Demagnetization Dynamics and Spin-dependent Lifetimes in Ferromagnets

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Thanks

Theory

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Benedikt Müller

Experiment

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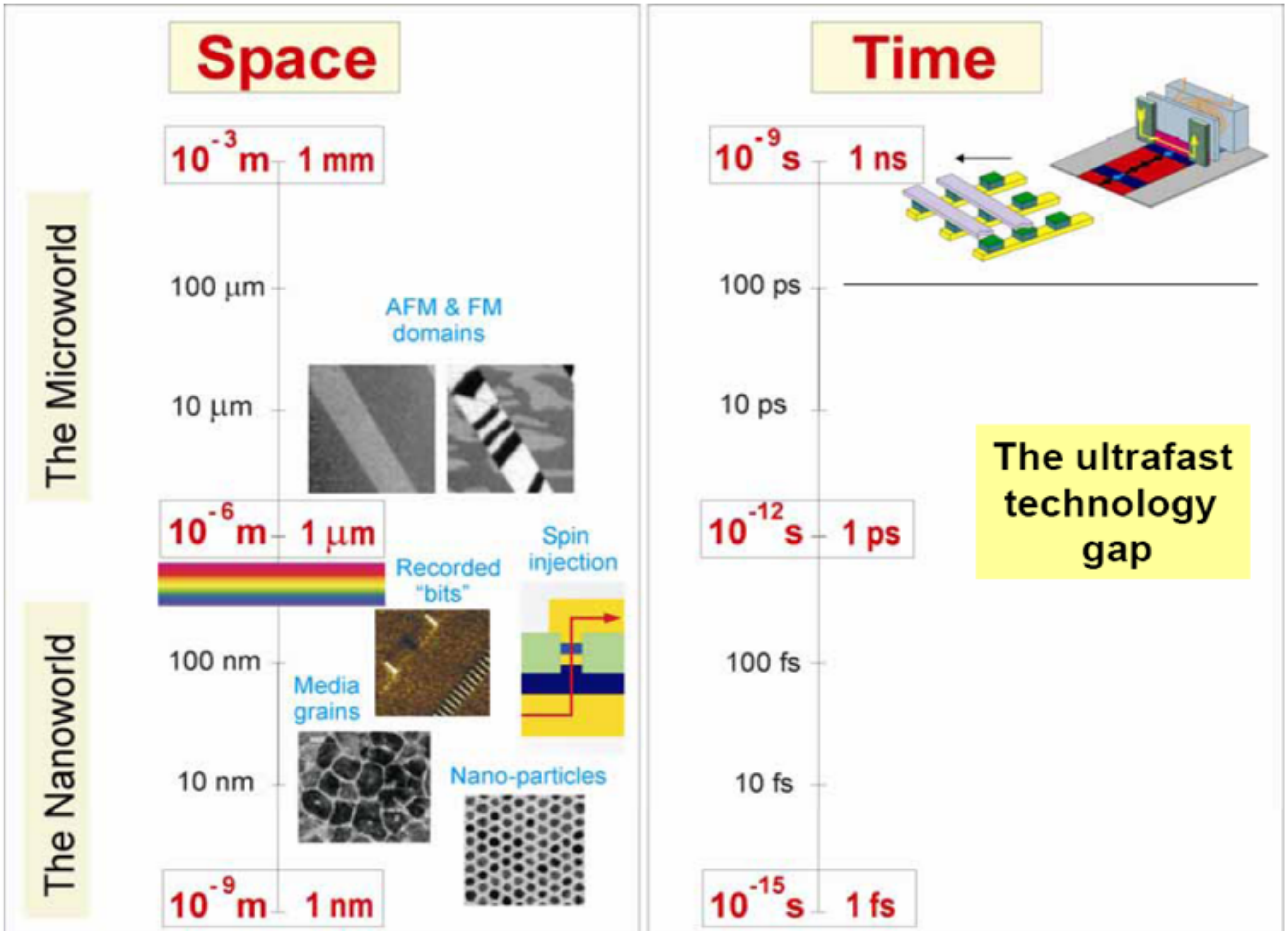
Mirko Cinchetti

Outline

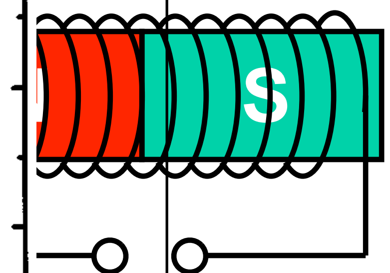
1. Introduction & What is ultrafast demagnetization in ferromagnets?
2. Elliott-Yafet mechanism for electron-phonon scattering and dynamical Stoner model
3. Spin-dependent lifetimes in ferromagnets
4. Spin-dependent transport (in normal metals)

How Small & Fast Can Magnetism/Spintronics Get?

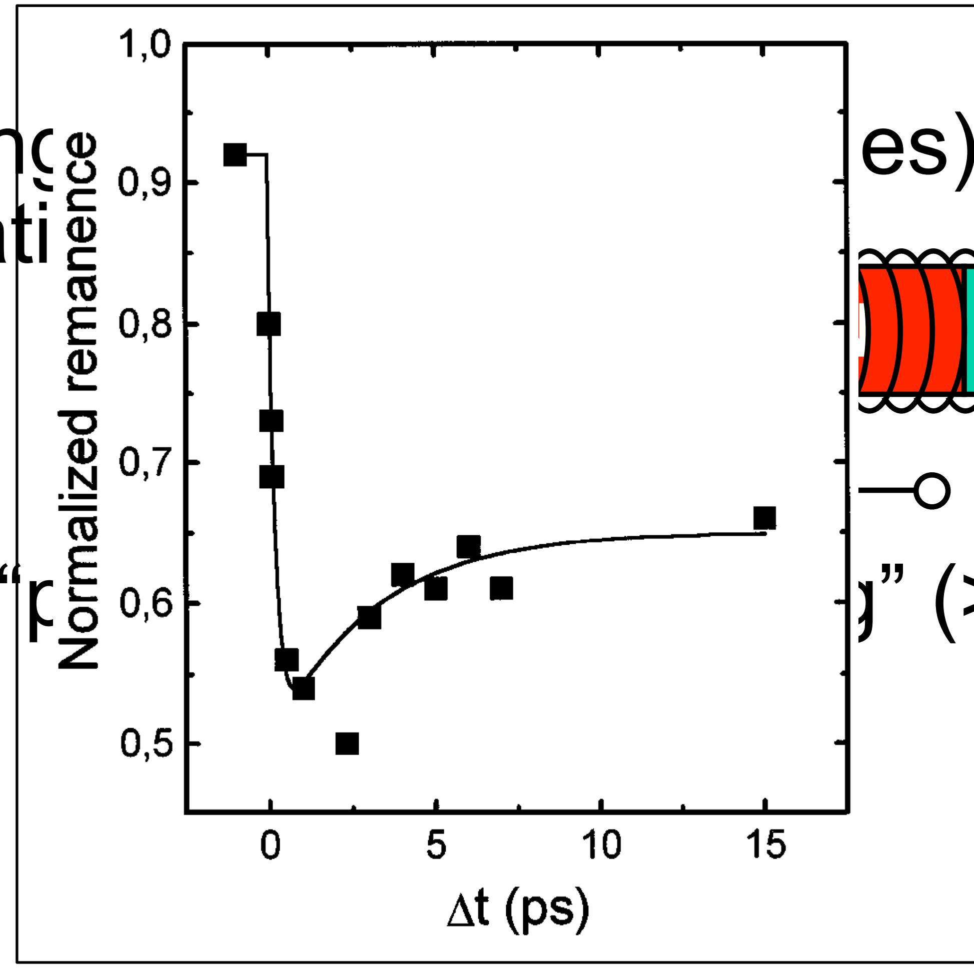


Magnetization Dynamics: Scenarios in Fe, Co, Ni

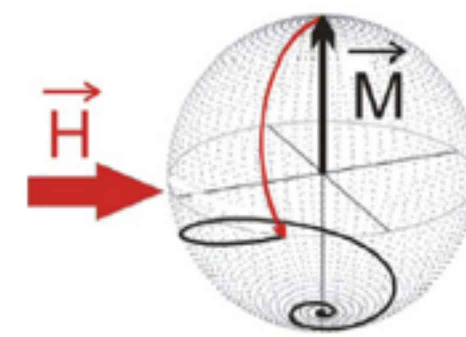
- Conventional switching ... es) →
  Domain-wall propagati...



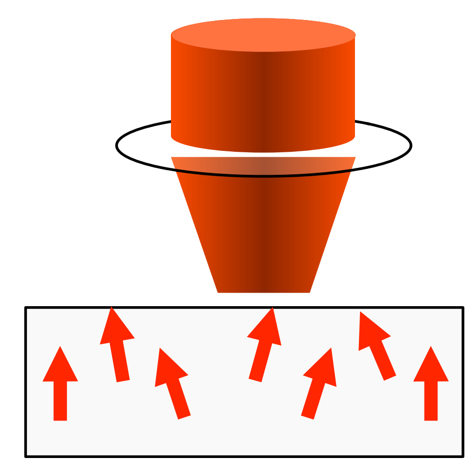
slow!



- Coherent rotation → "p... g" (>10ps)



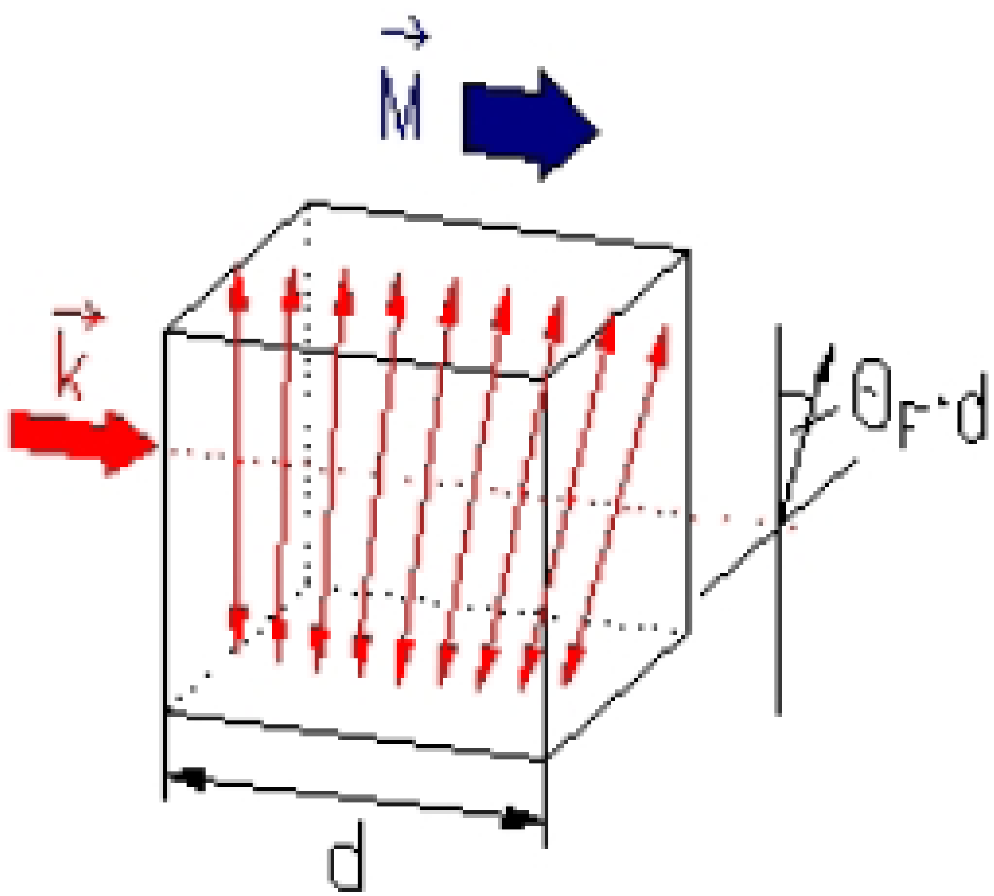
- Optically induced magnetization dynamics



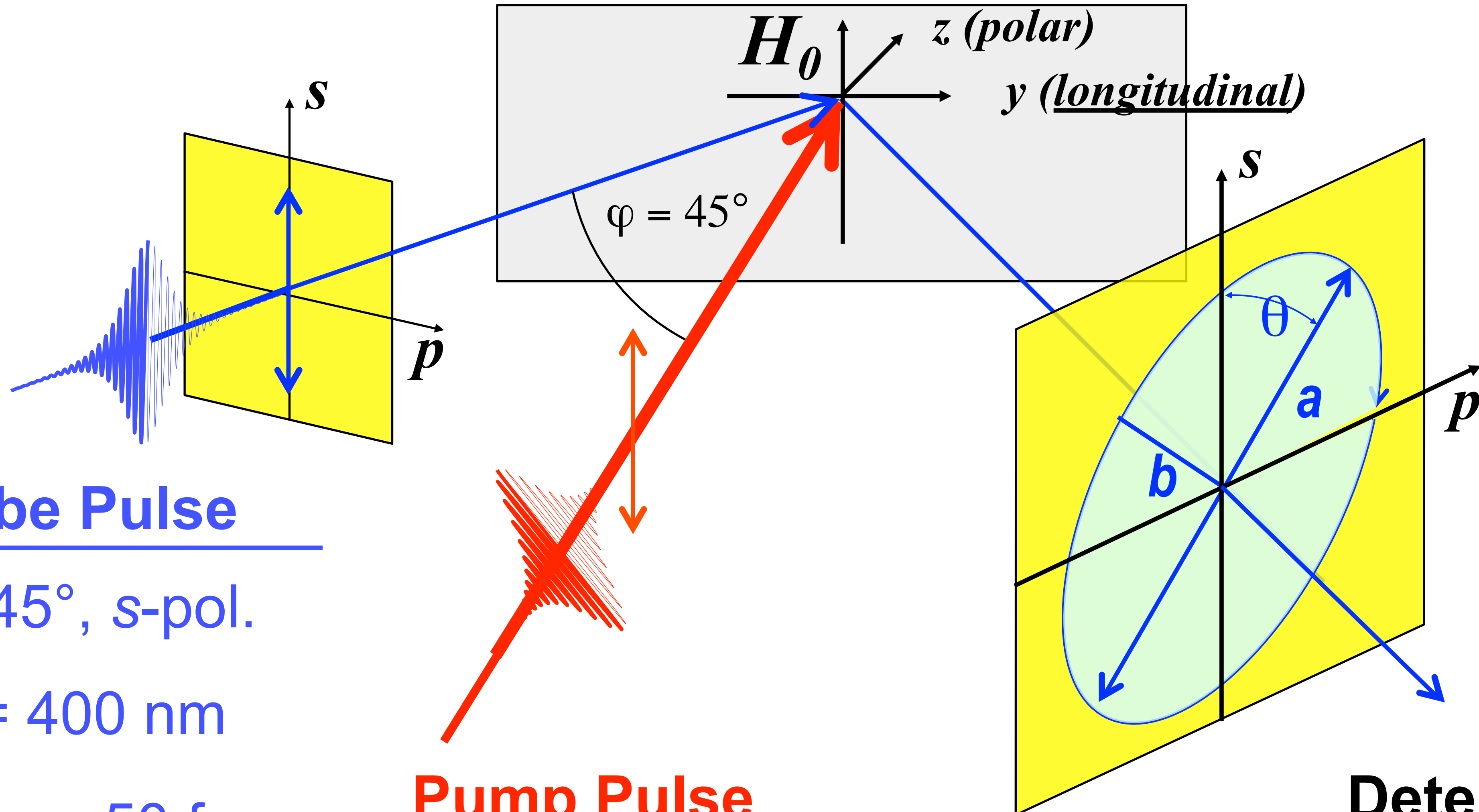
Beaurepaire, Merle, Daunois, Bigot, Phys. Rev. Lett. **76**, 4250 (1996)

Magneto-Optical Kerr Effect: MOKE

- Magneto-optical effects: dielectric function depends on magnetization $\varepsilon = \varepsilon(M)$
- Influences reflected (*Kerr* effect) and transmitted light (*Faraday* effect) and
- MOKE: Light polarization angle rotated by $\Theta_F(M)$
- Faraday geometry: Intensity changes = magnetic contrast



Experimental TR-MOKE setup



$$\Theta_K = \theta_K + i\varepsilon_K$$

$$\theta_K \propto \vec{k} \bullet \vec{M}$$

Probe Pulse

φ_i = 45°, *s*-pol.

λ_0 = 400 nm

τ_{FWHM} = 50 fs

weak intensity

Pump Pulse

φ_i = 2°, *s*-pol.

λ_0 = 800 nm

τ_{FWHM} = 50 fs

high intensity
(F = 1 - 5 mJ/cm^2)

Detection Scheme

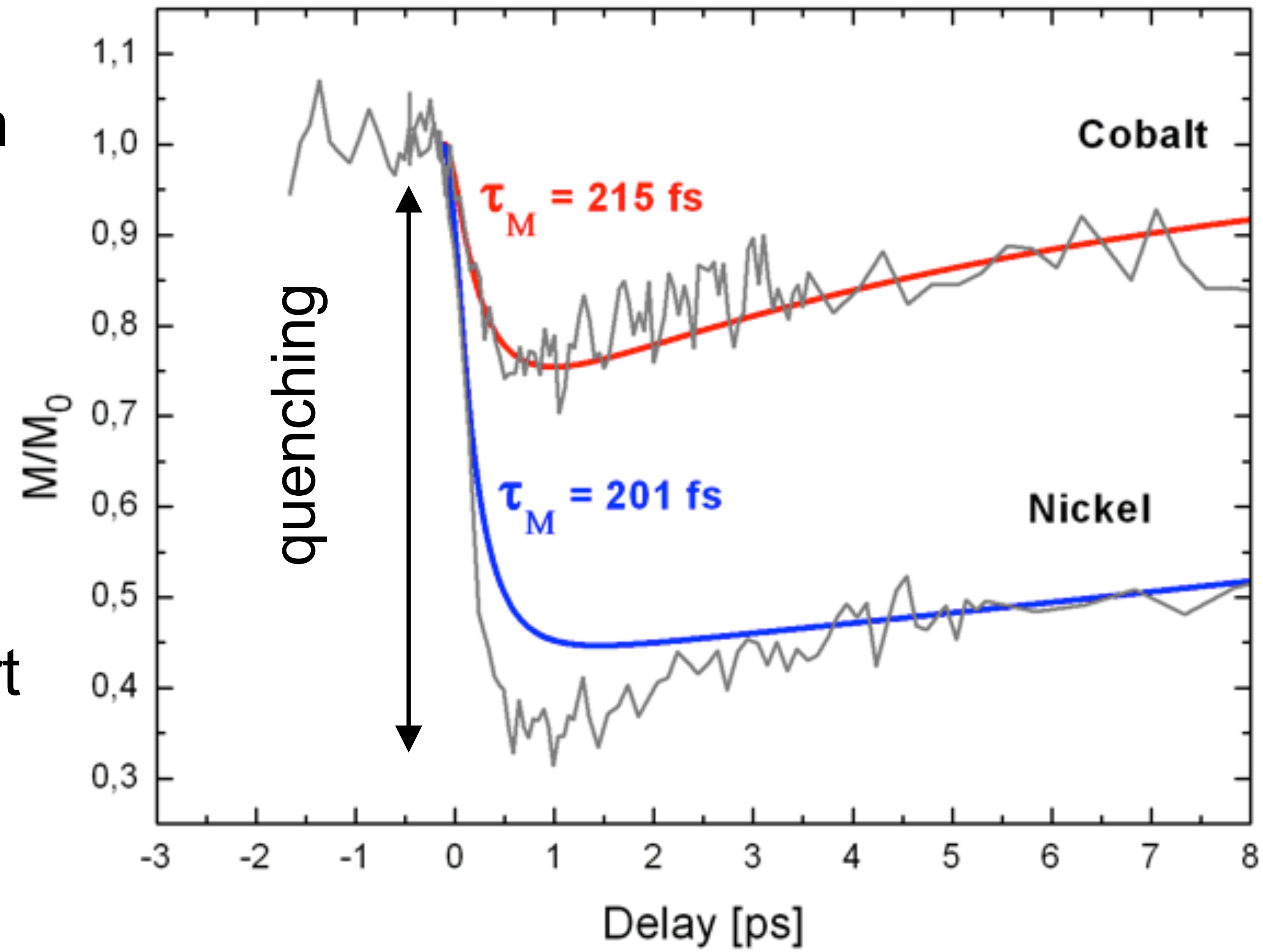
Balanced optical bridge

Lock-In filtering

Data analysis 2σ-acceptance window

Ultrafast Demagnetization in Experiment

- Pump-Probe-Measurement of the Magneto-optical Kerr Effect (MOKE)
- Magnetization changes on ultrafast timescales ("quenching")

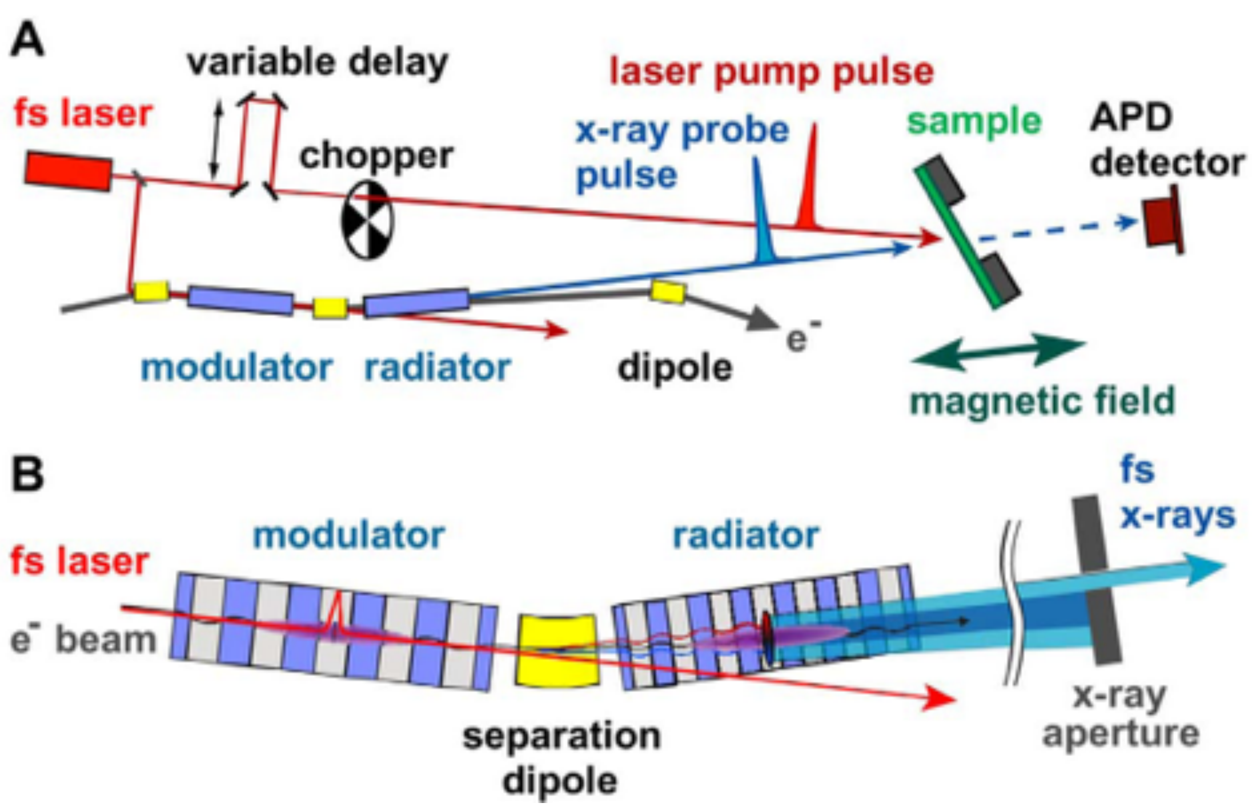


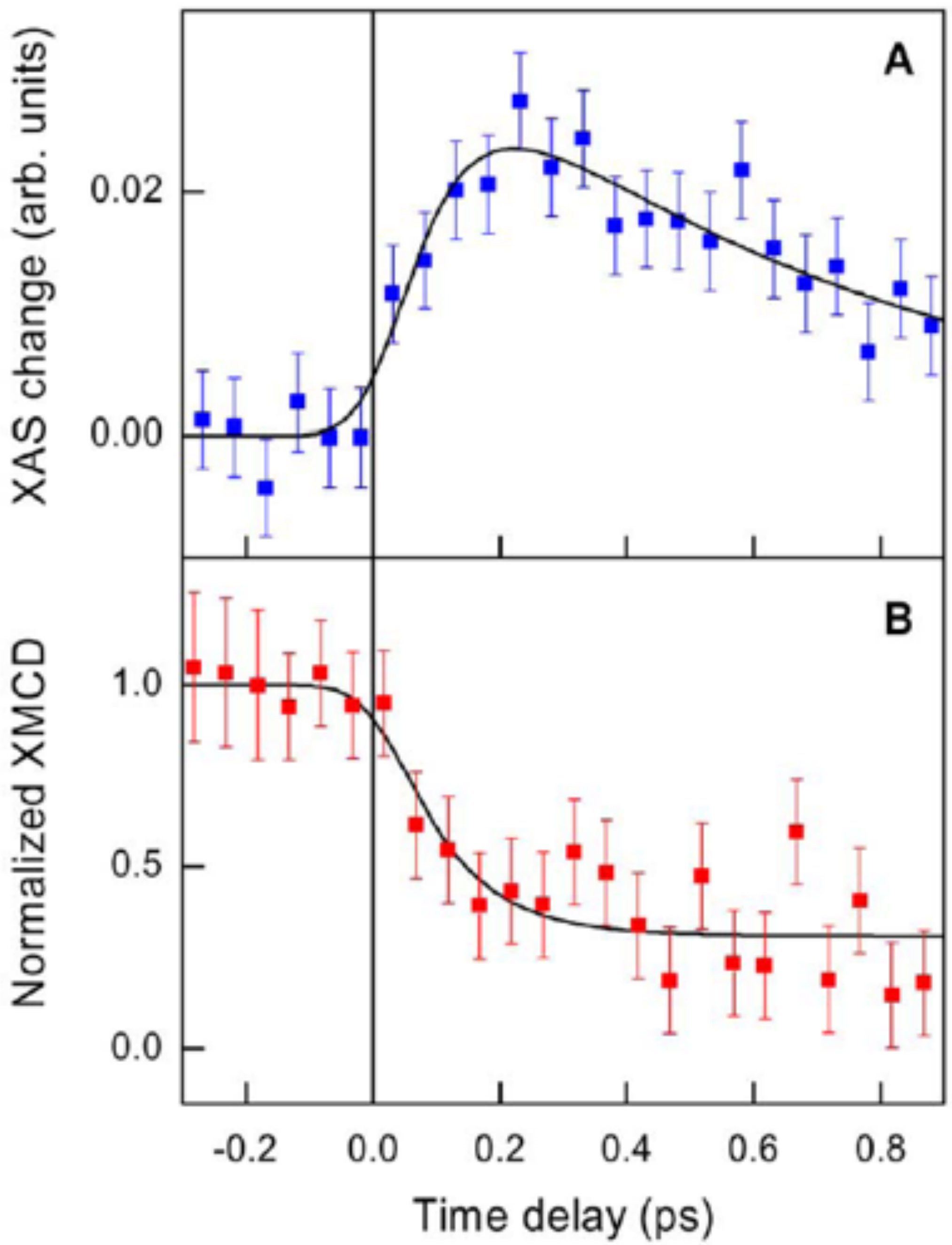
- No coherent artifacts
- MOKE measures magnetization on ultrashort timescales

