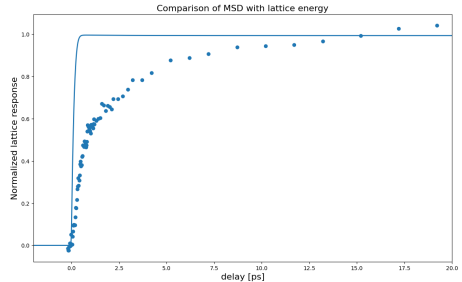
New fits respecting absorbed energies

parameter [units]	used	Fe for ref
$\gamma [\frac{kJ}{m^3 K^2}]$	0.2	≈ 0.8
$C_{p,max} [\frac{MJ}{m^3 K}]$	4	3.4
$g_{ep} [\frac{EW}{m^3 K}]$	0.44	≈ 1.5



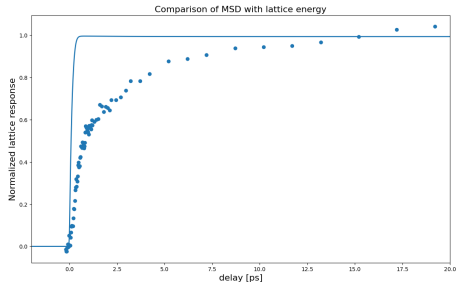
Lattice response

- fitted is norm.
 $\Delta(C_p T_p)$ to norm.
MSD
- above simulation
parameters do not fit
lattice response



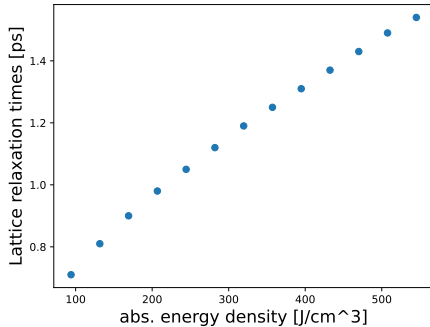
Lattice response

- lattice equilibrates on similar timescale **as electron**
temperature ≤ 1 ps
- lattice temperature **decreases** slightly over time due to $\dot{Q}_{\text{es}} < 0$



Lattice relaxation times

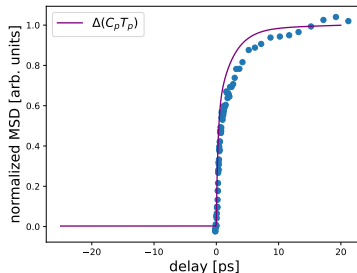
- lattice equilibrates way slower than electrons



Multi-lattice modeling

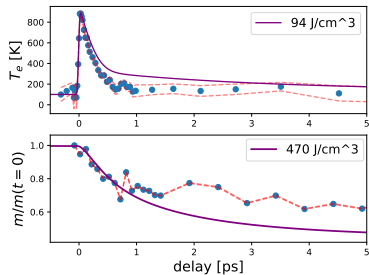
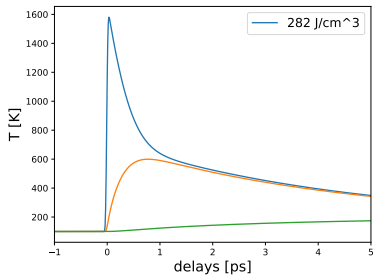
- assume not the full lattice is coupled to electrons
- two subsystems of phonons coupled through phonon-phonon coupling

$$\begin{aligned}C_{p,e} T_{p,e} &= k C_p(T_{p,e}) T_{p,e} \\C_{p,p} T_{p,p} &= (1 - k) C_p(T_{p,p}) T_{p,p} \\C_{p,e} \frac{dT_{p,e}}{dt} &= g_{ep}(T_e - T_{p,e}) + g_{pp}(T_{p,p} - T_{p,e}) \\C_{p,p} \frac{dT_{p,p}}{dt} &= g_{pp}(T_{p,e} - T_{p,p})\end{aligned}$$



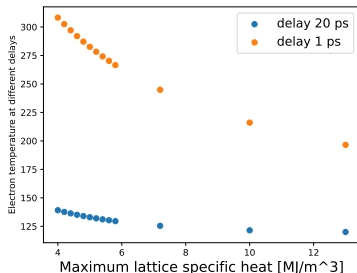
$$k = 0.1$$

Magnetization and electron temperature in multi-lattice approach

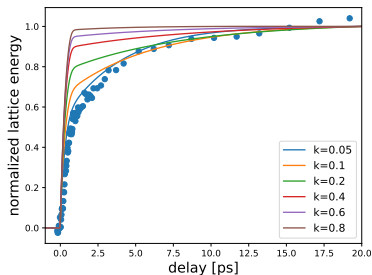


Lattice heat capacity

Maximum lattice heat capacity for $k = 0.1$



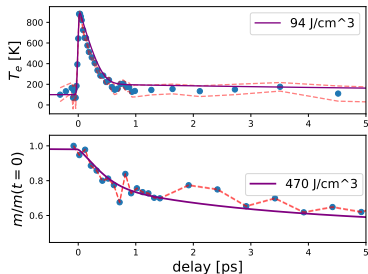
Distribution of lattice heat capacity



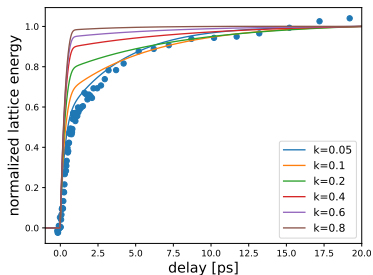
$$C_{po} = kC_p(T_{po})T_{po}$$

Lattice heat capacity

Electron and spin systems

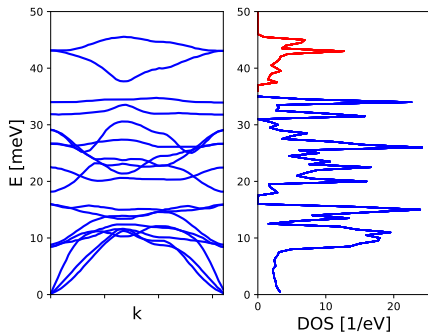


Distribution of lattice heat capacity



$$C_{po} = kC_p(T_{po})T_{po}$$

Band structure to density of states



$$DOS = \sum_{\mu, k} \frac{\delta k}{\Delta E} \delta(E - E_{\mu}(k))$$

δk unitless, grainsize
 10^{-4} on a range of
[0,16]

$\Delta E = 0.5$ eV

separation of phonon packages at
the band gap at 35
meV

From DOS to C_p

$$C_p = \frac{(2\pi)^3}{V_{UC}} \partial_{T_p} \int dE E f_{BE}(E, T_p) DOS(E)$$

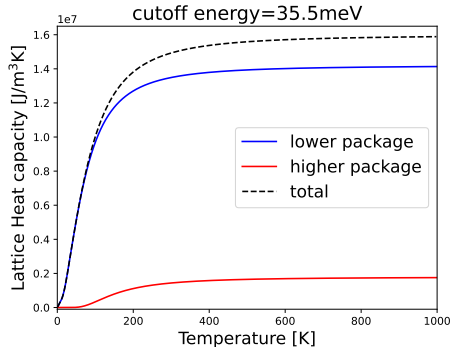
V_{UC} Volume of the unit cell

$f_{BE}(E, T_p)$ Bose Einstein distribution

total C_p agrees actually very well to what I used

ratio of C_p s fits to what I used

total C_p reference I have not found any, there is this paper, where they claim to have measured it, but I cannot access it



From DOS to C_p

