CGT M3TM simulations

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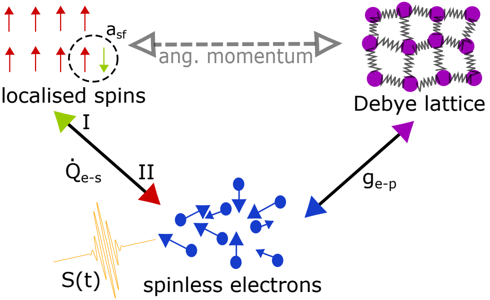
M3TM model concept



- 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 CGT: no remagnetization so energy flow $\dot{Q}_{es}$ (see next slide) unidirectional e $\longrightarrow$ s)
- spin flips (/magnon excitations) upon e-p scattering event from Elliott-Yafet spin mixing
- implicit angular momentum exchange between spins and lattice

Calculation of dynamics

Energy dynamics

$$C_{\mathrm{e}} \frac{dT_{\mathrm{e}}}{dt} = g_{\mathrm{e-p}}(T_{\mathrm{p}} - T_{\mathrm{e}}) + S_0 G(t,z)) + \dot{Q}_{\mathrm{es}}$$

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

Angular momentum dynamics

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

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

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

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

g_{ep} electron phonon coupling

$\dot{Q}_{es}$ $= Jm\dot{m}/V_{at}$ energy exchange of spin-and electron system (mean field energy cost of spin flip)

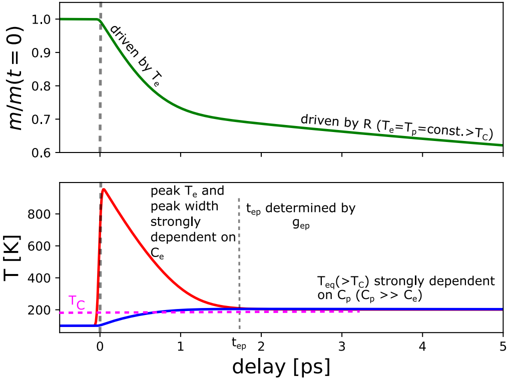
R $= 8\frac{a_{sf} g_{ep} T_C^2 V_{at}}{\mu_{at} k_B T_{Deb}^2}$ magnetization rate parameter

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

S $= 3/2$ effective spin

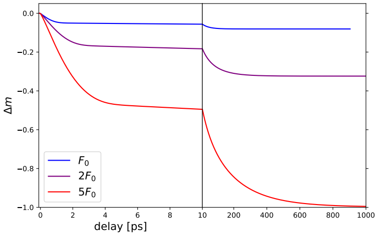
$W^{\pm}$ transition rates for down/up spin flip between S_z components m_s

Example (with **FGT** parameters)

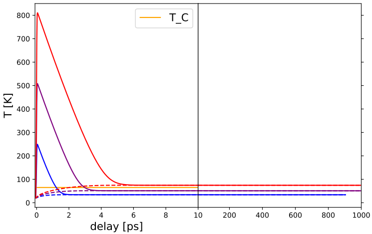


Simulations for CGT for different fluences, $T_0 = 20$ K

Magnetization dynamics

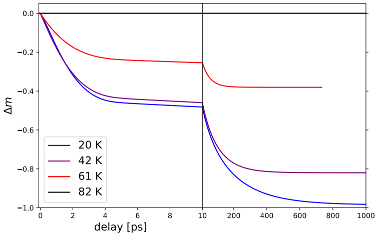


Temperature dynamcis

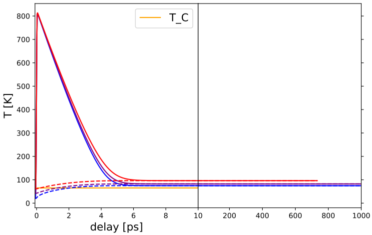


Simulations for CGT for different temperatures, $F = 5F_0$

Magnetization dynamics



Temperature dynamcis



Parameters used

$\gamma_e[\frac{J}{m^3K^2}]$	736.87
$C_{p\infty}[10^6\frac{J}{m^3K}]$	8.9
$g_{\mathrm{ep}}[10^15\frac{W}{m^3K}]$	150
$R[\frac{1}{ps}]$	0.06
T_C [K]	65
T_{Deb} [K]	175
T_{ein} [K]	131

electronic heat capacity: Sommerfeld approximation: $C_e = \gamma_e T_e$

lattice heat capacity: Einstein model:

$$C_p = C_{p\infty}\frac{T_{\mathrm{ein}}^2}{T_p^2}\frac{\exp\left(\frac{T_{\mathrm{ein}}}{T_p}\right)}{(\exp\left(\frac{T_{\mathrm{ein}}}{T_p}\right)-1)^2}$$

g_{ep}: $\approx$ three times larger than in the supplementary material you sent, basically to speed up the initial demagnetization ($\approx 2ps$), which are driven by the electron dynamcis. The faster $T_e \approx T_p$ is achieved, the faster the initial demag. phase

R: rate parameter (for comparison:
Nickel: $R \approx 18/ps$, Type I behaviour
Gadolinium: $R \approx 0.1/ps$, Type II behaviour)

Comments

As I have/could not run the simulations for a wide range of fluences yet, the absolute values of magnetization quenching between simulations is not as in the paper draft you sent us. Especially the temperature dependence for 20 K/42 K deviates for the fluence I have chosen here ($T_\infty > T_C$). I will work on this and update you with better 'fits'. I hope there is still something to gain from this summary.