Beaurepaire, Merle, Daunois, Bigot, Phys. Rev. Lett. **76**, 4250 (1996)
these data: M. Krauß et al., Phys. Rev. B **80**, 180407(R) (2009)

Ultrafast Demagnetization in Experiment

- X-ray magnetic circular dichroism (XMCD)





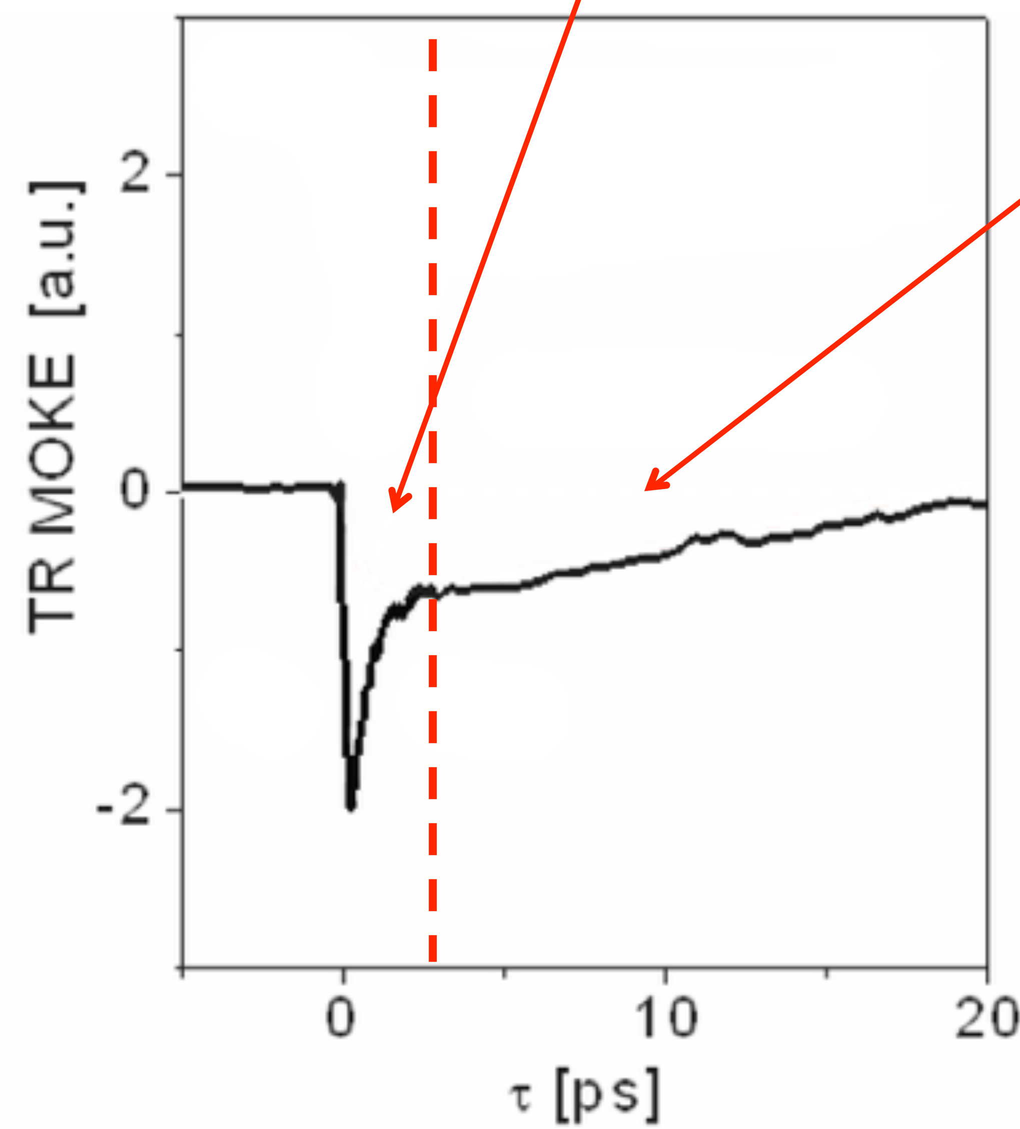
Stamm et al., Nature Materials **6**, 740 (2007)

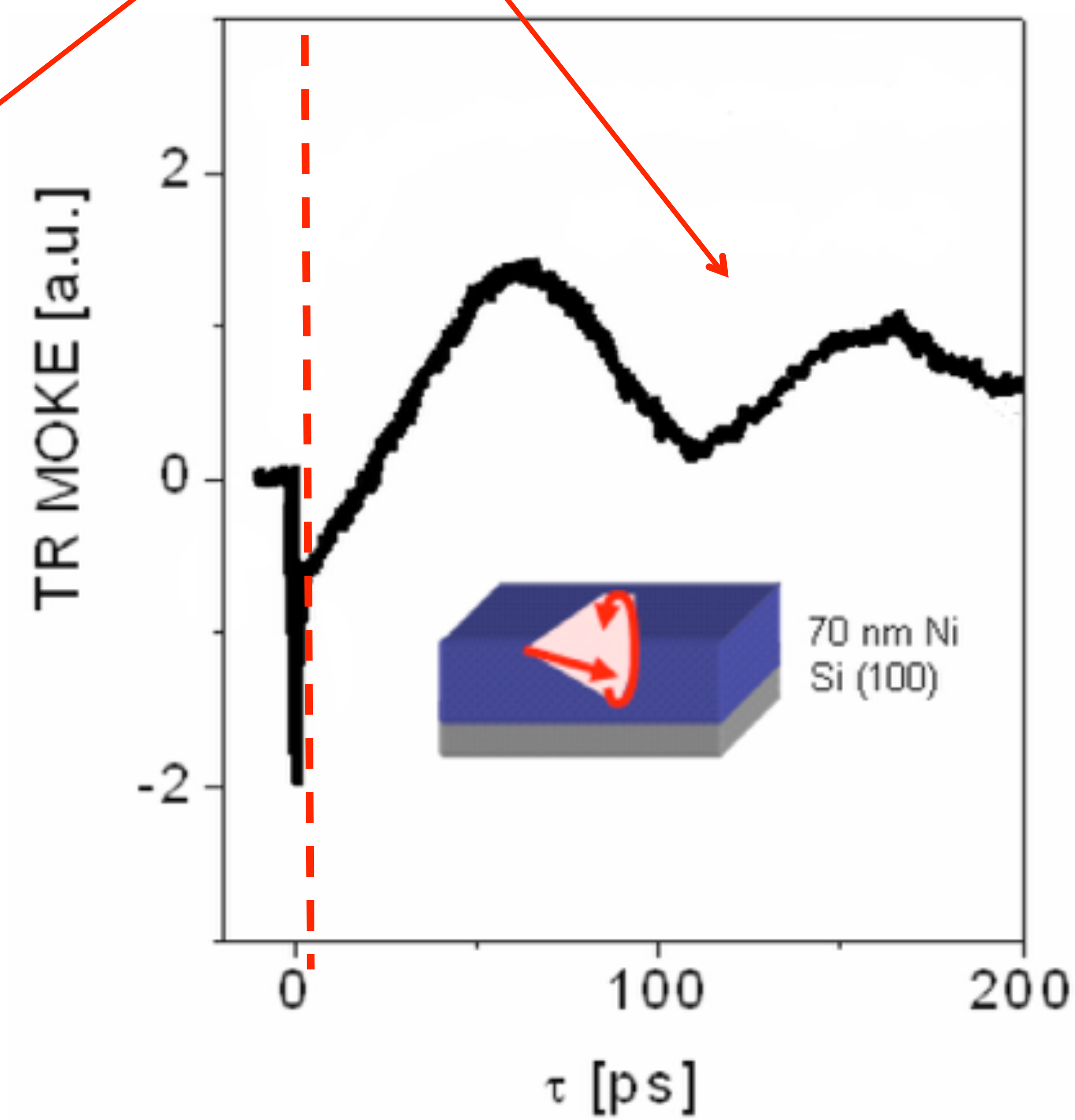
Magnetization Dynamics on Different Time Scales

- Experimental TR-MOKE result on different time scales

- non-equilibrium dynamics
- temperature not well defined

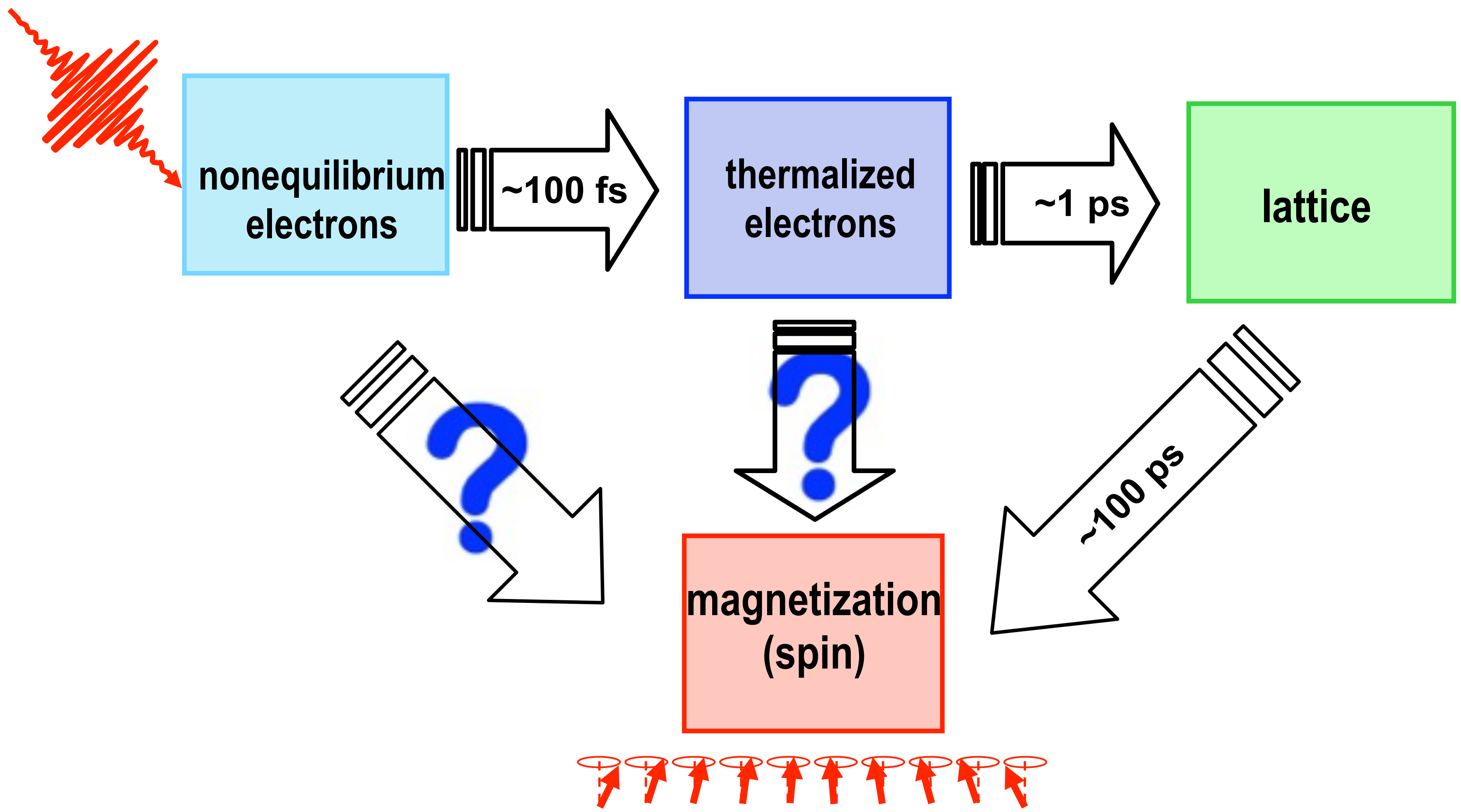
- quasi-equilibrium dynamics
- temperature $T=T(\mathbf{r},t)$





Djordjevic et al., phys. stat. sol. (c) 3, 1347 (2006)

Time Scales of Magnetization Dynamics



- Coherent regime (~10 fs)
- Incoherent “thermalization” dynamics of nonequilibrium electrons (100 fs)
- Quasi-thermal regime: electron temperature, lattice temperature (1 ps)
- Spin-lattice equilibration (100 ps)

- Ultrafast magnetization (spin) dynamics surprising!

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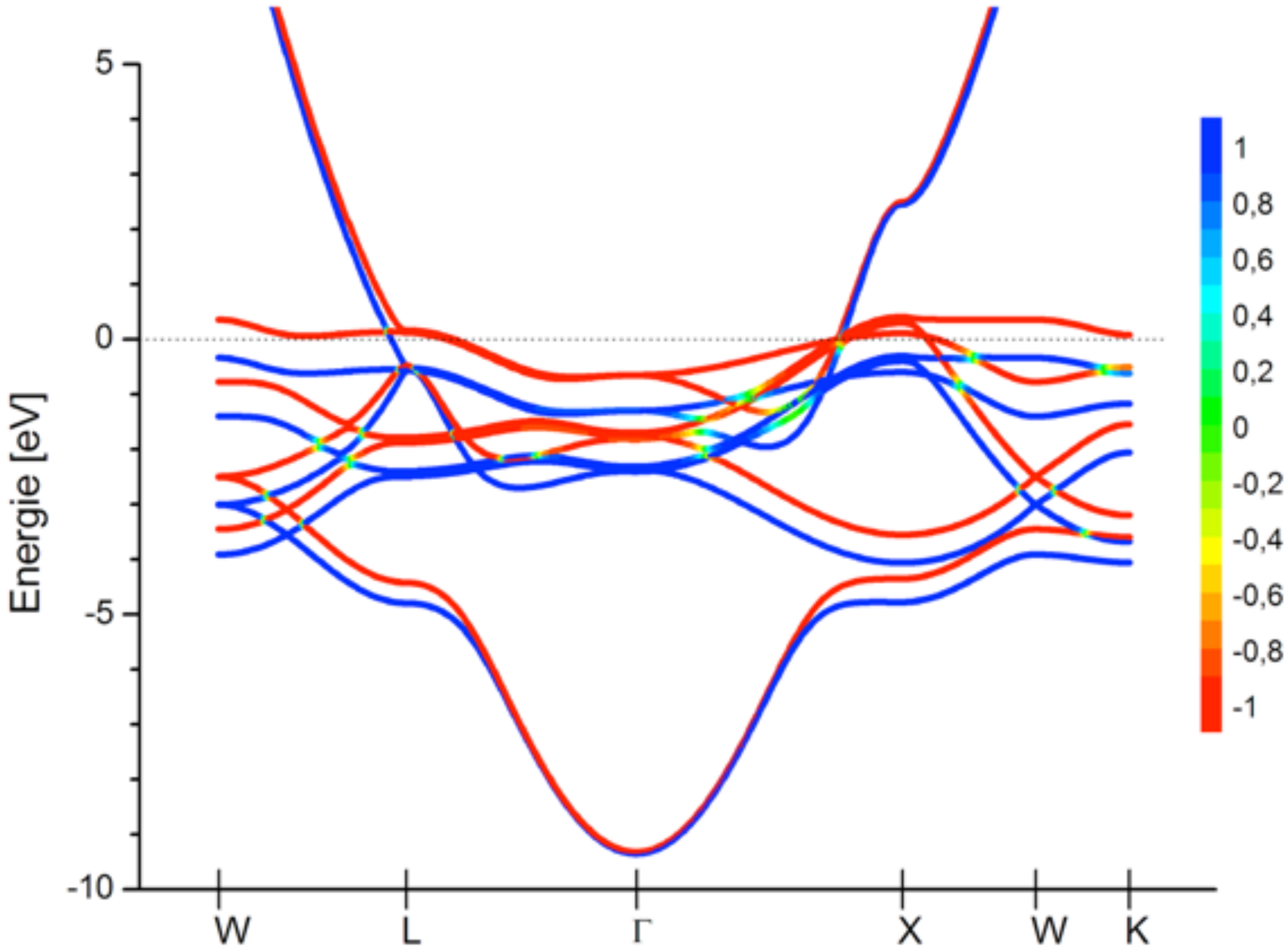
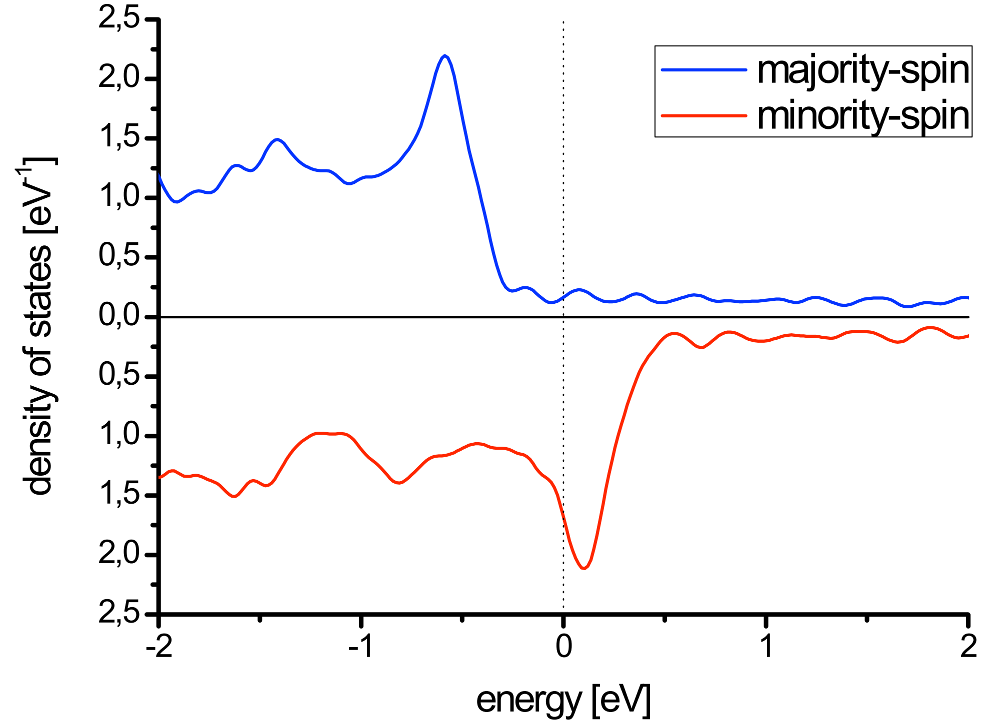
Relevant Facts

Nickel band structure @ T = 0K
including spin-orbit coupling



Nickel Density of States
@ T=0K



Ultrashort Magnetization Dynamics (Theory)

Question(s) Microscopic mechanism behind the magnetization quenching on ultrashort timescales?

1. Role of coherent effects in the presence of the pulse
2. Role of band-structure details
3. Role of non-equilibrium electrons
4. Role of “true” (correlated) magnetization dynamics
5. Role of spin-dependent transport processes

This talk (items 2–4)

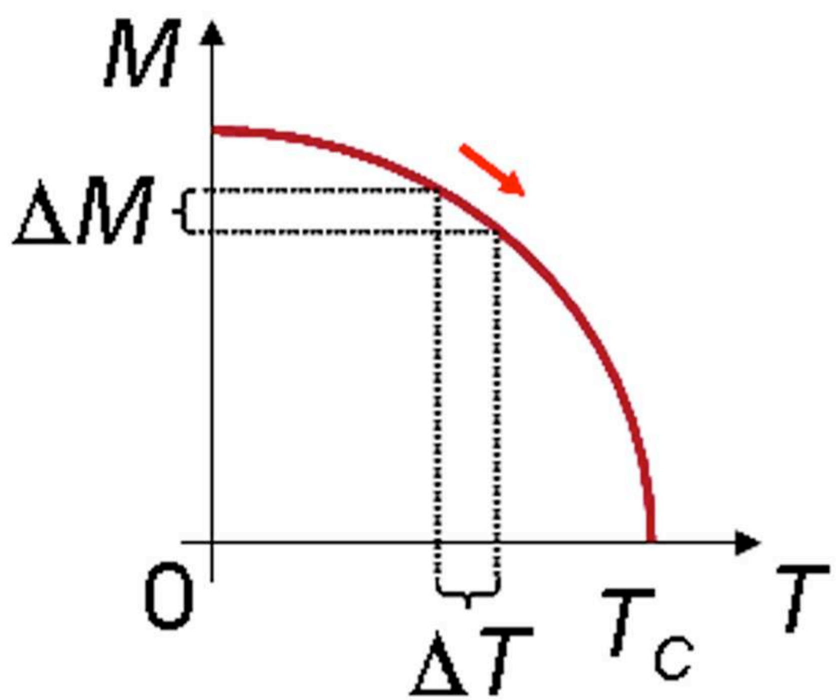
Answer Probably: “All of the above”

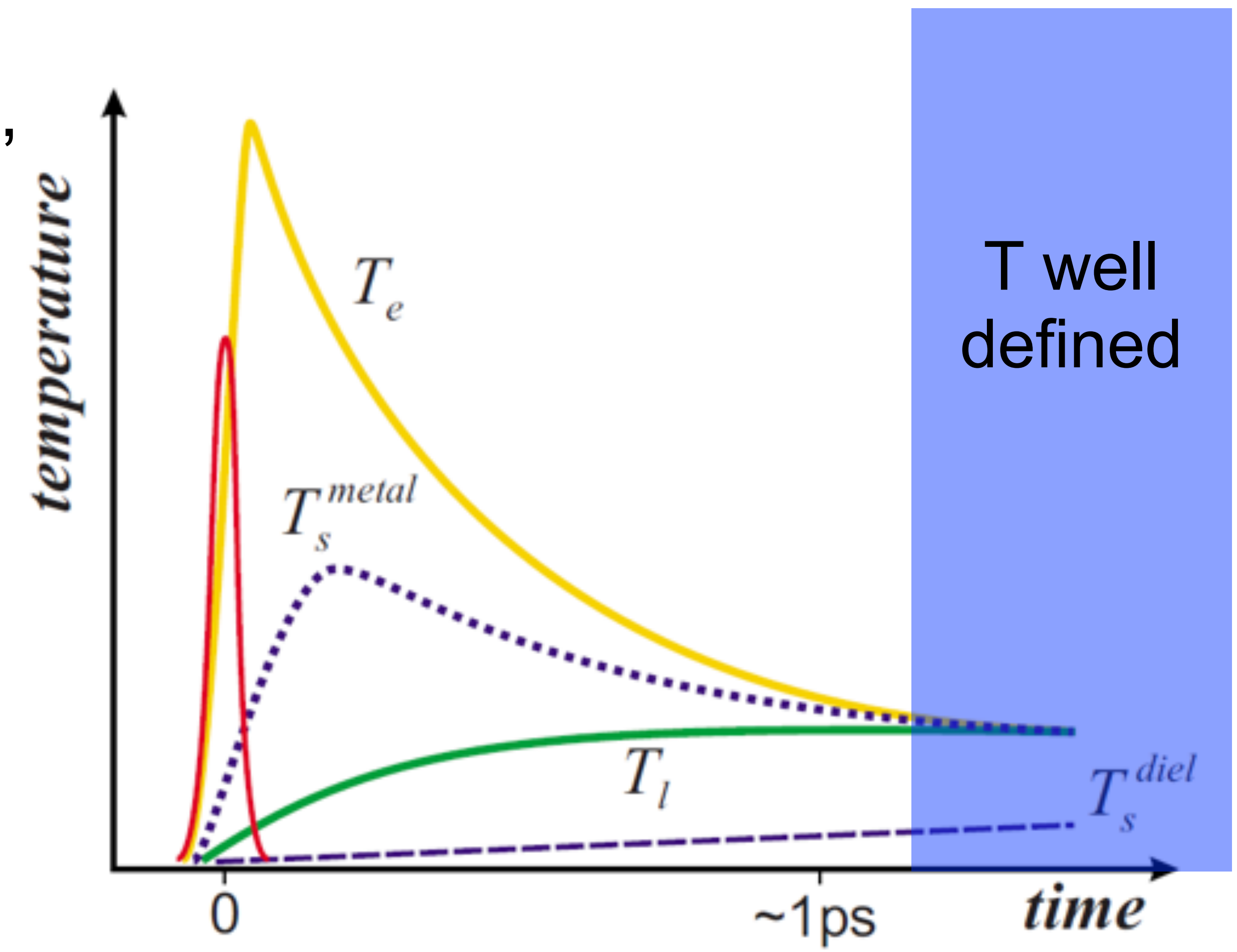
Agreement Spin-orbit interaction has something to do with it

Problem Usually “agreement with experiment” for 1-5;
BUT dependence on parameters

(Phenomenological) Three-Temperature Model

- Three systems (electrons, lattice, and spins) in quasi-equilibrium: assign temperatures





from: Kirilyuk et al., Rev. Mod. Phys. **82**, 2731 (2010)

- Separation and quasi-equilibrium assumption OK for picosecond time scale. But:

  How to describe ultrafast dynamics in the correlated electron system of the ferromagnet <u>microscopically</u>?

Other Approaches

- Coherent effects: Important for (few) localized levels with strong spin-orbit coupling

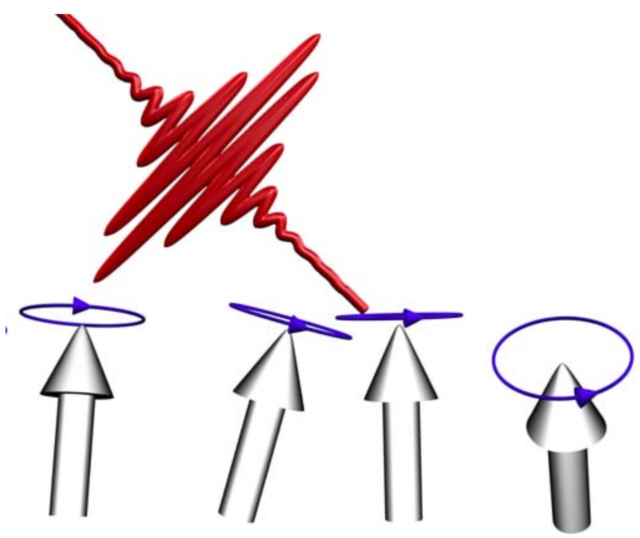
Zhang and Hübner, Phys. Rev. Lett. **85**, 3025 (2000)

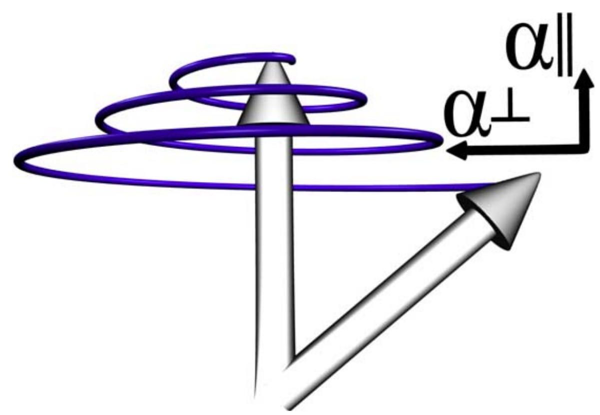
Bigot, Vomir, Beaurepaire, Nature Phys. **5**, 515 - 520 (2009)

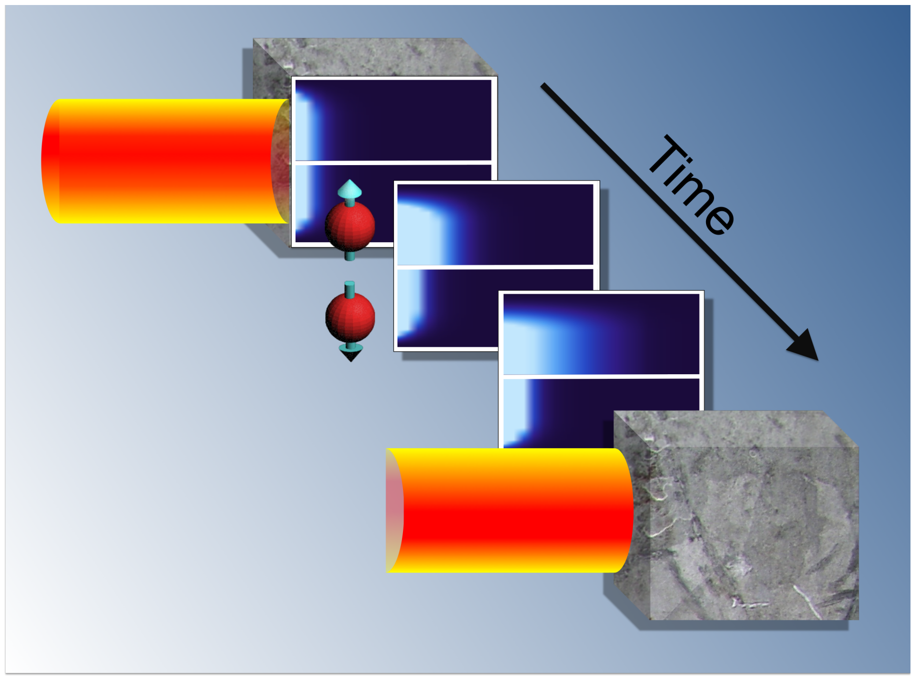
- Landau-Lifshitz-Bloch equations: assume electronic temperature; effective spin-orbit coupling includes spin-fluctuations (around T_c)

Chubykalo-Fesenko et al, Phys. Rev. B **74**, 094436 (2006)

Atxitia, Chubykalo-Fesenko, Walowski, Mann and Münzenberg Phys. Rev. B **81**, 174401 (2010)







- Superdiffusive transport: electrons with different spin leave spot with different velocities

Battiato, Carva, and Oppeneer, PRL **105**, 027203 (2010)

Spin Mixing in Transition Metals

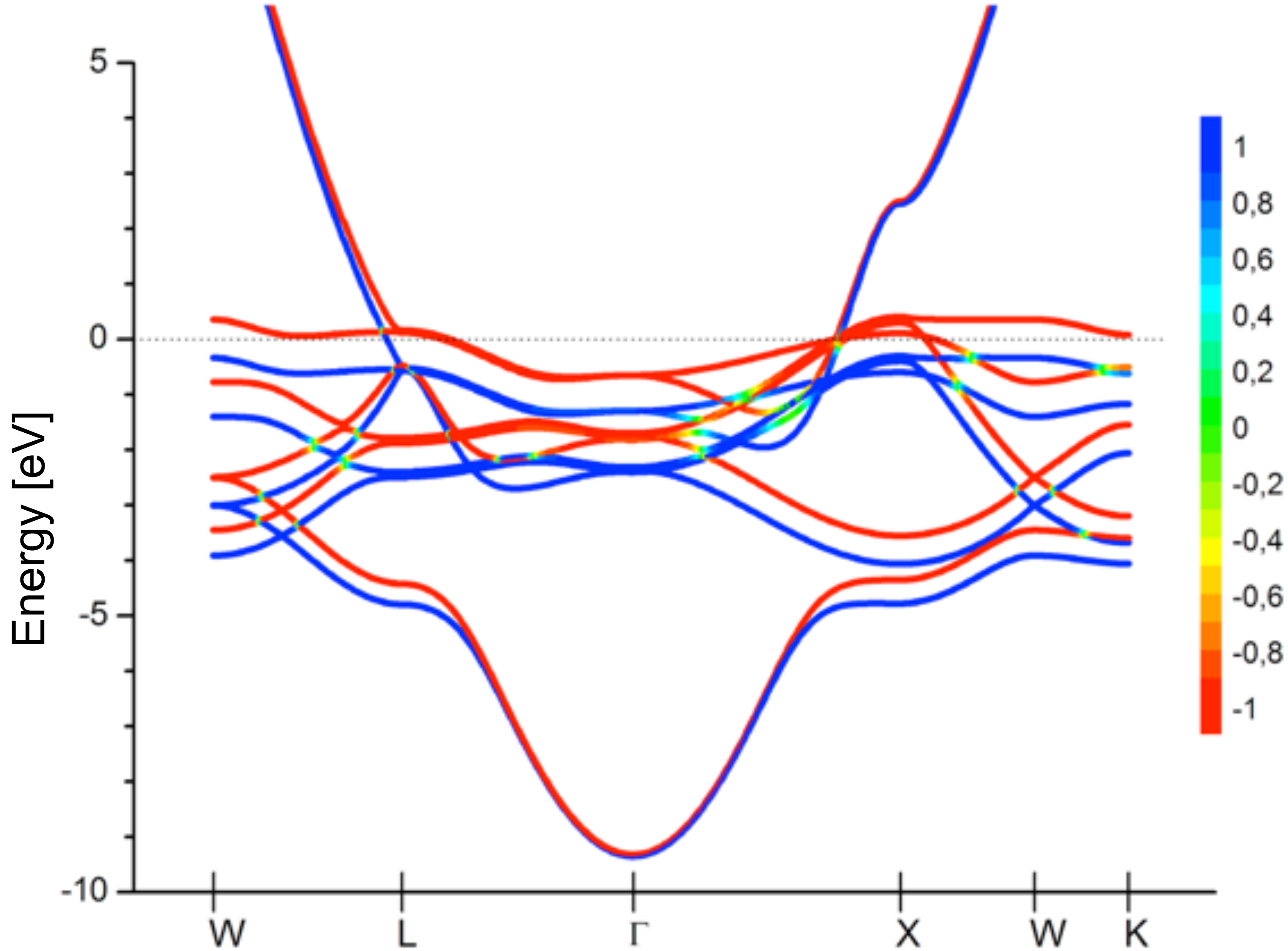
- Spin mixing important for optical excitation and scattering
- Spin mixing anisotropic ("spin hot-spots")?

  Fabian & Das Sarma, Phys. Rev. Lett. **81**, 5624 (1998)

- Keep band structure fixed!
- Goal: Obtain quantitative results!

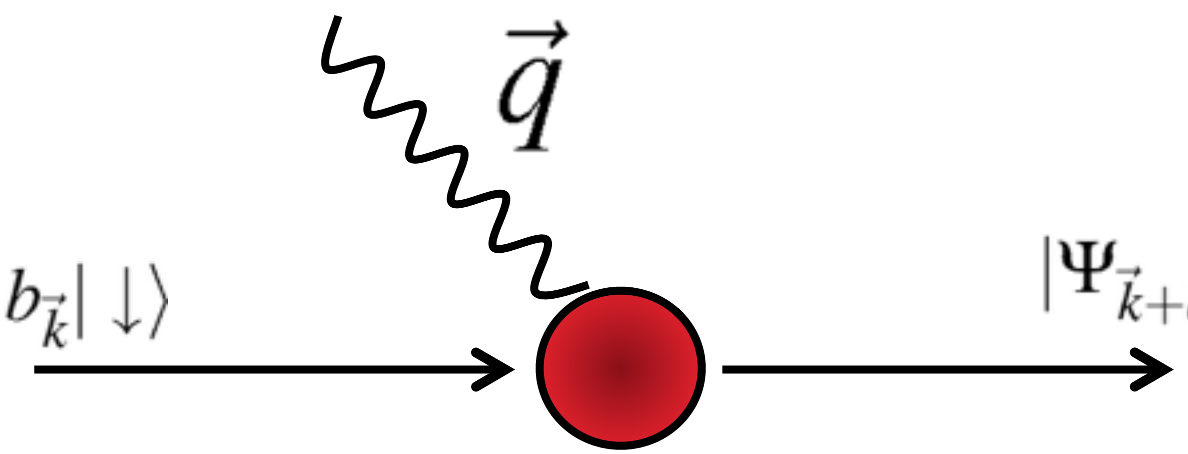
Nickel band structure

with "spin hot-spots"



Elliott-Yafet Mechanism: Spin Relaxation due to Electron-Phonon Scattering

$|\Psi_{\vec{k}}\rangle = a_{\vec{k}}|\uparrow\rangle + b_{\vec{k}}|\downarrow\rangle$



$|\Psi_{\vec{k}+\vec{q}}\rangle = a_{\vec{k}+\vec{q}}|\uparrow\rangle + b_{\vec{k}+\vec{q}}|\downarrow\rangle$

Spin mixing + electron-phonon scattering = spin relaxation

$$\left\langle \Psi_{\vec{k}} \middle| \hat{S}_z \Psi_{\vec{k}} \right\rangle \neq \left\langle \Psi_{\vec{k}+\vec{q}} \middle| \hat{S}_z \Psi_{\vec{k}+\vec{q}} \right\rangle \Rightarrow \frac{d}{dt}\left\langle S_z \right\rangle \neq 0$$

- Phonons do <u>not</u> carry angular momentum (spin-diagonal interaction)

Yafet, Solid State Physics, **14** (1963)

Koopmans et al., Nature Mat. **9**, 256 (2010)

k-resolved Electron Scattering Dynamics

- Equation of motion for electronic dynamics

$$\frac{d}{dt}f^{\mu}(\vec{k}) = \left.\frac{d}{dt}f^{\mu}(\vec{k})\right|_{e-ph} + \left.\frac{d}{dt}f^{\mu}(\vec{k})\right|_{opt}$$

carrier distribution in
band μ with momentum k

- Optical excitation of carriers

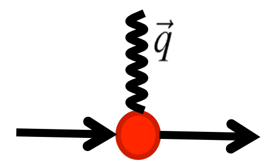
$$\left.\frac{d}{dt}f^{\mu}(\vec{k})\right|_{opt} = \frac{2\pi}{\hbar}\sum_{\nu\neq\mu}\left|\vec{d}_{\mu\nu}\cdot\vec{E}\right|^2\left(f^{\nu}(\vec{k}) - f^{\mu}(\vec{k})\right) g\left(\left|\epsilon^{\nu}(\vec{k}) - \epsilon^{\mu}(\vec{k})\right| - \hbar\omega\right)$$

k-Resolved Electron-Phonon Scattering

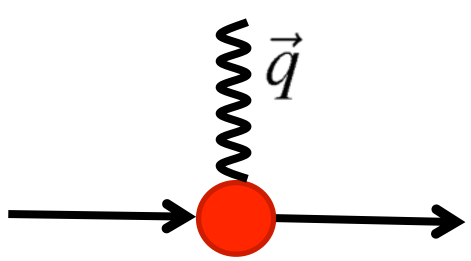
- Electron-phonon Boltzmann scattering integrals

$$\frac{d}{dt} f^{\mu}(\vec{k}) = \sum_{\lambda} \sum_{\vec{q}} \left[w^{\lambda}_{\vec{k}+\vec{q},\mu' \to \vec{k},\mu} f^{\mu'}(\vec{k}+\vec{q}) \left(1 - f^{\mu}(\vec{k})\right) - w^{\lambda}_{\vec{k},\mu \to \vec{k}+\vec{q},\mu'} f^{\mu}(\vec{k}) \left(1 - f^{\mu'}(\vec{k}+\vec{q})\right) \right]$$

$$w^{\lambda}_{\vec{k},\mu \to \vec{k}+\vec{q},\mu'} = \frac{2\pi}{\hbar} \left| \quad \right|^{2} \left[\tilde{n}^{\lambda}_{\vec{q}} \delta\left(\epsilon^{\mu'}(\vec{k}+\vec{q}) - \epsilon^{\mu}(\vec{k}) - \hbar\omega^{\lambda}_{\vec{q}}\right) + \left(\tilde{n}^{\lambda}_{-\vec{q}} + 1\right) \delta\left(\epsilon^{\mu'}(\vec{k}+\vec{q}) - \epsilon^{\mu}(\vec{k}) + \hbar\omega^{\lambda}_{-\vec{q}}\right) \right]$$



- Two contributions to spin-flip matrix element



$$\propto \sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} \left\langle \psi_f \middle| \vec{\epsilon}_{\vec{q}} \cdot \nabla_{\vec{R}} \left(V + \frac{\hbar}{4m^2c^2} (\nabla_{\vec{r}} V \times \vec{p}) \cdot \vec{\sigma} \right) \middle| \psi_i \right\rangle$$

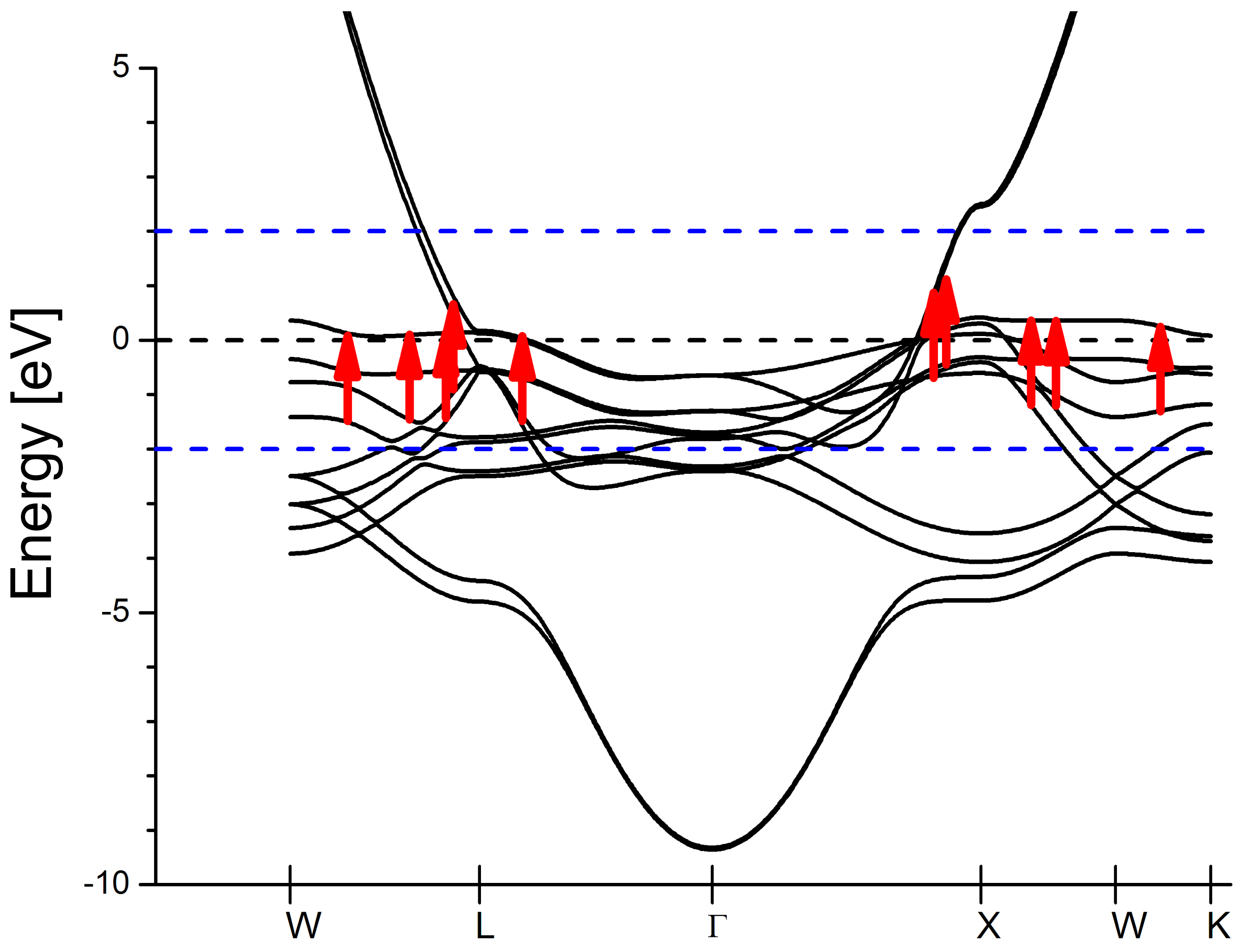
ab-initio input

S. Essert & H. C. Schneider,
Phys. Rev. B **84**, 224405 (2011)

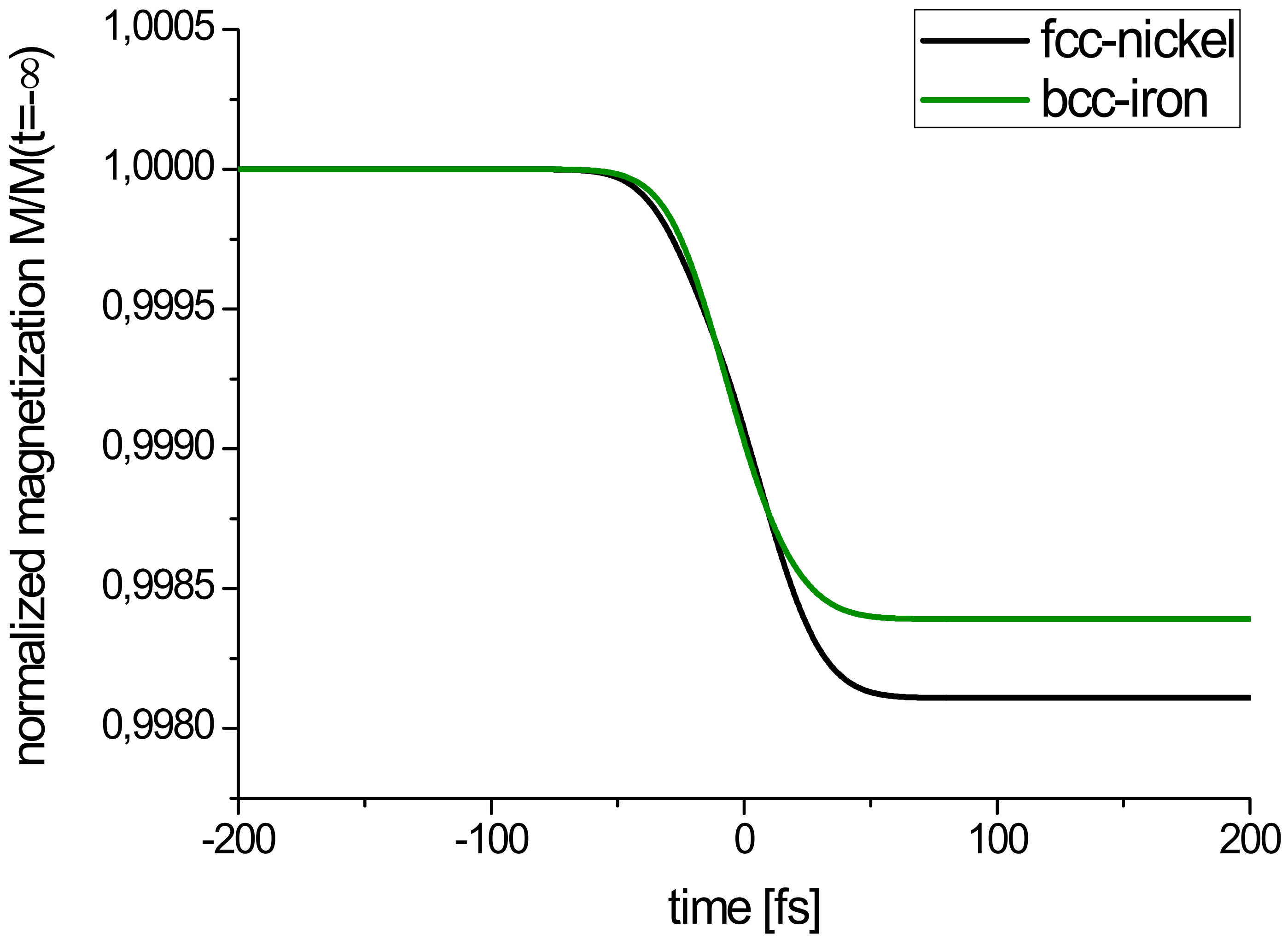
- Band structure @ T = 0K: $\epsilon^{\mu}(\vec{k})$
- Phonon dispersion $\omega^{\lambda}_{\vec{q}}$
- Transition dipole matrix elements $\vec{d}_{\mu\nu}$
- Electron-phonon matrix elements $M^{\lambda}_{\vec{k},\mu;\vec{k}',\mu'}$

Optical Excitation: Dipole Transitions in Nickel

- Dipole transitions with photon energy 1.55 eV in different regions of the Brillouing zone



Optical Excitation (2)

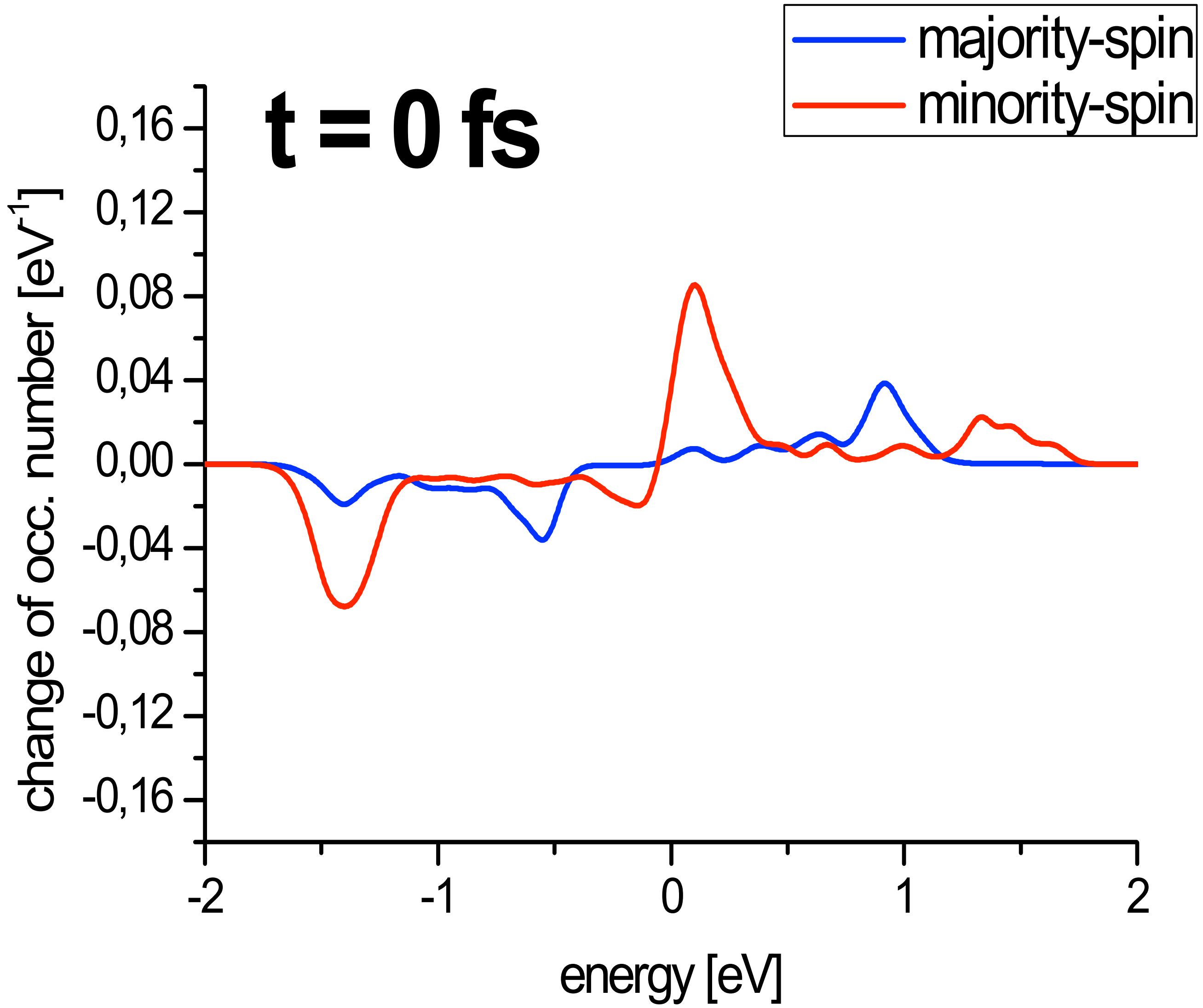


- Optical excitation using ultrashort pulse (1.55 eV, 50fs, 4 mJ/cm^{-2})
- Demagnetization is not caused by spin mixing during optical excitation

S. Essert & H. C. Schneider,
Phys. Rev. B **84**, 224405 (2011)

Optical Excitation in Nickel

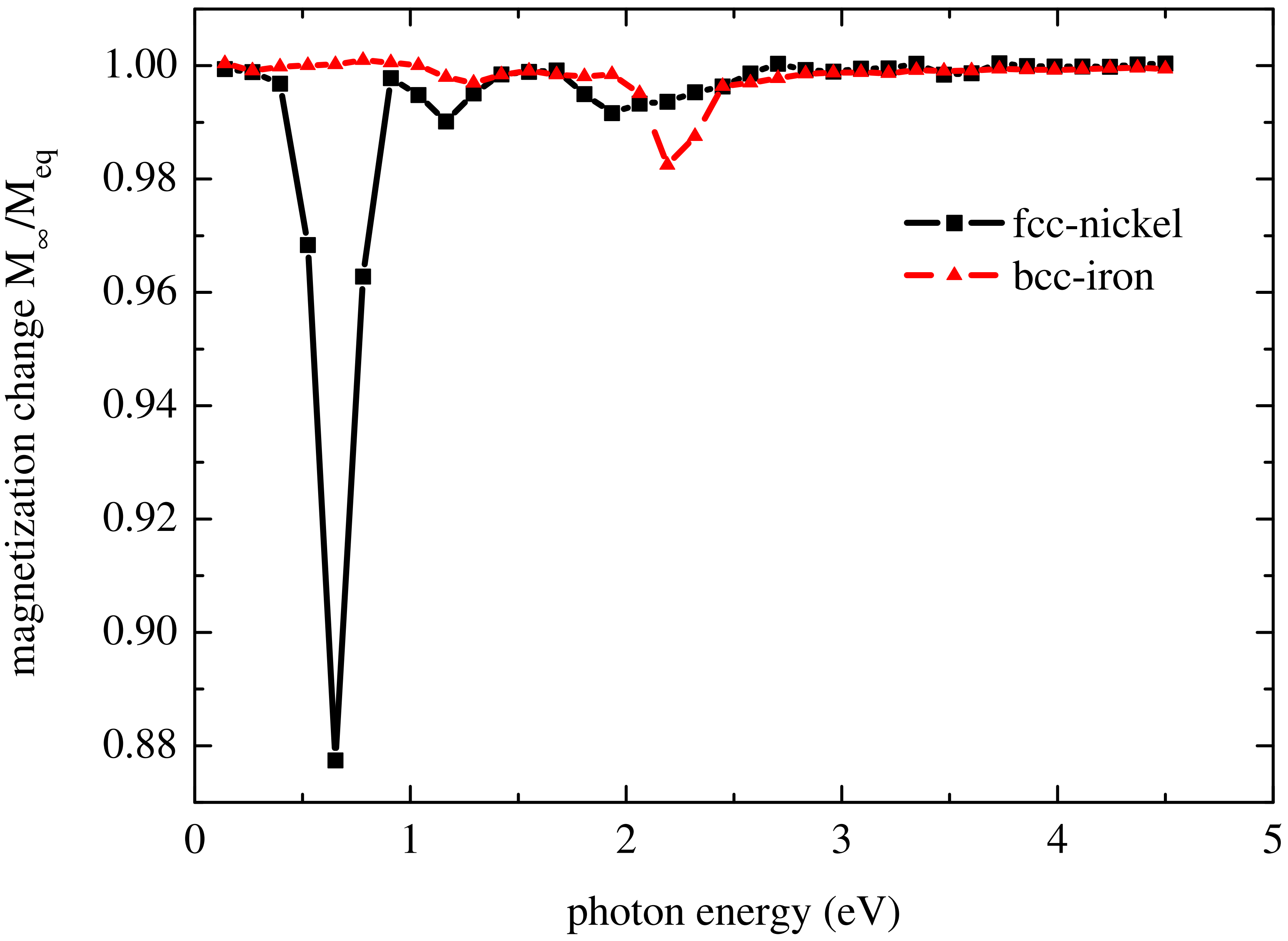
- Energy resolved change in carrier occupation
- Optical excitation using ultrashort pulse (1.55 eV, 50fs, 4 mJ/cm^{-2})
- Mainly minority electrons (and holes!) excited



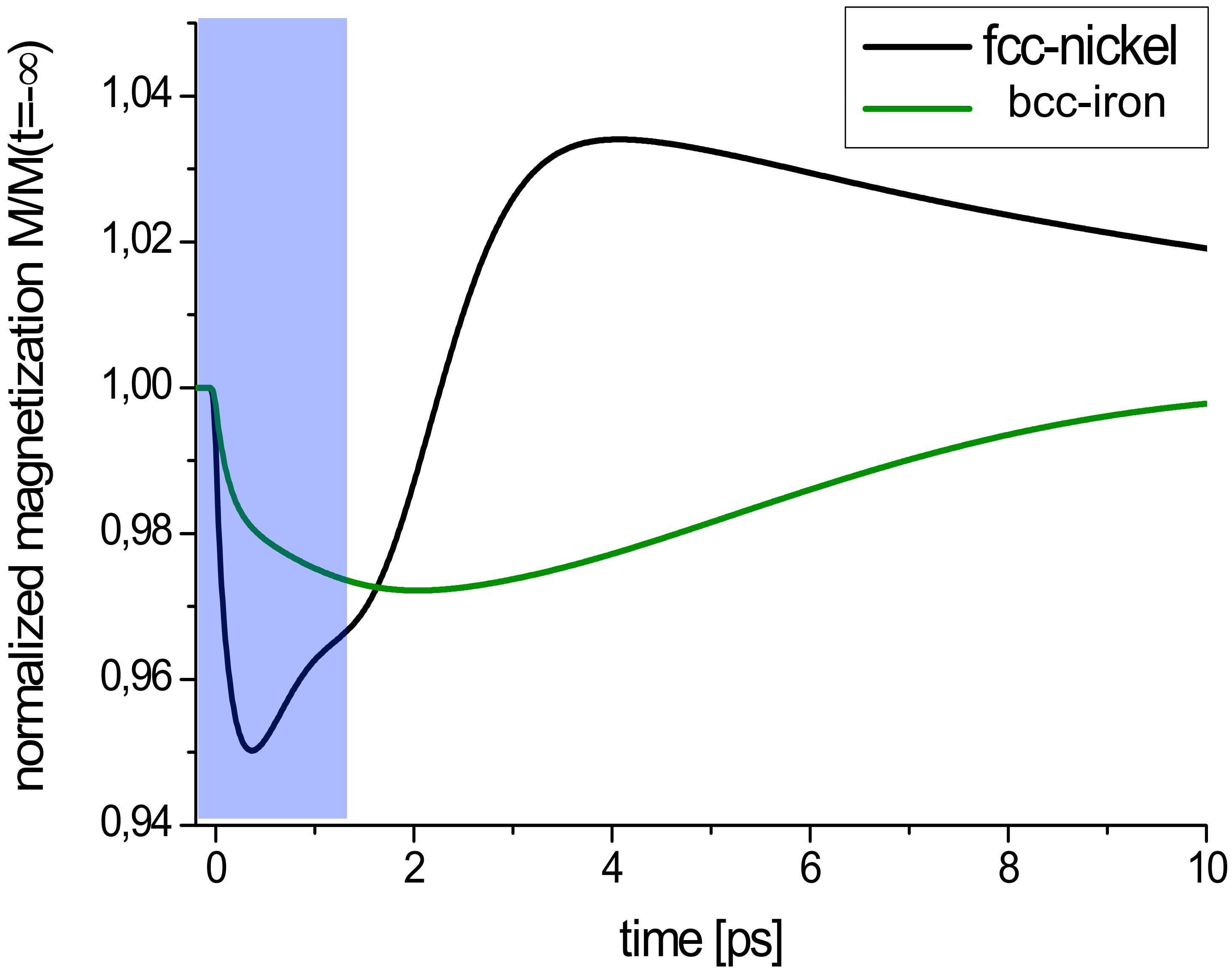
$$\Delta N_\tau(E) = \sum_{\vec{k}} \sum_{\mu} \delta(E - \varepsilon_k^\mu) \langle \sigma_\tau \rangle_k^\mu \left[f_{\vec{k}}^\mu(t) - F(\varepsilon_{\vec{k}}^\mu, T_0) \right]$$

Optical Excitation: Frequency Dependence

- Influence of band structure/spin-mixing on optical excitation



Magnetization Dynamics after Optical Excitation



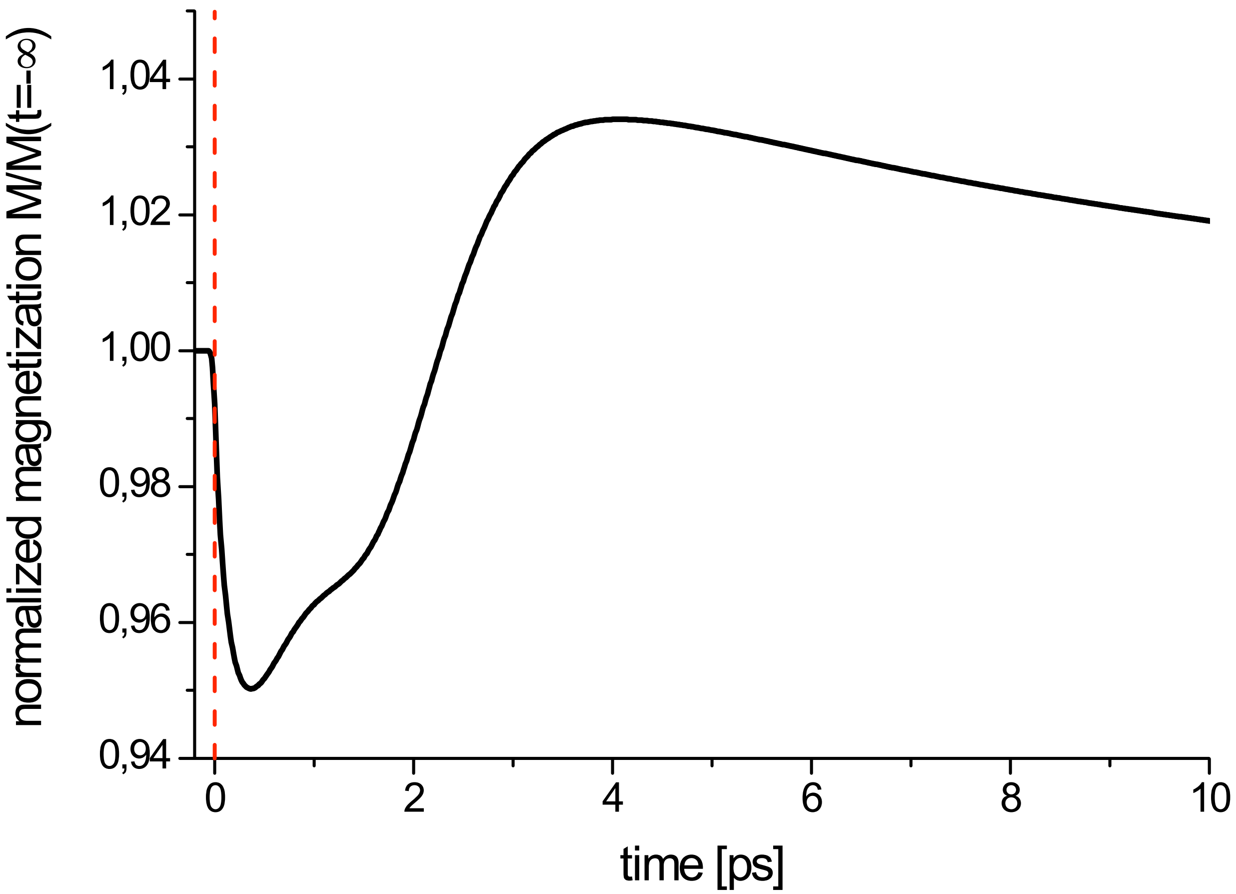
Essert & Schneider, Phys. Rev. B **84**, 224405 (2011)

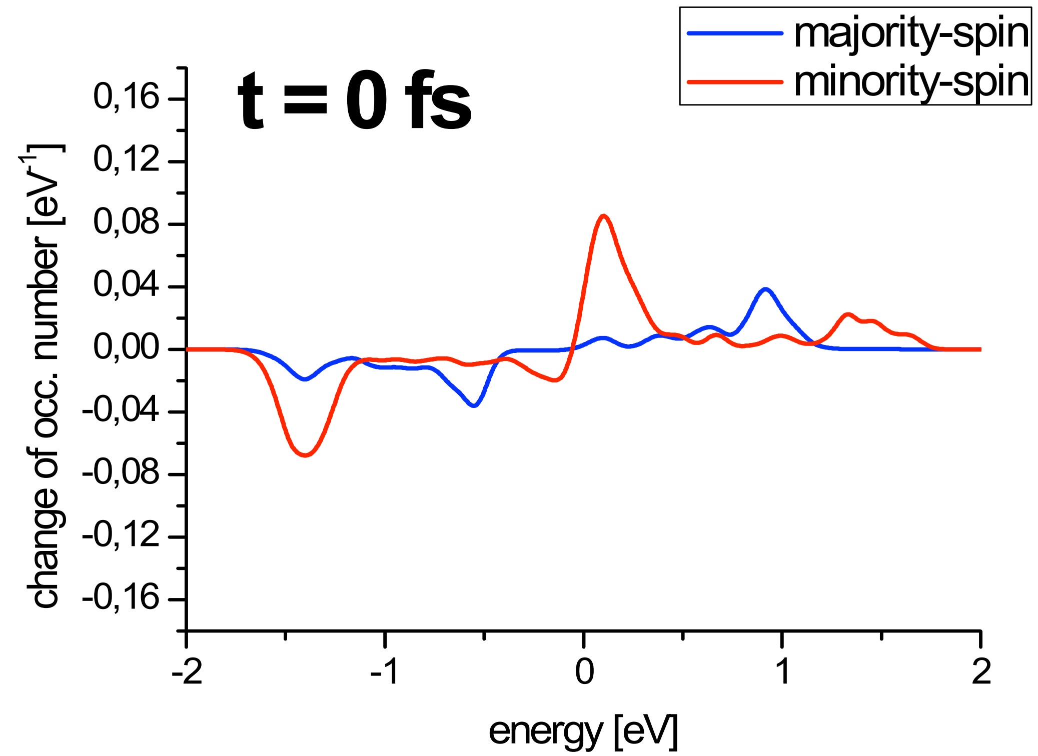
agreement with Carva, Battiato and Oppeneer, PRL **107**, 207201 (2011)

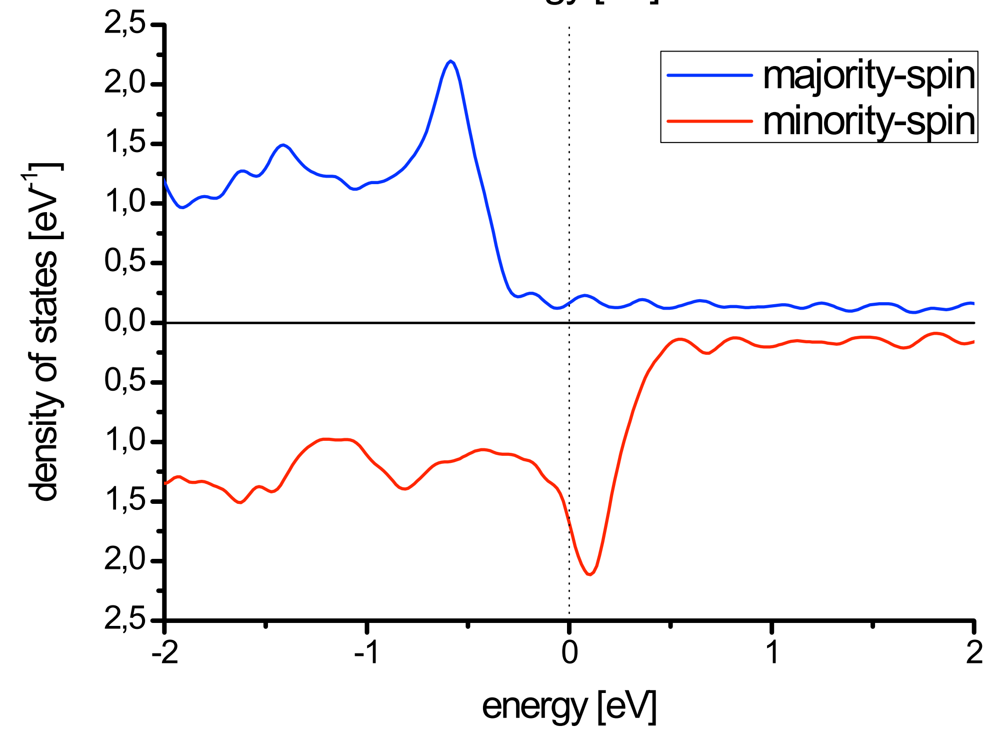
- Demagnetization mainly due to hole scattering
- Optical excitation and electron-phonon-scattering cannot explain the observed demagnetization
- Other scattering mechanisms?

Energy-Resolved Dynamics: fcc nickel

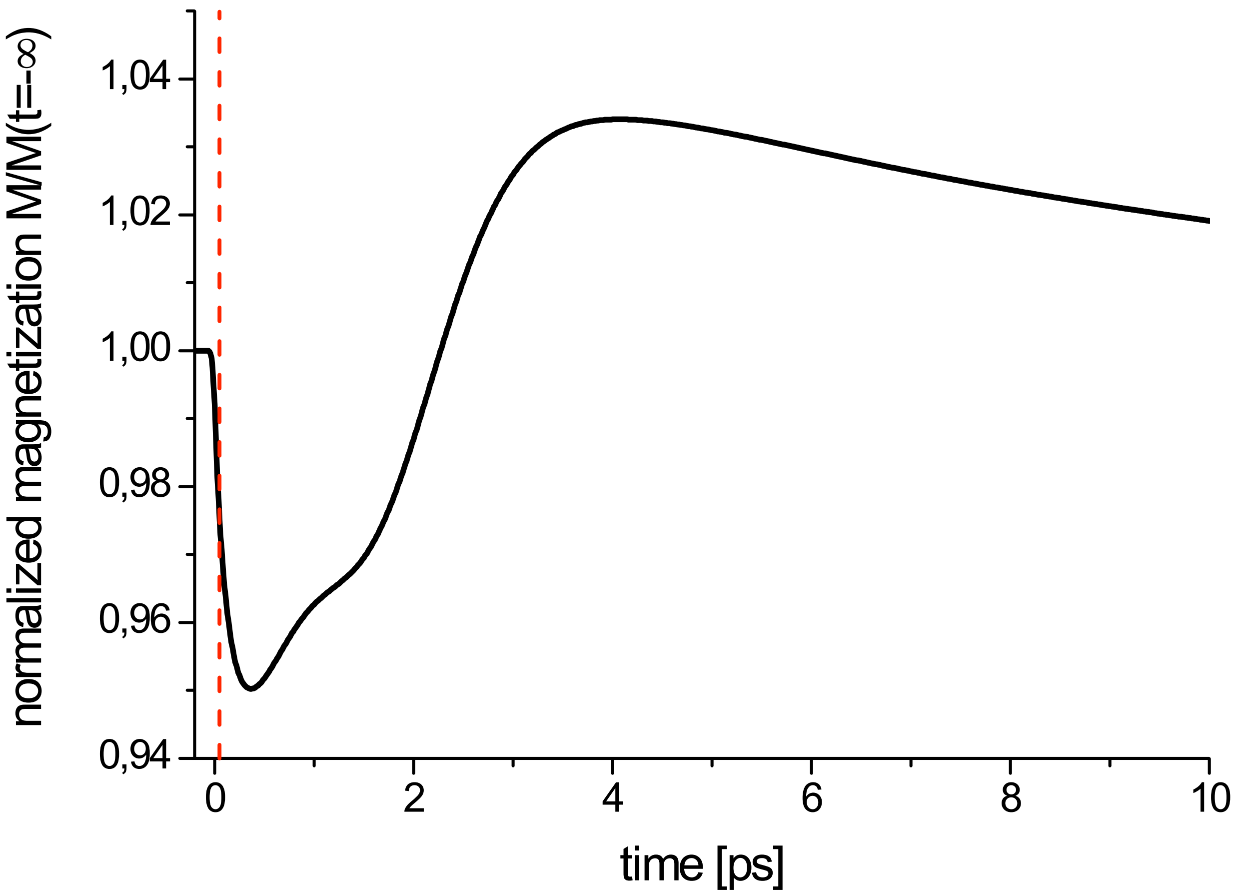
- Microscopic energy resolved dynamics

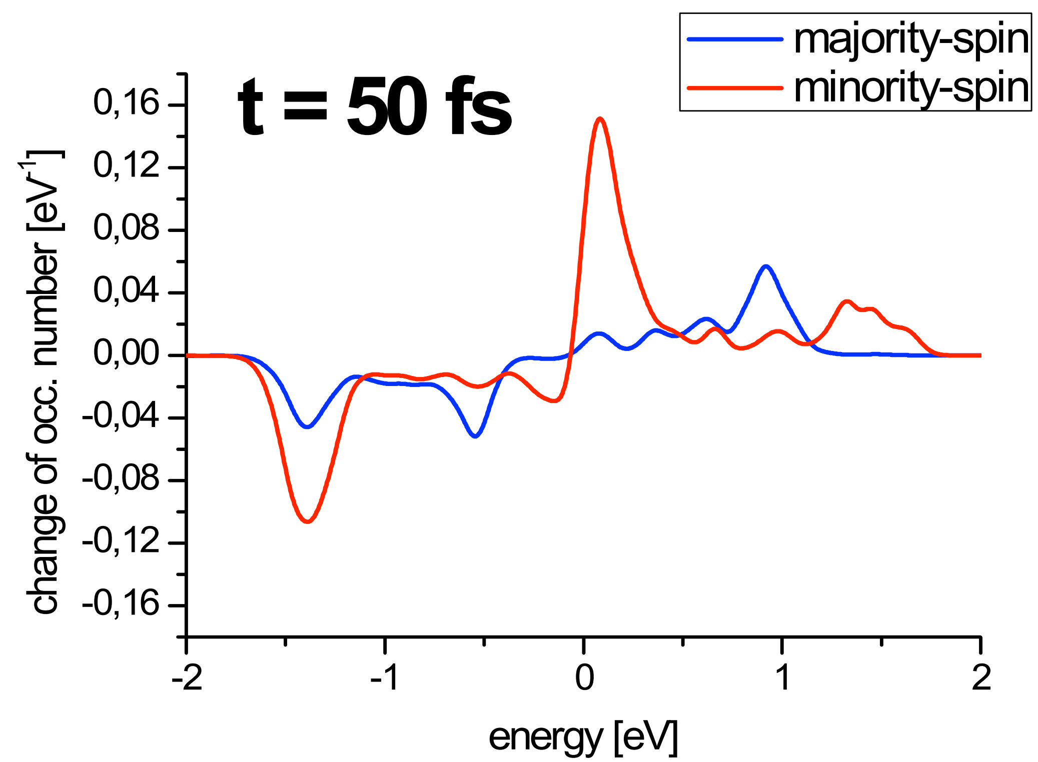


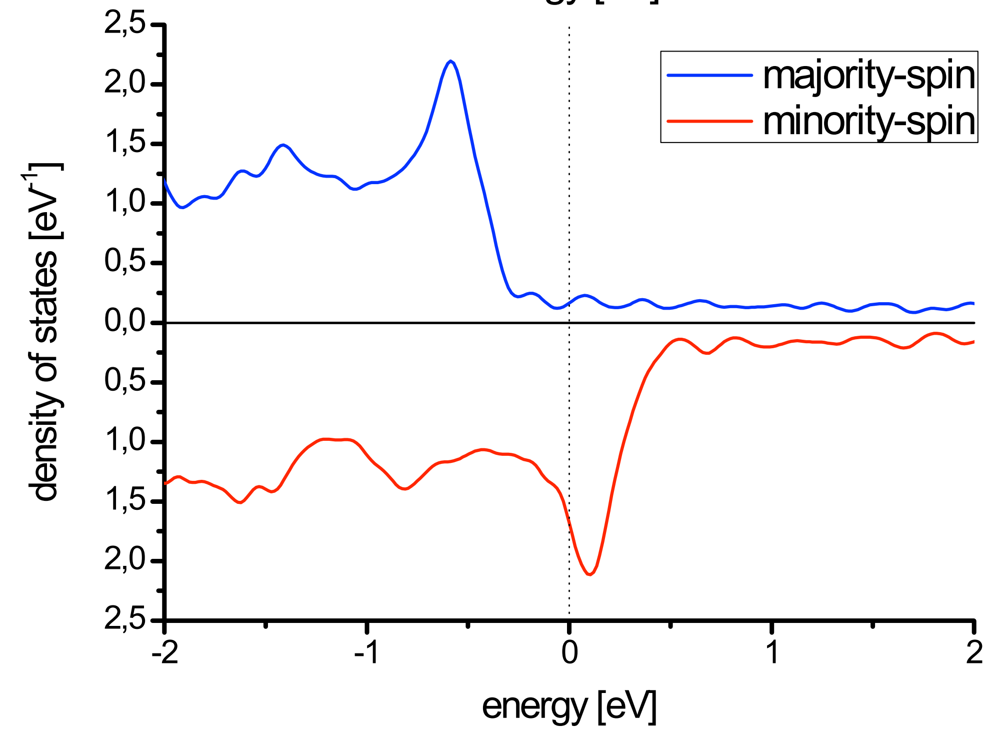




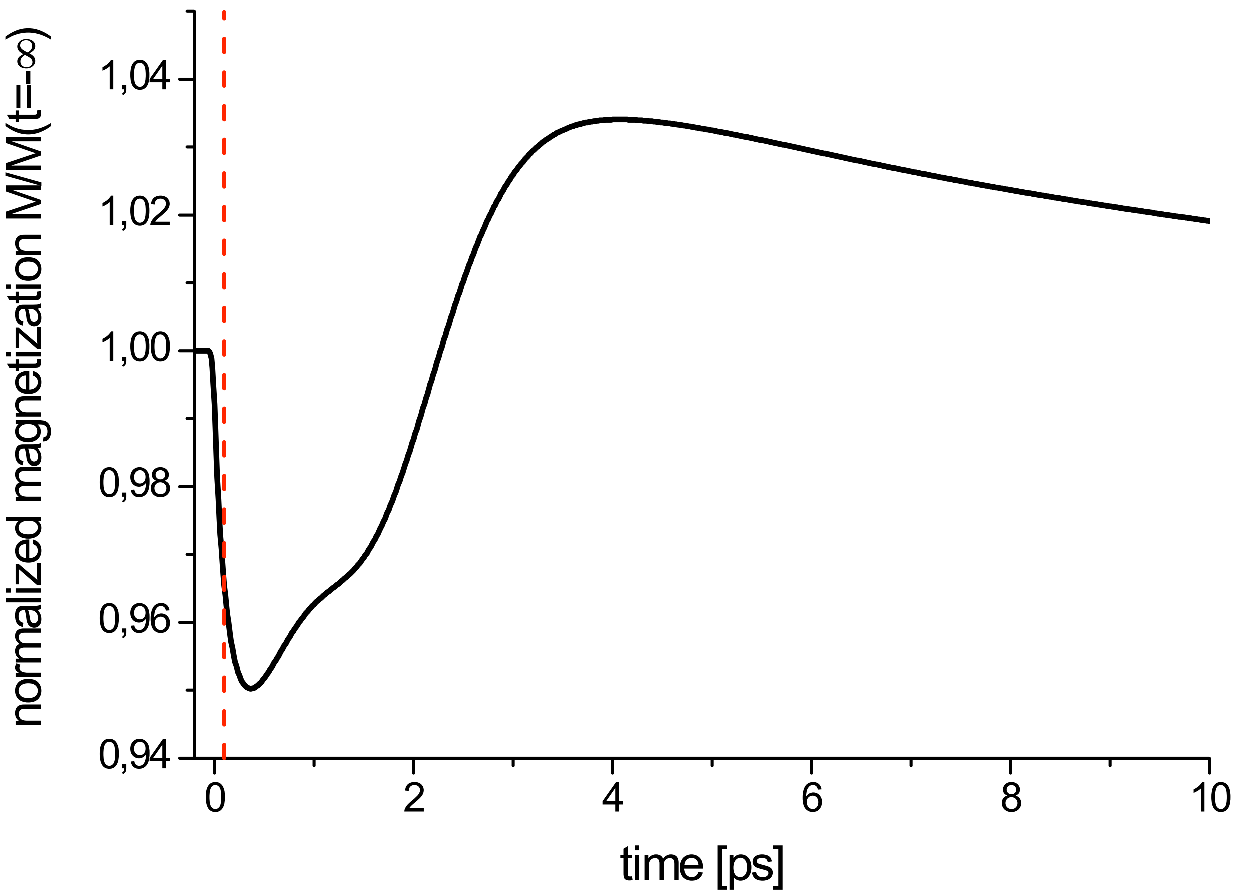
Energy-Resolved Dynamics: fcc nickel

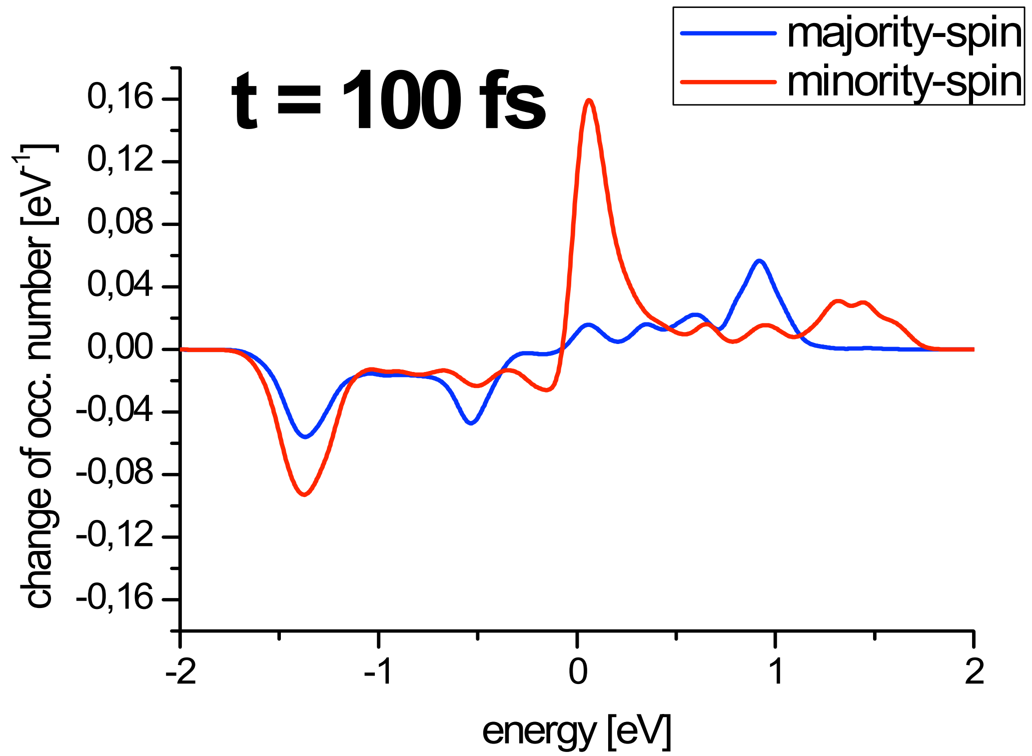


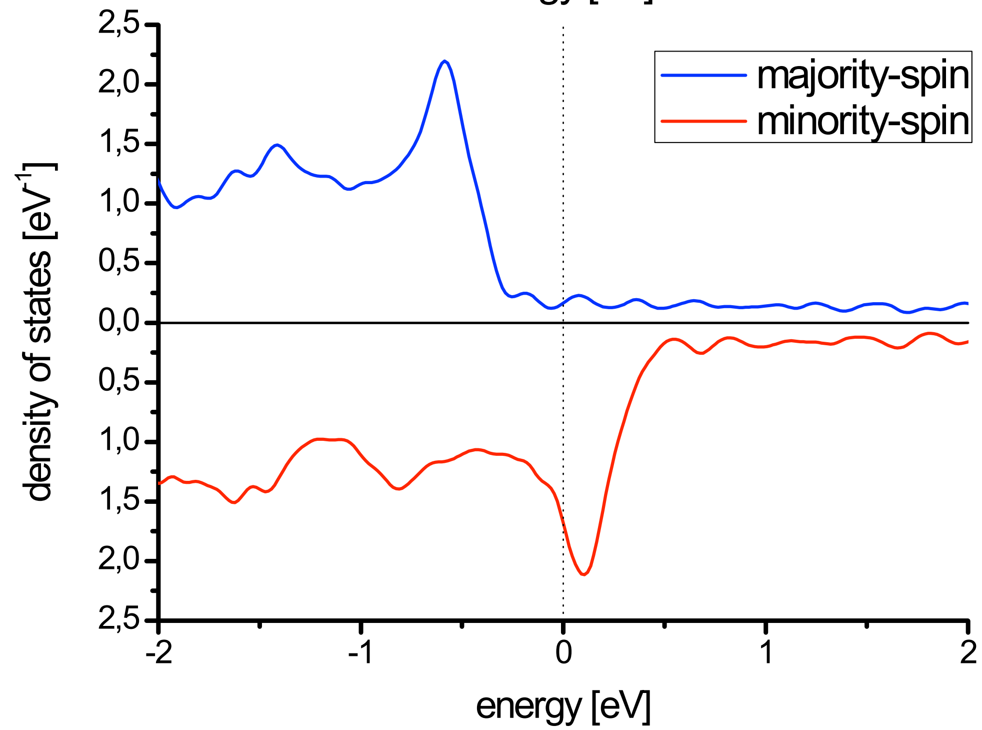




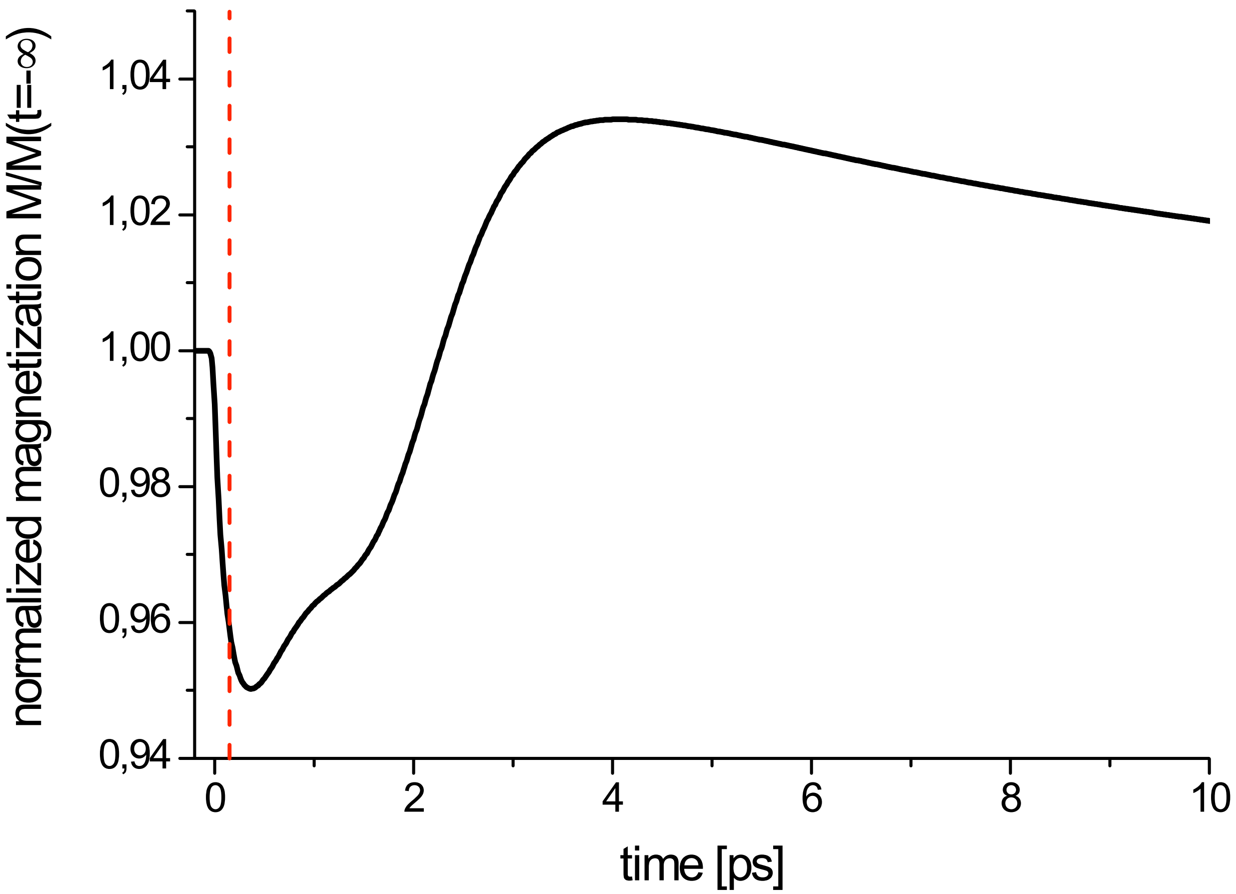
Energy-Resolved Dynamics: fcc nickel

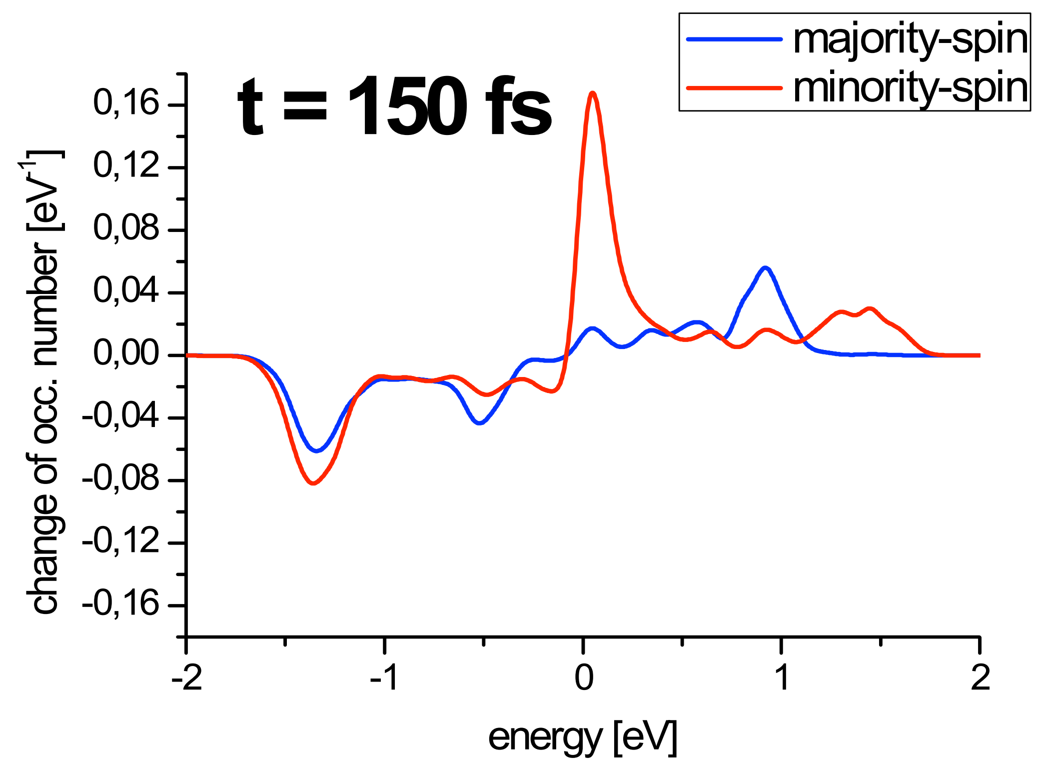


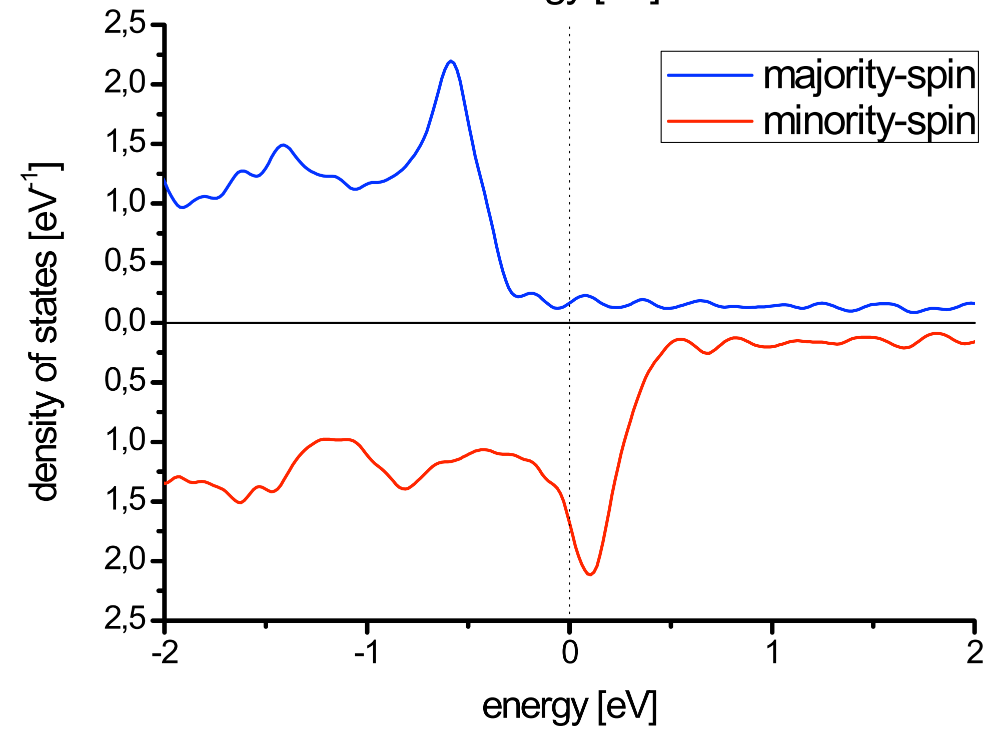




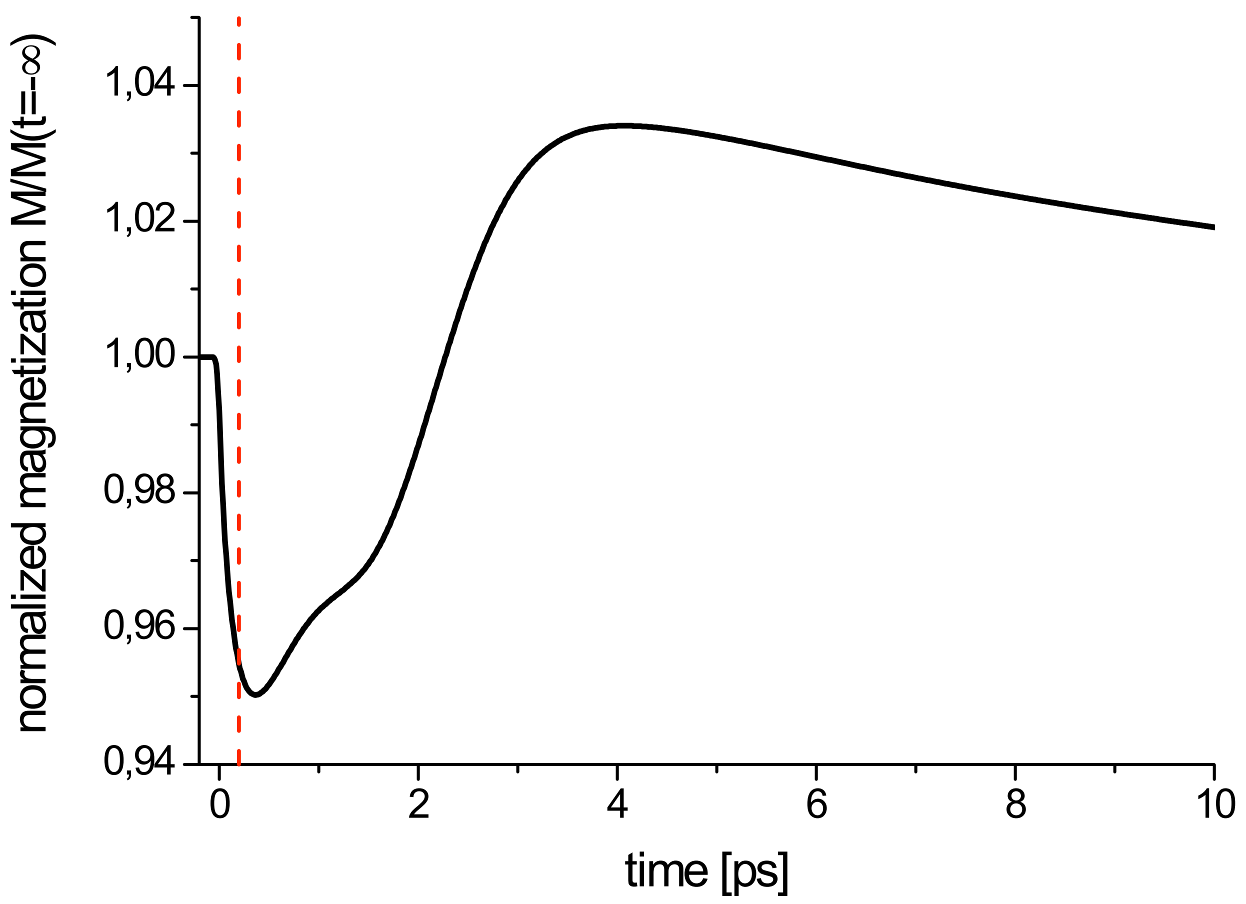
Energy-Resolved Dynamics: fcc nickel

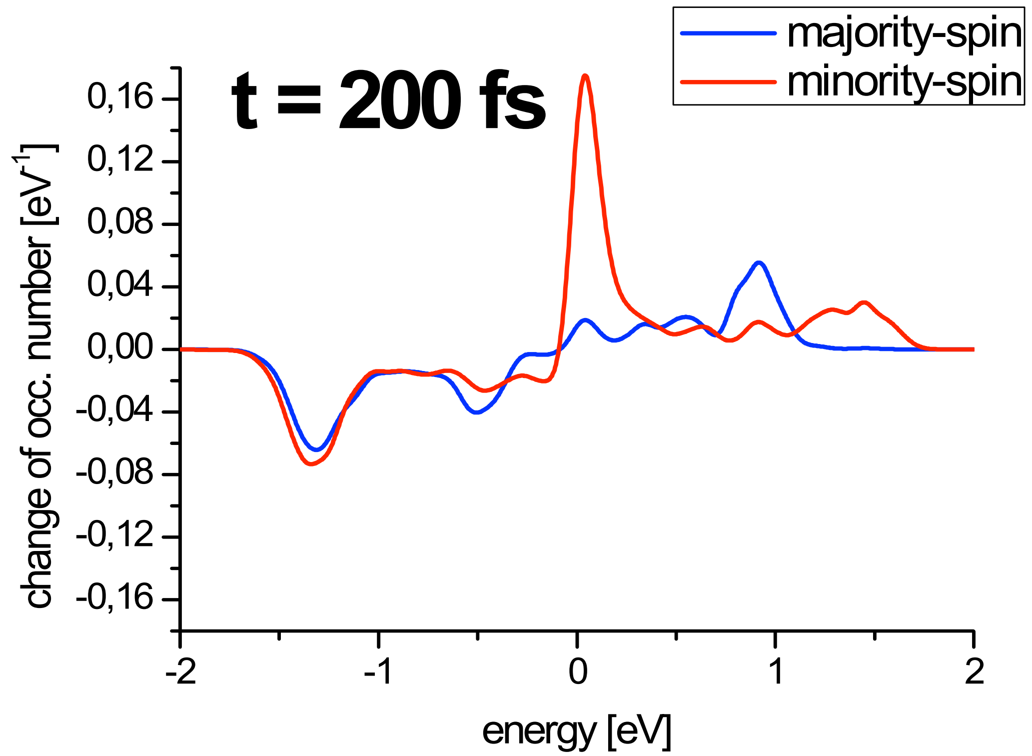


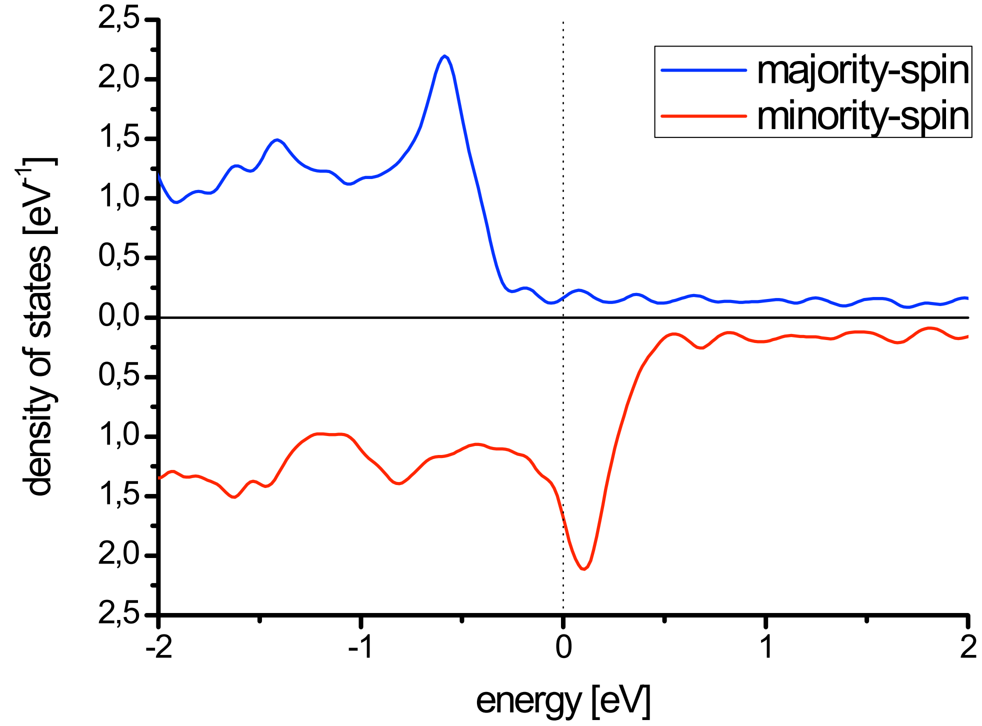




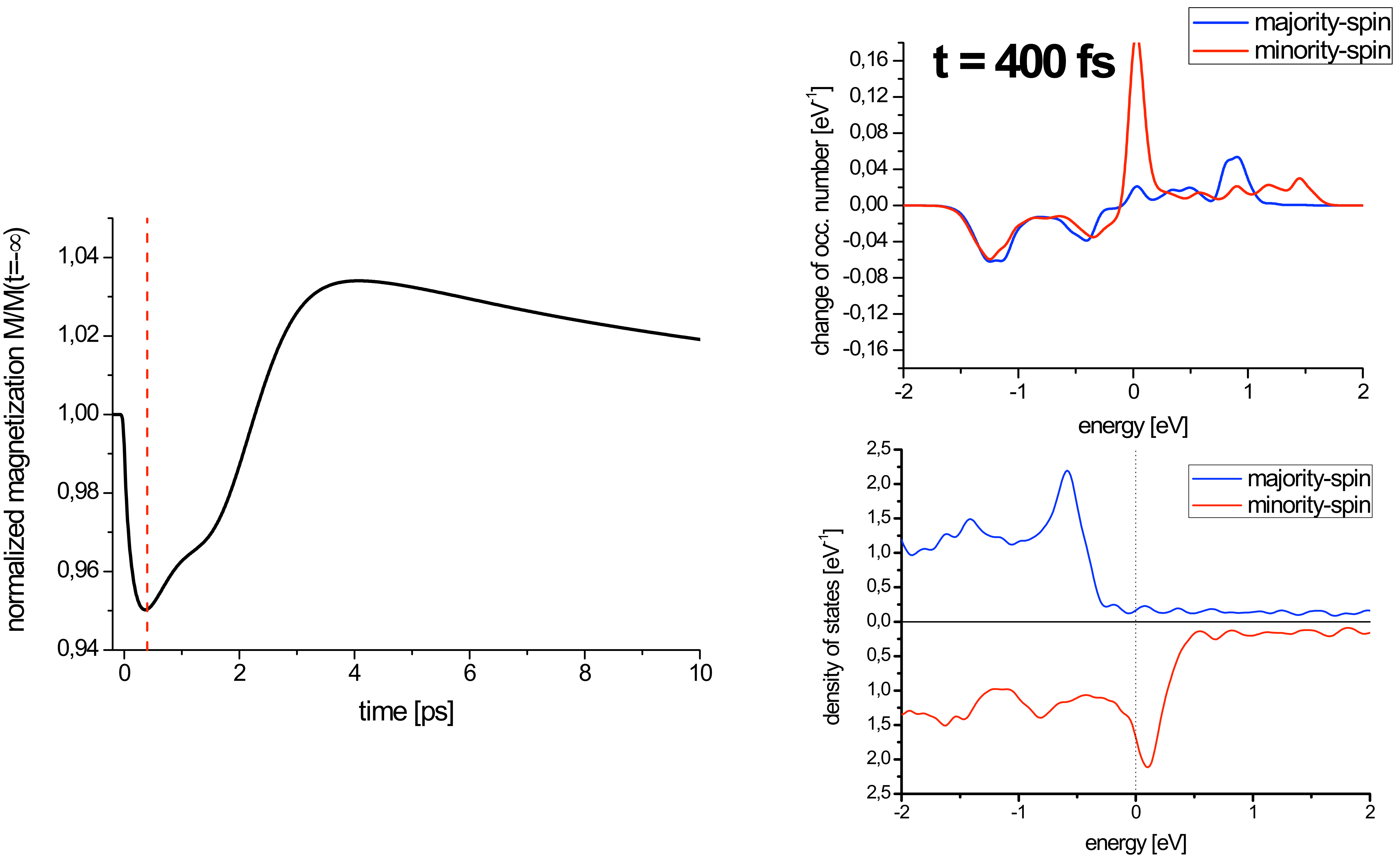
Energy-Resolved Dynamics: fcc nickel







Energy-Resolved Dynamics: fcc nickel



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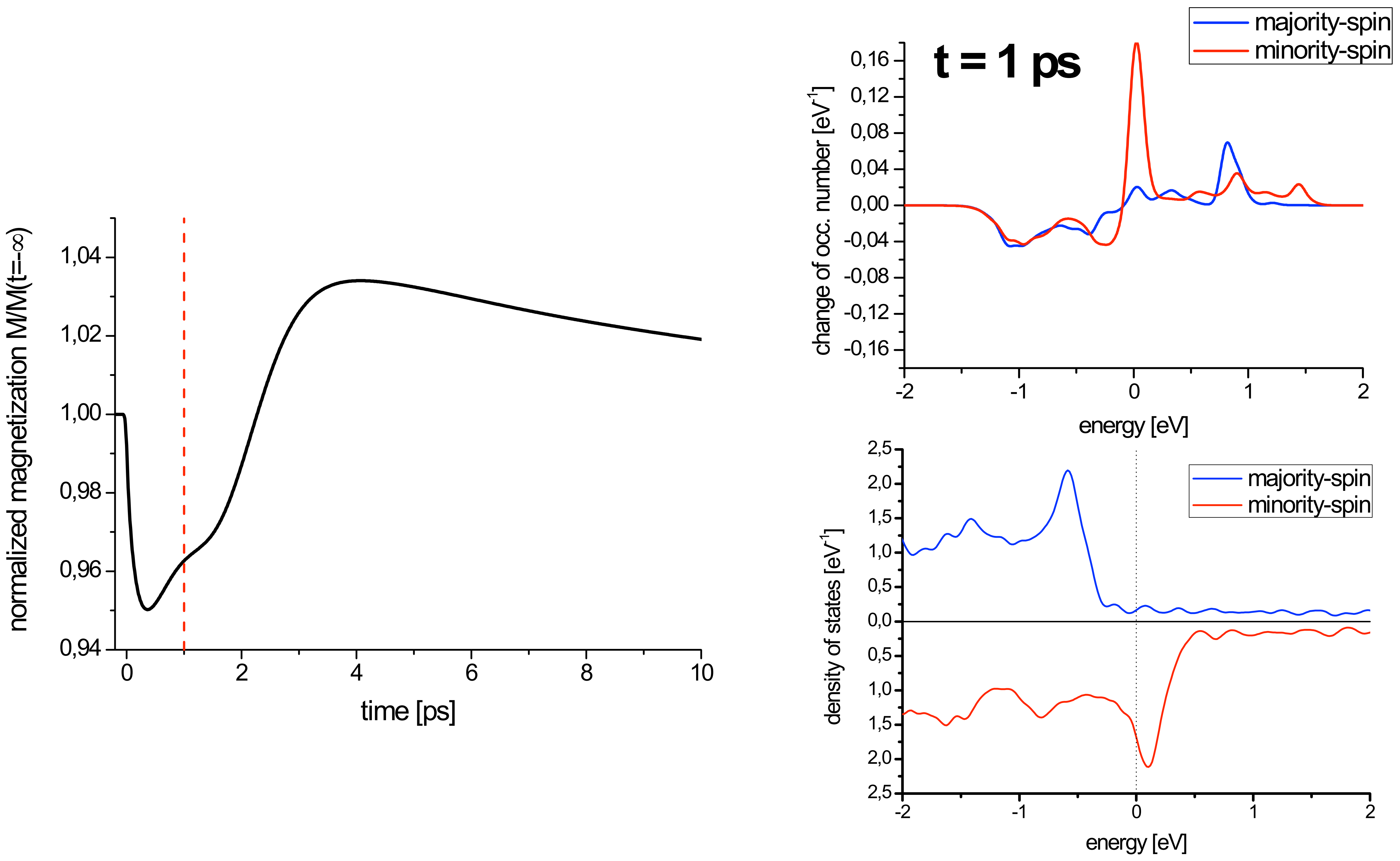
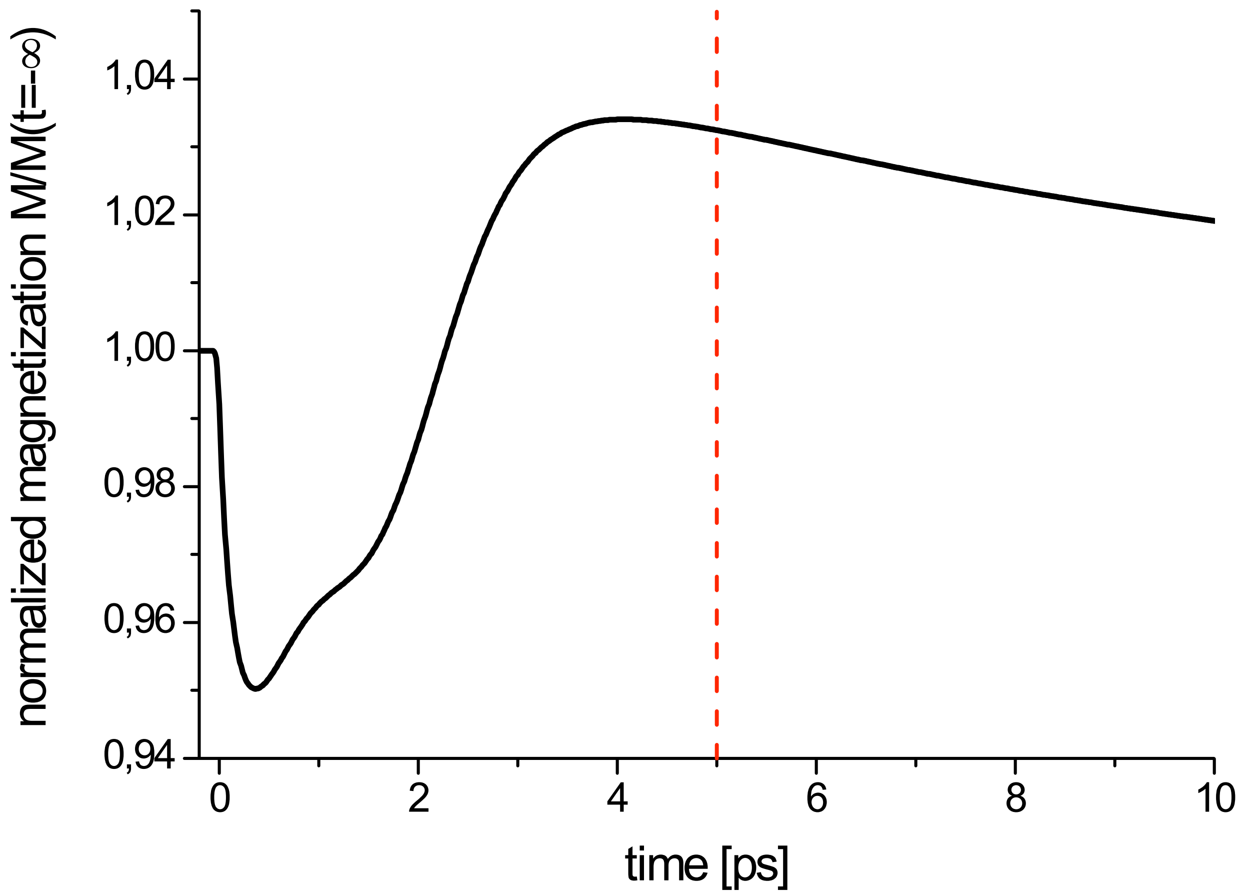
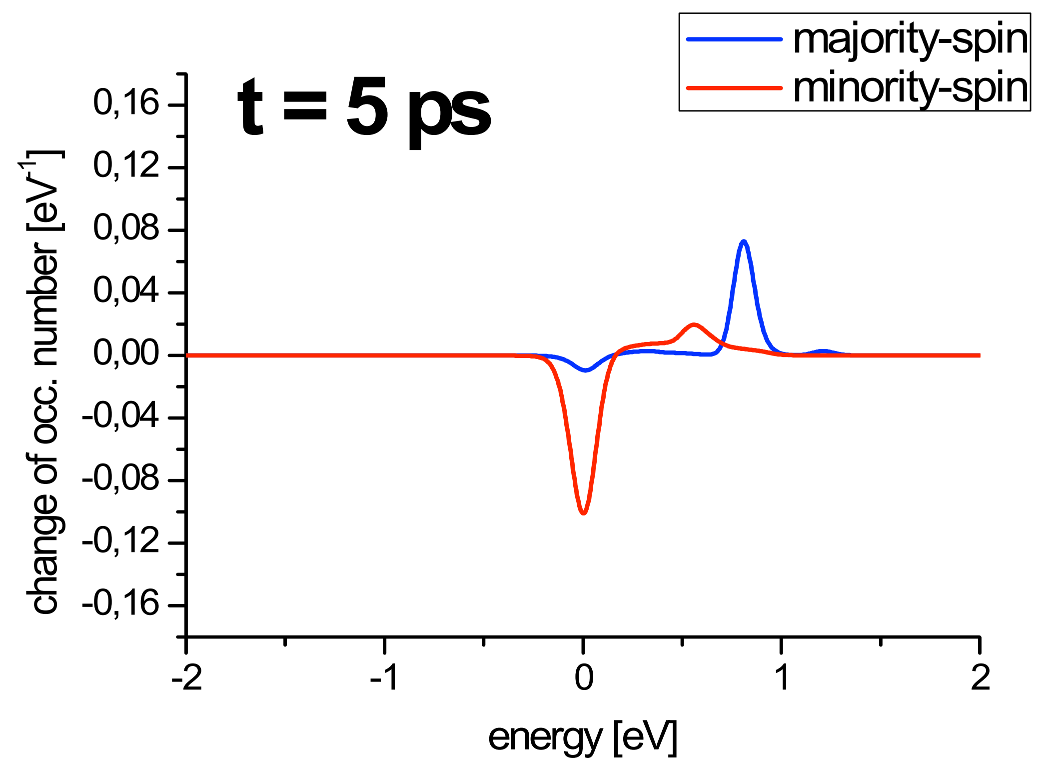
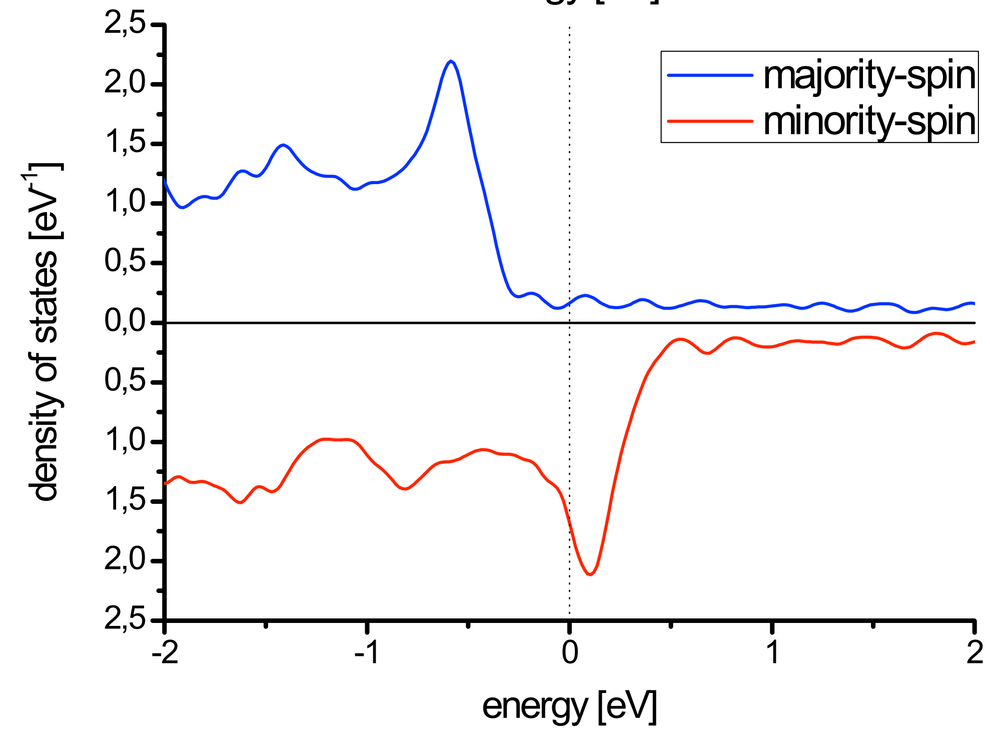


Energy-Resolved Dynamics: fcc nickel

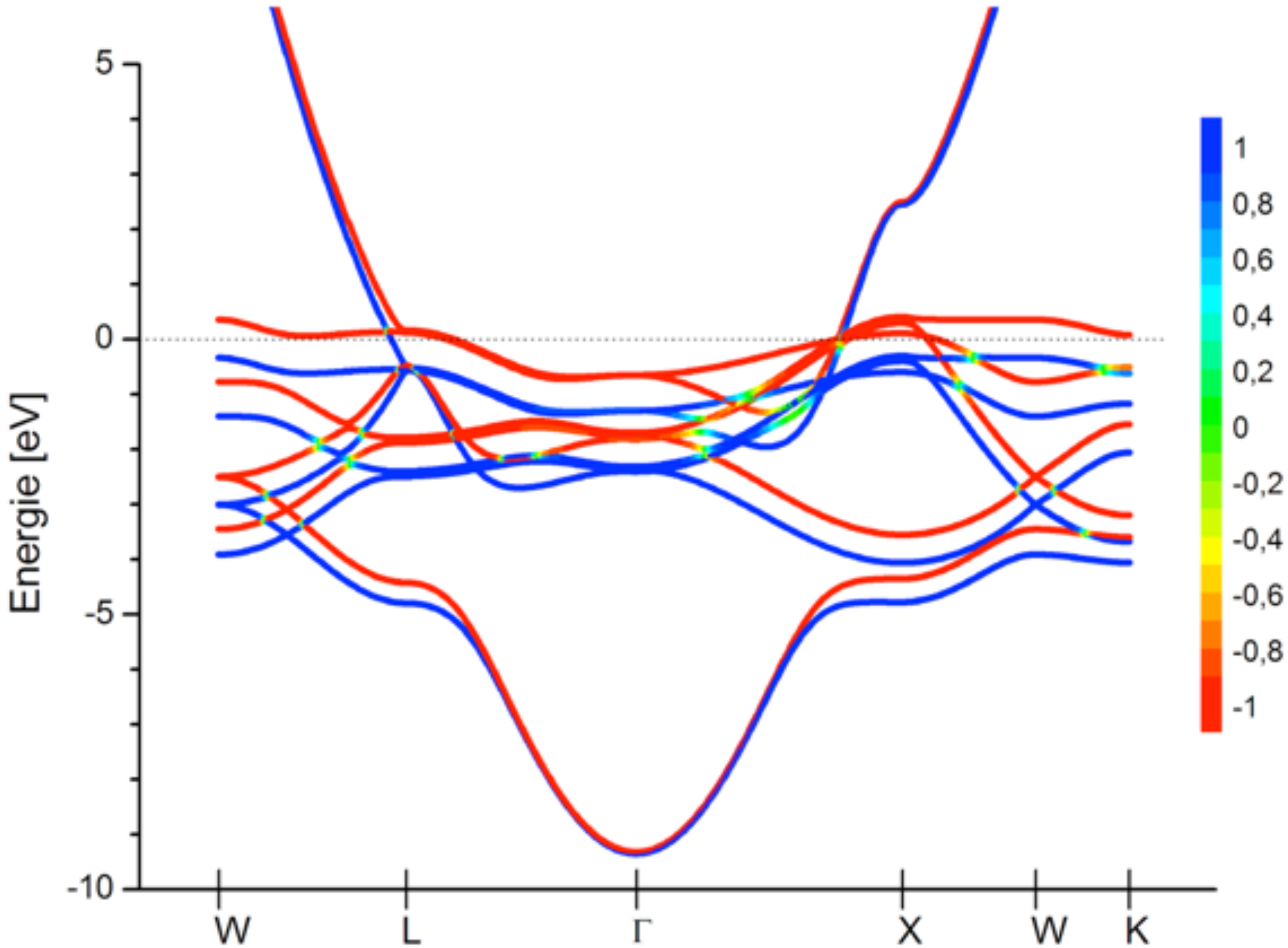




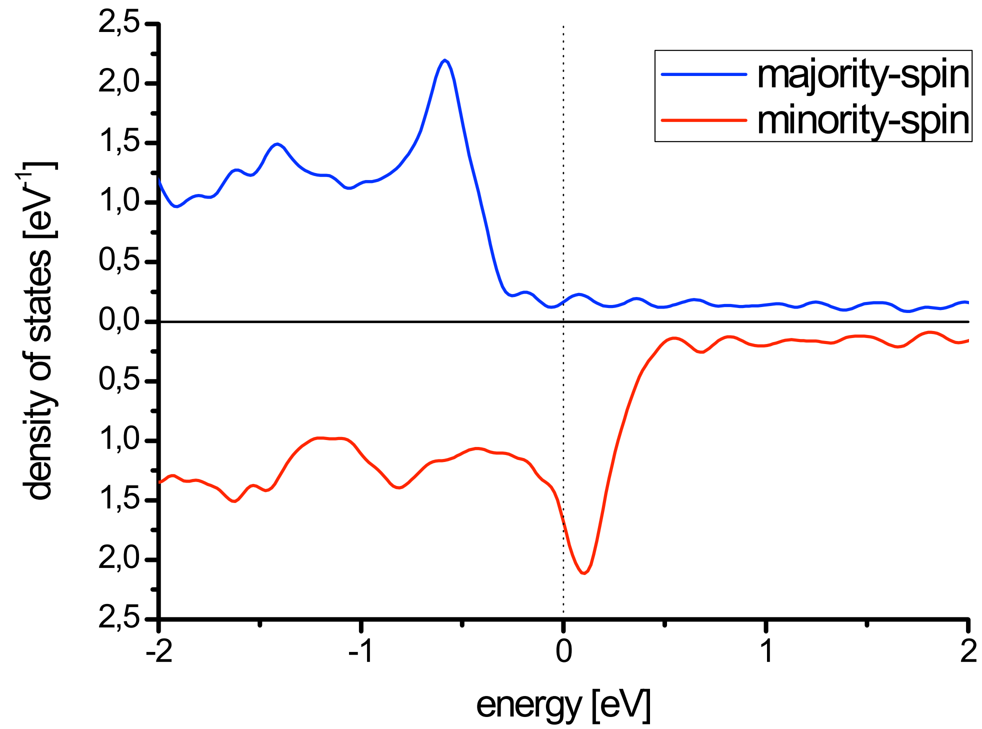


Band Structure Properties

Nickel band structure @ T = 0K
with "spin hot-spots"



Nickel Density of States
@ T=0K



- Demagnetization requires energy (delivered by pulse)
- <u>Any</u> scattering process = dynamical redistribution of excited carriers

How Accurate Can Scattering in a Fixed Band Structure Be?

- Minimal magnetization (maximal demagnetization) by "optimization" for the energy deposited by laser pulse in a fixed band structure

$$\min_{\{n^{\mu}_{\vec{k}}:0\le n^{\mu}_{\vec{k}}\le 1\}} \sum_{\vec{k}}\sum_{\mu} n^{\mu}_{\vec{k}} \langle S_z\rangle^{\mu}_{\vec{k}}$$

- Constraints $$\sum_{\vec{k}}\sum_{\mu} n^{\mu}_{\vec{k}} = N_{\mathrm{eq}}$$

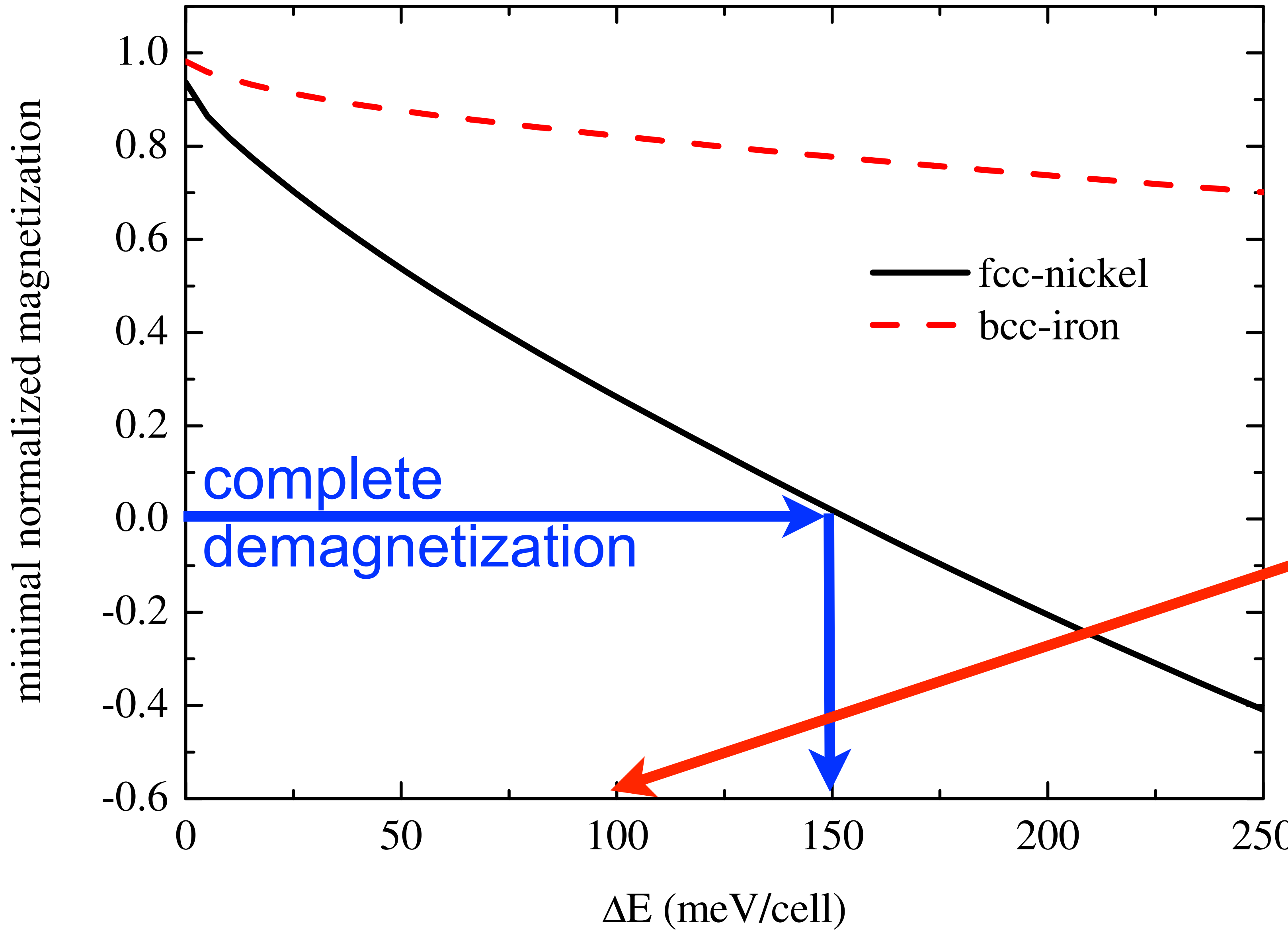
$$\sum_{\vec{k}}\sum_{\mu} n^{\mu}_{\vec{k}}\epsilon^{\mu}_{\vec{k}} \le E_{\mathrm{eq}} + \Delta E$$

- Deposited energy $$\Delta E = \int_{300\,\mathrm{K}}^{T(5\,\mathrm{ps})} dT C_{\mathrm{p}}(T)$$

Essert & Schneider, Phys. Rev. B **84**, 224405 (2011)

How Accurate Can Scattering in a Fixed Band Structure Be?

- Minimal magnetization (maximal demagnetization) by “optimization” for the energy deposited by laser pulse in a <u>fixed</u> <u>band structure</u>



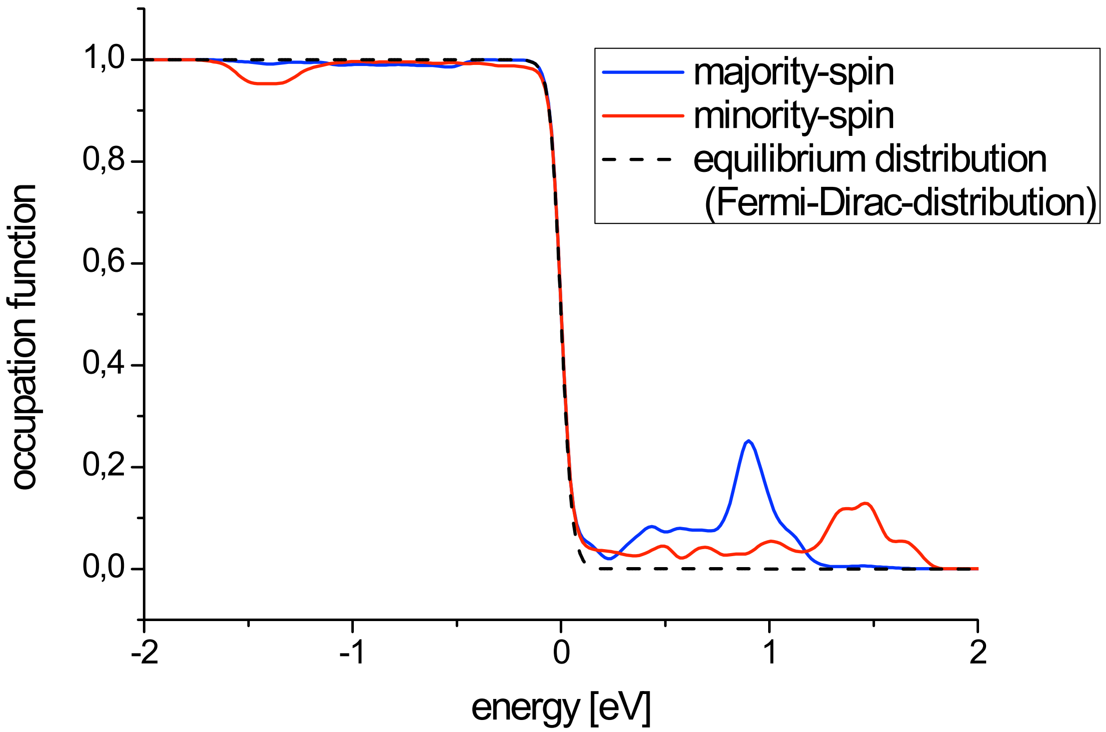
Essert & Schneider, Phys. Rev. B **84**, 224405 (2011)

ΔE from experiment for complete demagnetization:

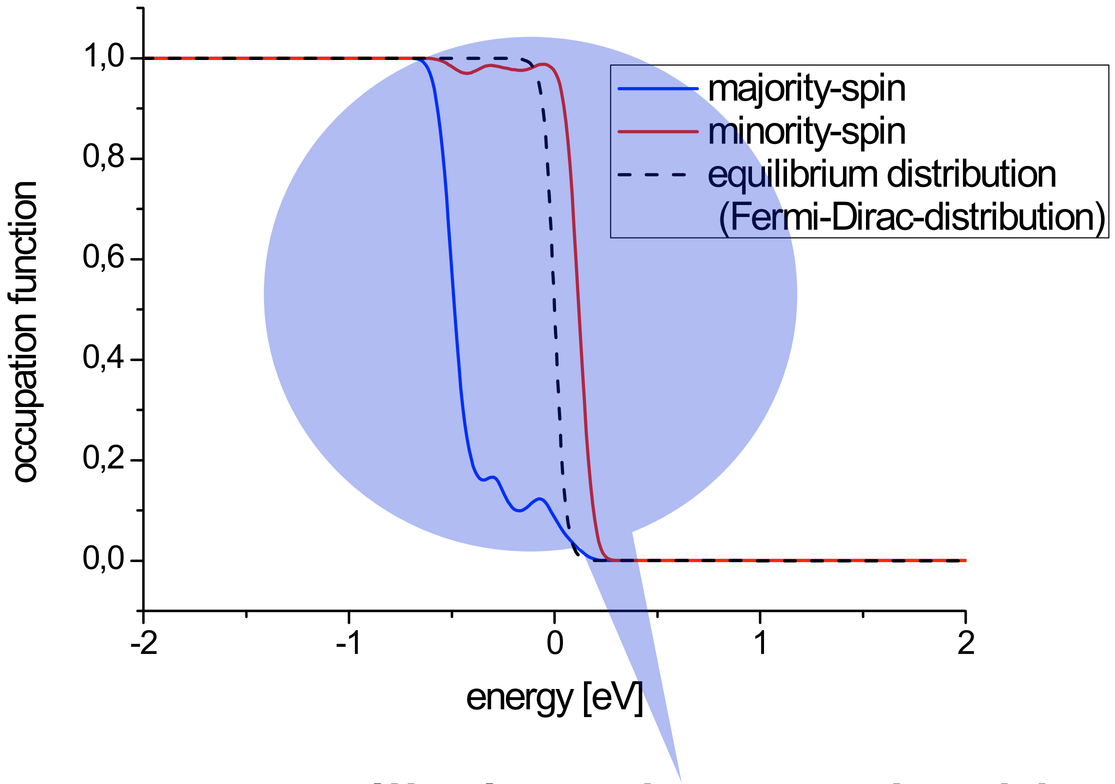
inconsistent with experiment!!!

Distribution Functions

after optical excitation



minimal magnetization



unlikely to be reached by physical scattering processes

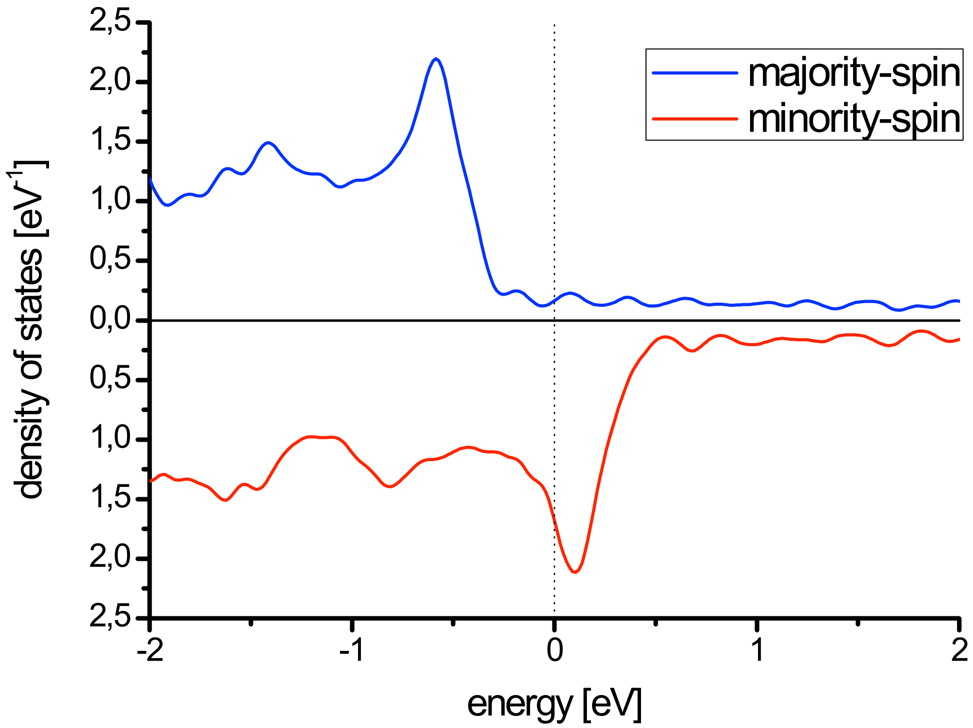
- Scattering in DFT band structure in general <u>not</u> sufficient to explain demagnetization
- Exchange splitting change/spin fluctuations must occur on ultrafast timescale <u>in addition to scattering</u>

agreement with Carva, Battiato and Oppeneer, PRL **107**, 207201 (2011)

Rhie et al., Phys. Rev. Lett. **90**, 247201 (2003)

Effective Stoner Model (1)

- Model based on nickel spin-dependent density of states
- Effective two-band model: Distribution functions $f_{\downarrow}(E)$ and $f_{\uparrow}(E)$ spin and energy dependent

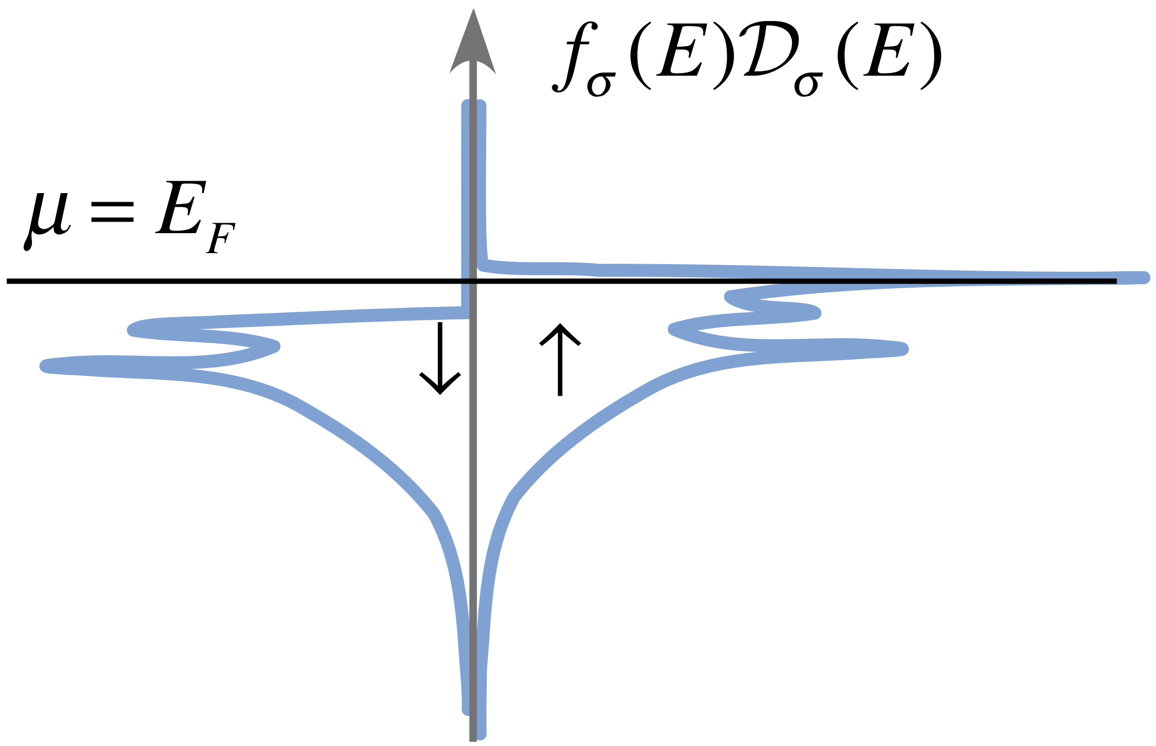


- Stoner model with effective Coulomb energy U=5.04 eV
- Exchange splitting

$$\Delta = U_{\text{eff}} M = 0.26\,\text{eV}$$

- Density of states

$$\mathcal{D}_\sigma(E) = \mathcal{D}_\sigma^{(0)}(E \pm \Delta)$$

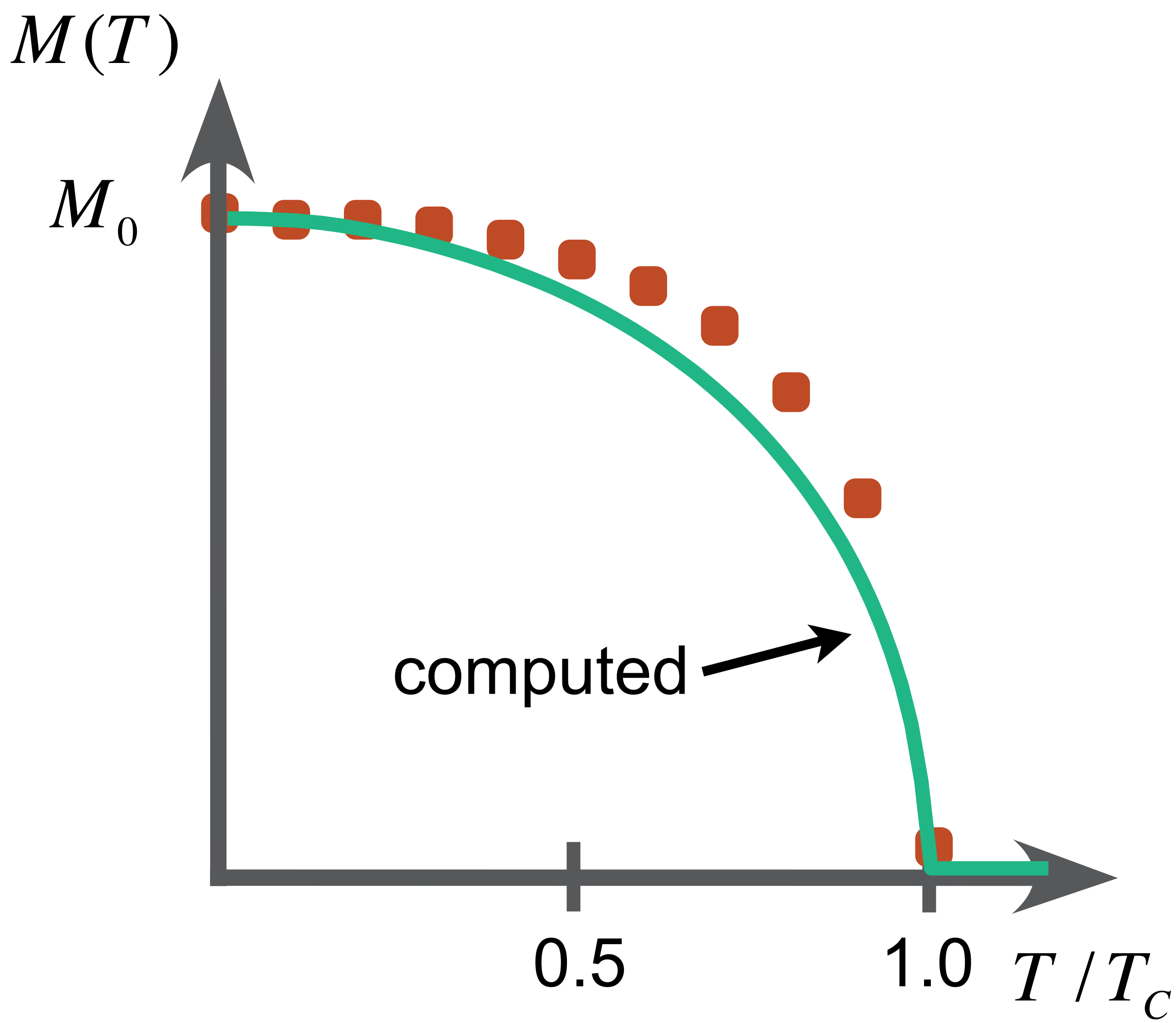


Effective Stoner Model (2)

- "Realistic" equilibrium magnetization curve

  $T_C = 631\mathrm{K}$

- Dynamics: Influence of "hot electrons"? ⇒ Include carrier-carrier and carrier-phonon scattering
- "Non-equilibrium generalization of 3-temperature model"

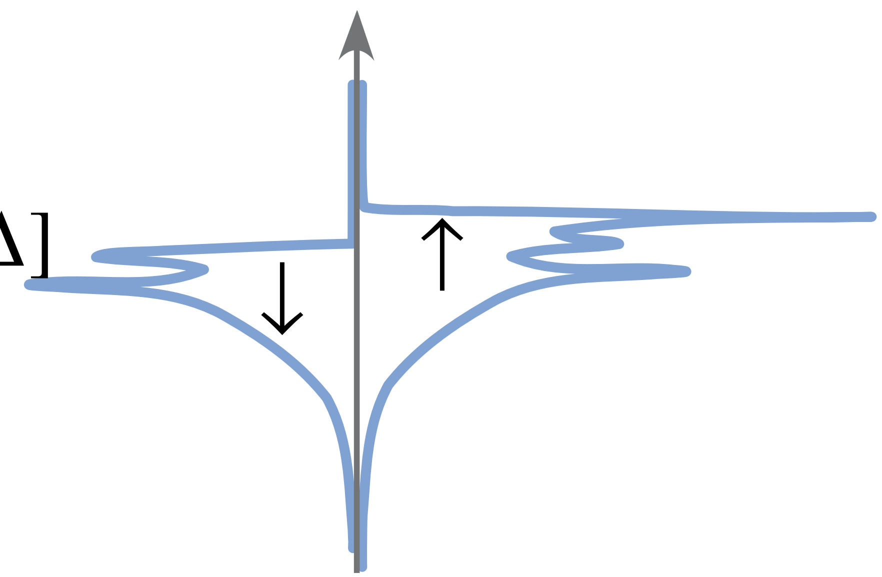


Dynamical Stoner Model

wave-function overlap — exchange splitting

$$\frac{\partial f_\eta}{\partial t} = \sum_{\sigma,\nu,\lambda} |\langle \eta,\sigma | \nu,\lambda\rangle|^2 \, \Gamma^{\eta,\sigma,\nu,\lambda}_{\text{el-el}}[\Delta] n + \sum_{\sigma} |\langle \eta | \sigma\rangle|^2 \, \Gamma^{\eta,\sigma}_{\text{el-ph}}[\Delta] + \sum_{\sigma} |\langle \eta | \sigma\rangle|^2 \, \Gamma^{\eta,\sigma}_{\text{exc}}[\Delta]$$

$$\frac{\partial g}{\partial t} = \sum_{\eta,\sigma} |\langle \eta | \sigma\rangle|^2 \, \Gamma^{\eta,\sigma}_{\text{ph-el}}[\Delta]$$



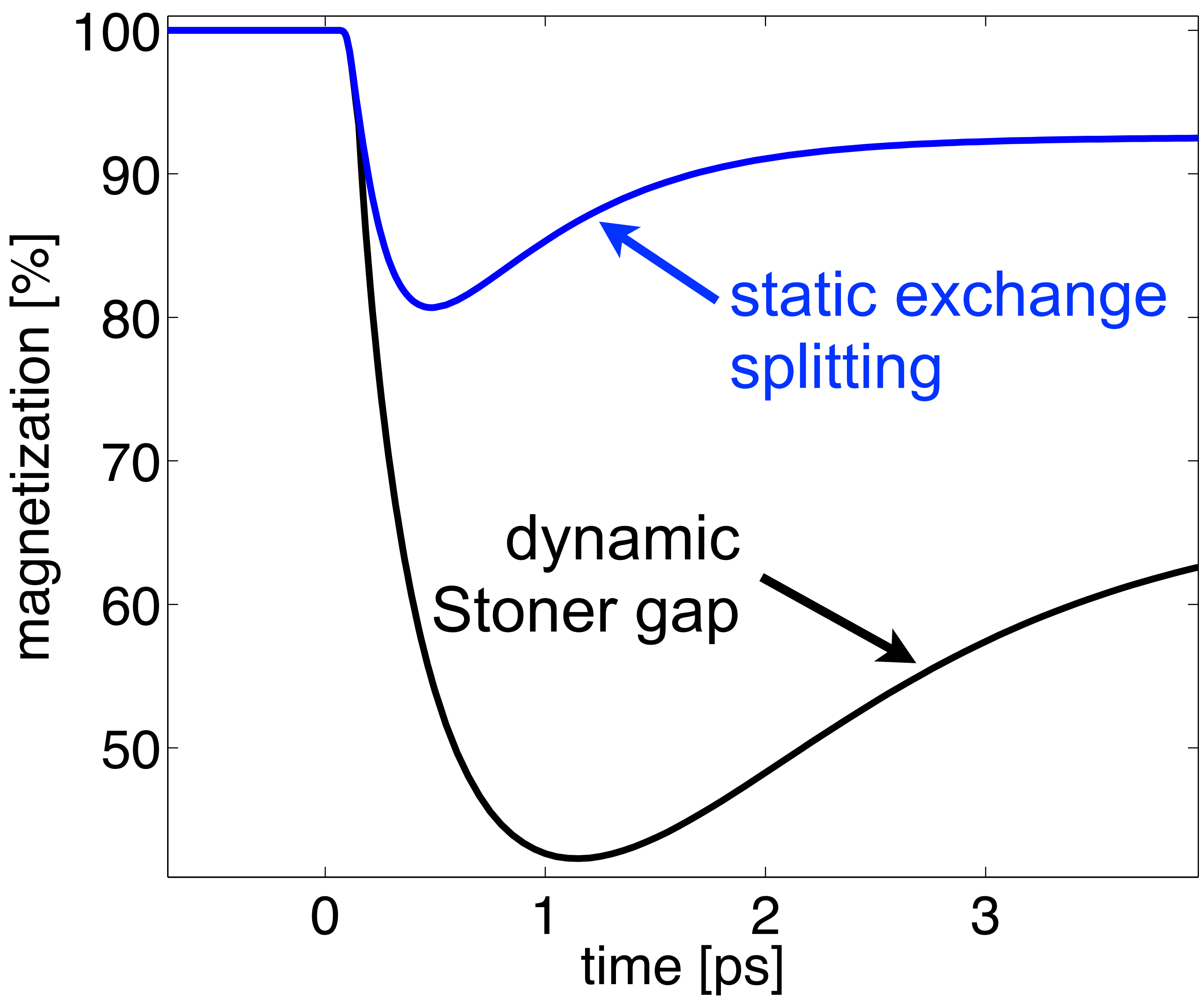
$$\Delta(t) = U_{\text{eff}} M(t)$$

- Boltzmann scattering integrals for carrier-carrier (static Coulomb), carrier-phonon (LA) interaction
- Optical excitation (plasma like)
- Dynamical energy dispersions

scattering integrals: M. Krauß et al, Phys. Rev. B **80**, 180407(R) (2009); dynamical exchange splitting: B. Mueller et al., PRL 111, 167204 (2013)

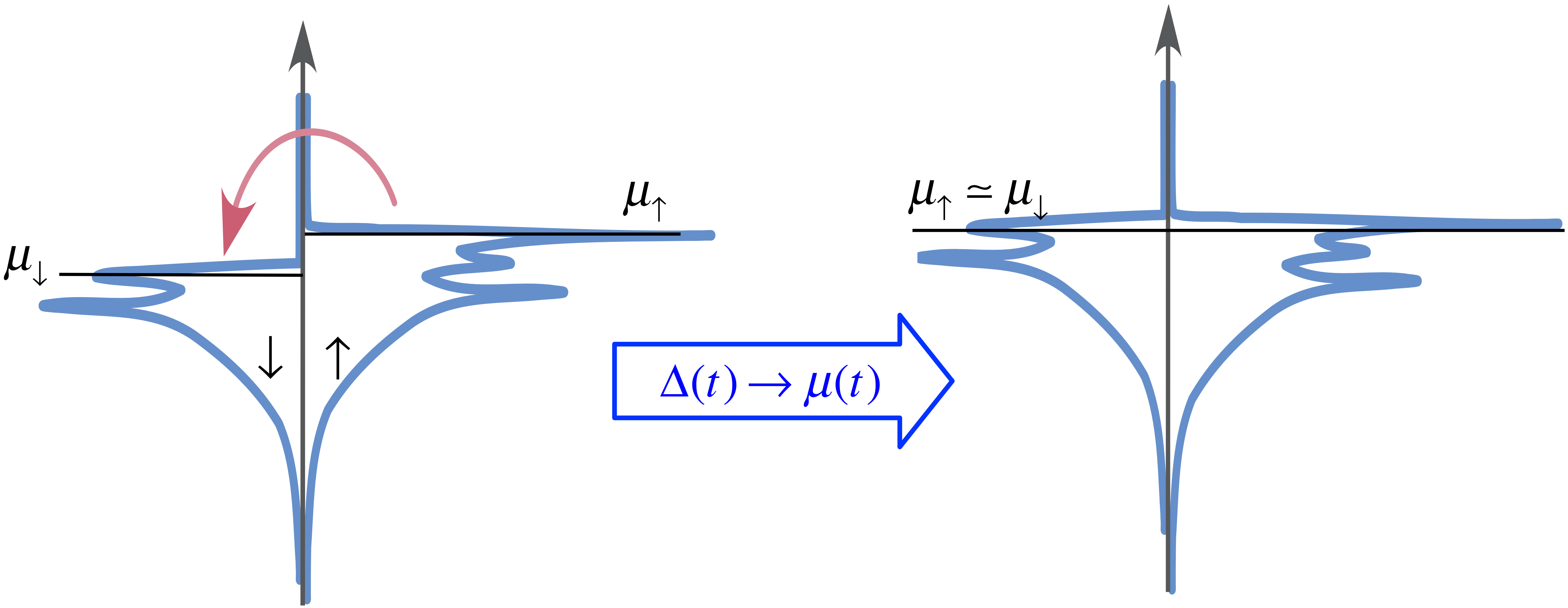
Stoner-Model Demagnetization Dynamics

- Dynamic exchange splitting "improves" quenching
- Temperature and chemical potential differences contribute to demagnetization dynamics
- Exchange splitting dynamics removes problem with spin-flip scattering across a static gap



Mueller et al., PRL 111, 167204 (2013)

Dynamical Exchange Splitting



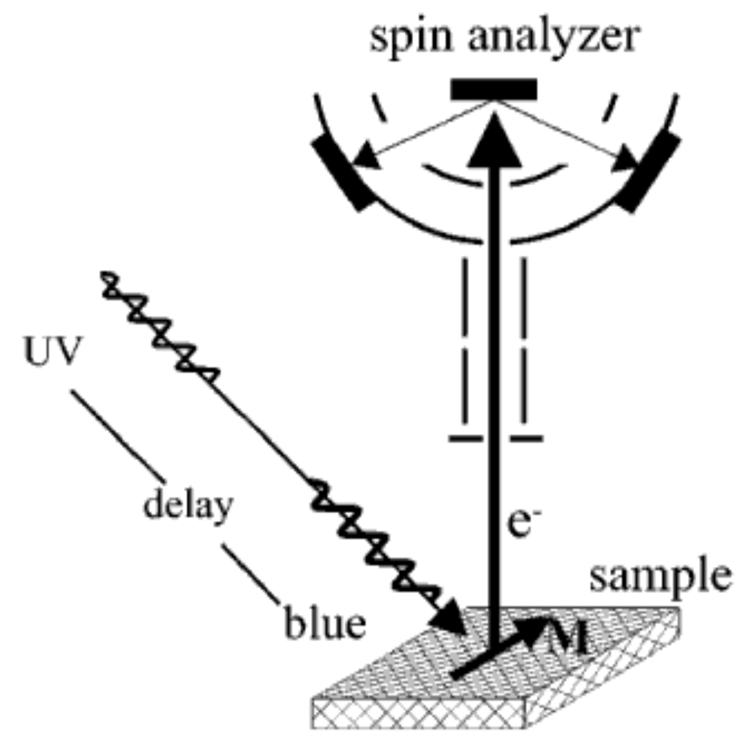
- Electrons heated up by optical exciation $\mu_\uparrow \neq \mu_\downarrow$
- Scattering equilibrates chemical potentials $\mu_\uparrow, \mu_\downarrow \to \mu$
- Dynamical exchange splitting shifts bands: changes quasi-equilibrium chemical potential μ

Outline

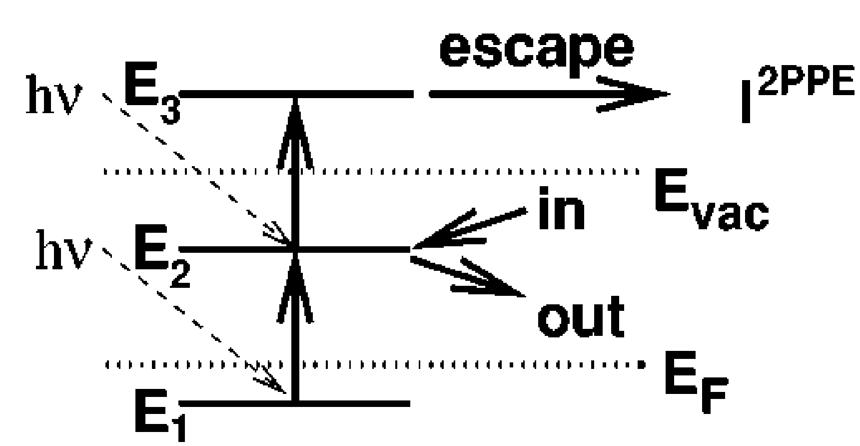
1. Introduction & What is ultrafast demagnetization in ferromagnets?
2. Elliott-Yafet mechanism for electron-phonon scattering and dynamical Stoner model
3. Spin-dependent lifetimes in ferromagnets
4. Spin-dependent transport (in normal metals)

Ferromagnet Lifetimes + "History"

- So far: measurement and calculation of demagnetisation dynamics fraught with inaccuracies
- Simpler(?) problem: Measure/calculate lifetimes



- Theory developed for electron gas in the 1950s and 1960 by Ritchie, Quinn & Ferrell, Ritchie, Quinn (see, e.g., Mahan: *Many-particle physics*)
- Surface states by Echenique, Chulkov and coworkers
- DFT + Many-Particle Theory community (Ambrosch-Draxl, Godby, Louie, Chulkov & Echenique)



Lifetimes: Theory

- Evaluate dielectric function

$$\varepsilon(\vec{q},\omega) = 1 - V_q \sum_{\mu\nu\vec{k}} |B^{\mu\nu}_{\vec{k}\vec{q}}|^2 \frac{f^{\nu}_{\vec{k}} - f^{\mu}_{\vec{k}+\vec{q}}}{\hbar\omega + \epsilon^{\nu}_{\vec{k}} - \epsilon^{\mu}_{\vec{k}+\vec{q}} + i\hbar\gamma}$$

- with wave function overlap $B^{\mu\nu}_{\vec{k}\vec{q}} = \langle \psi^{\mu}_{\vec{k}+\vec{q}} | e^{i\vec{q}\cdot\vec{r}} | \psi^{\nu}_{\vec{k}} \rangle$

- spin-mixing (spin-orbit) coupling included $|\psi^{\mu}_{\vec{k}}\rangle = a^{\mu}_{\vec{k}} \left|\uparrow\right\rangle + b^{\mu}_{\vec{k}} \left|\downarrow\right\rangle$

- Coulomb pot. $V_q = \dfrac{e^2}{\varepsilon_0 q^2}$

- Use q-dependent tetrahedron method (implemented by S. Kaltenborn)
- DFT code including spin-orbit coupling: ELK
- No local-field effects

Lifetimes: Theory

- Lifetimes from Fermi's Golden Rule, i.e., G_0W_0 approximation for self-energy
- momentum and band dependent rate: $(\nu,\vec{k}) \rightarrow (\mu,\vec{k}+\vec{q})$

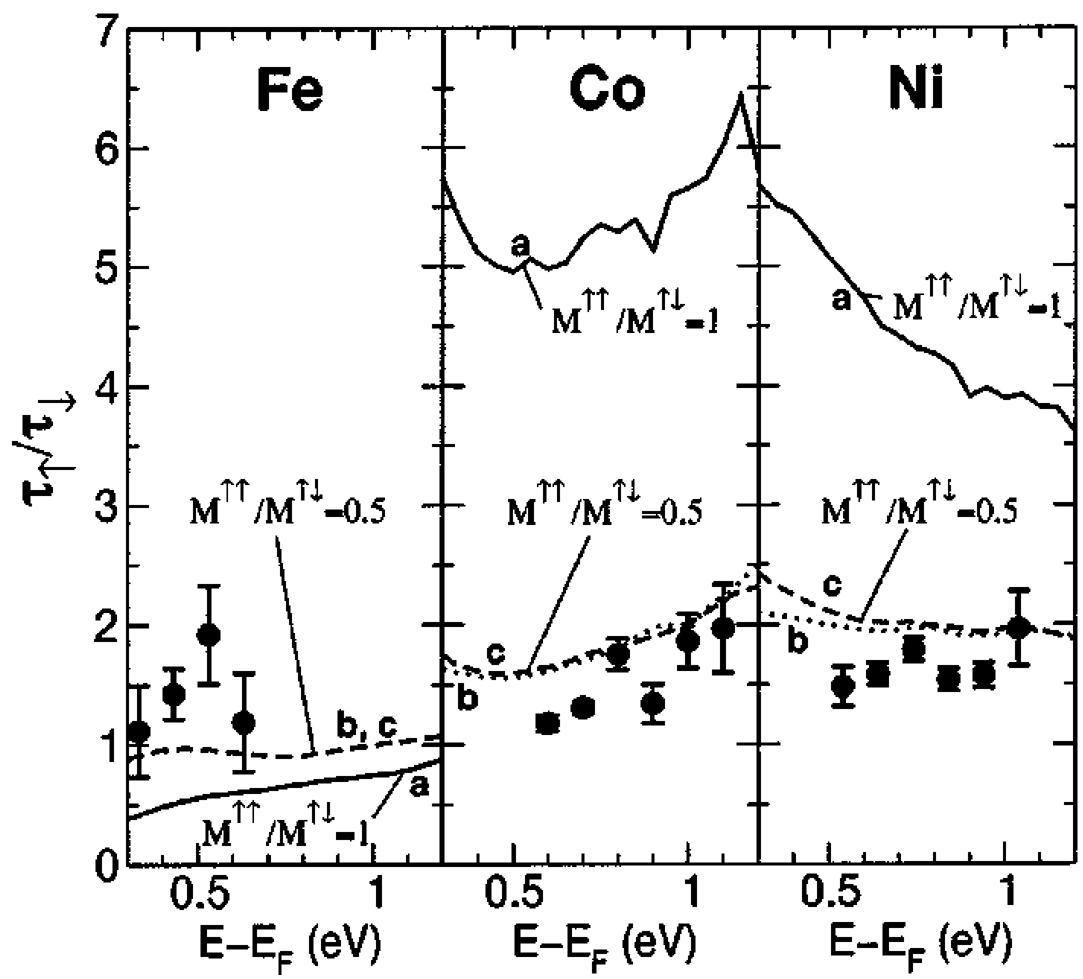
$$\gamma_{\vec{k}}^{\nu} = \frac{2}{\hbar}\sum_{\mu\vec{q}} \frac{\Delta q^3}{(2\pi)^3} V_q \,|\, B_{\vec{k}\vec{q}}^{\mu\nu} \,|^2\, f_{\vec{k}+\vec{q}}^{\mu} \frac{\operatorname{Im}\varepsilon(\vec{q},\Delta E)}{|\,\varepsilon(\vec{q},\Delta E)\,|^2}$$

- energy difference $\Delta E = \epsilon_{\vec{k}+\vec{q}}^{\mu} - \epsilon_{\vec{k}}^{\nu}$
- again, spin-orbit coupling included $|\,\psi_{\vec{k}}^{\mu}\rangle = a_{\vec{k}}^{\mu}\left|\uparrow\right\rangle + b_{\vec{k}}^{\mu}\left|\downarrow\right\rangle$

Spin-dependent Lifetimes in Ferromagnets

- Success explaining spin-integrated lifetimes
- Problems with spin dependence
- Reason: Singlet vs. triplet scattering??

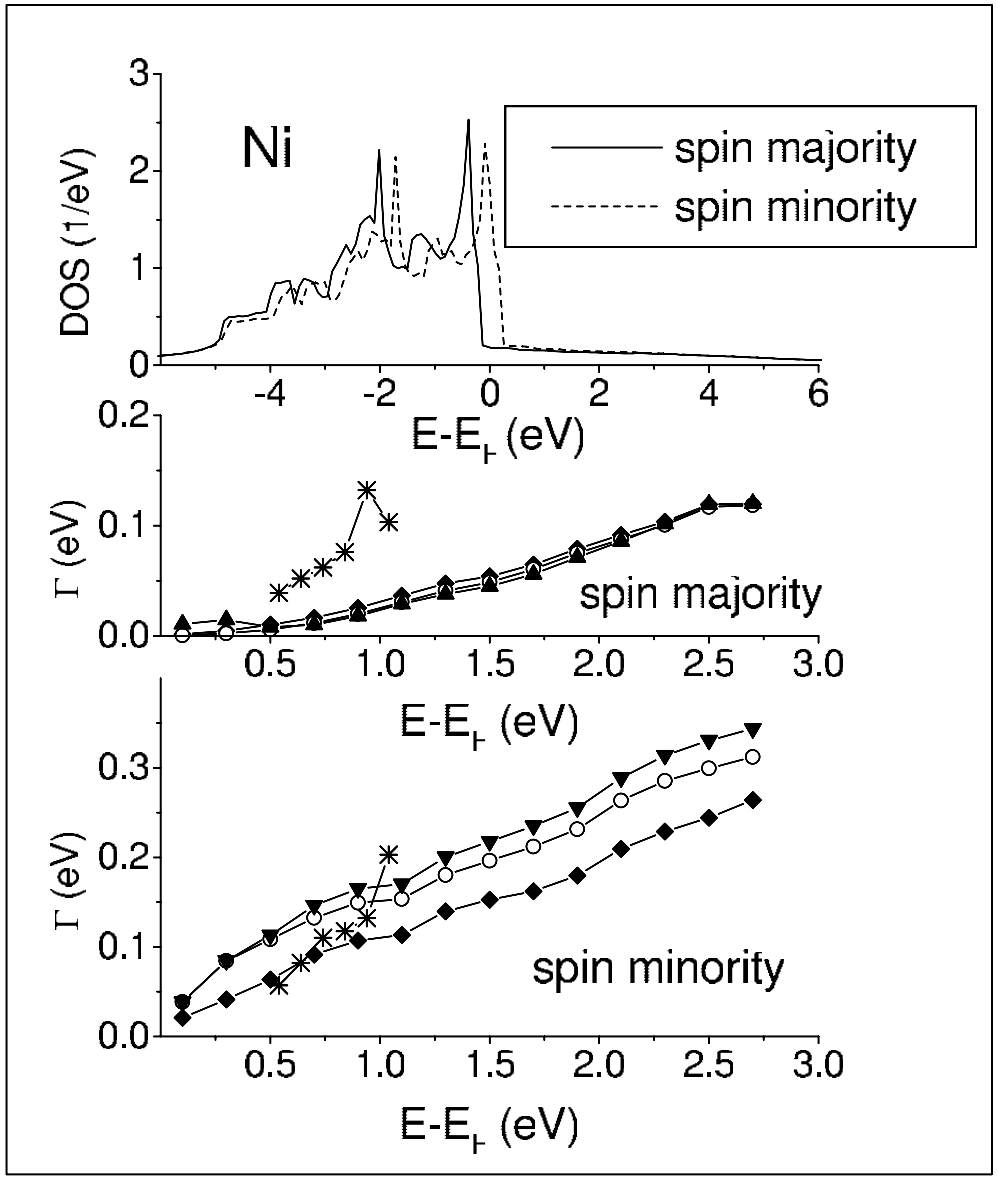
- Discrepancy with calculations; see also Goris *et al.*, Phys. Rev. Lett. 107, 026601 (2011)

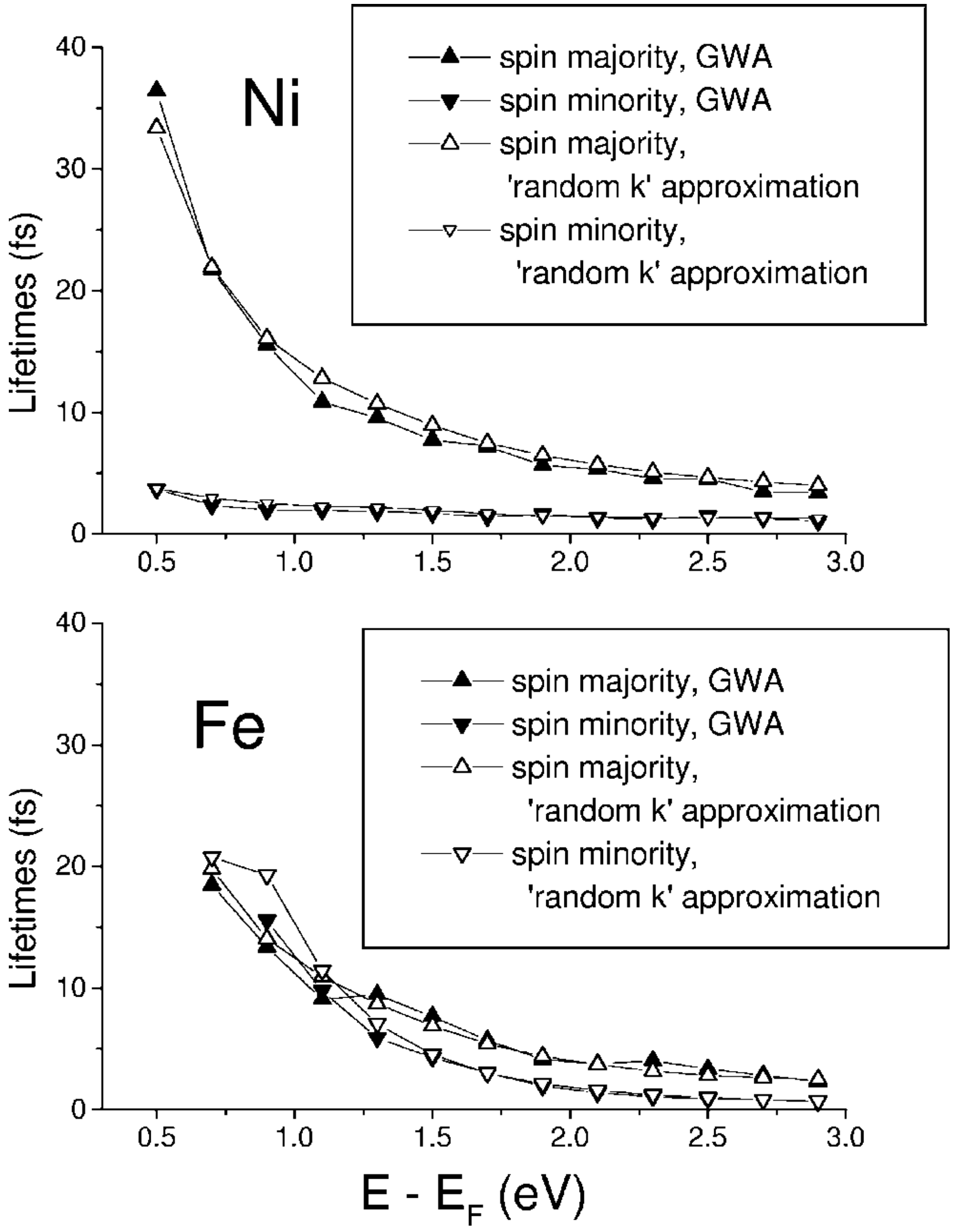


Knorren, Bennemann, Burgermeister, Aeschlimann, Phys. Rev. B 61, 9427 (2000)

Spin-dependent Lifetimes in Ferromagnets

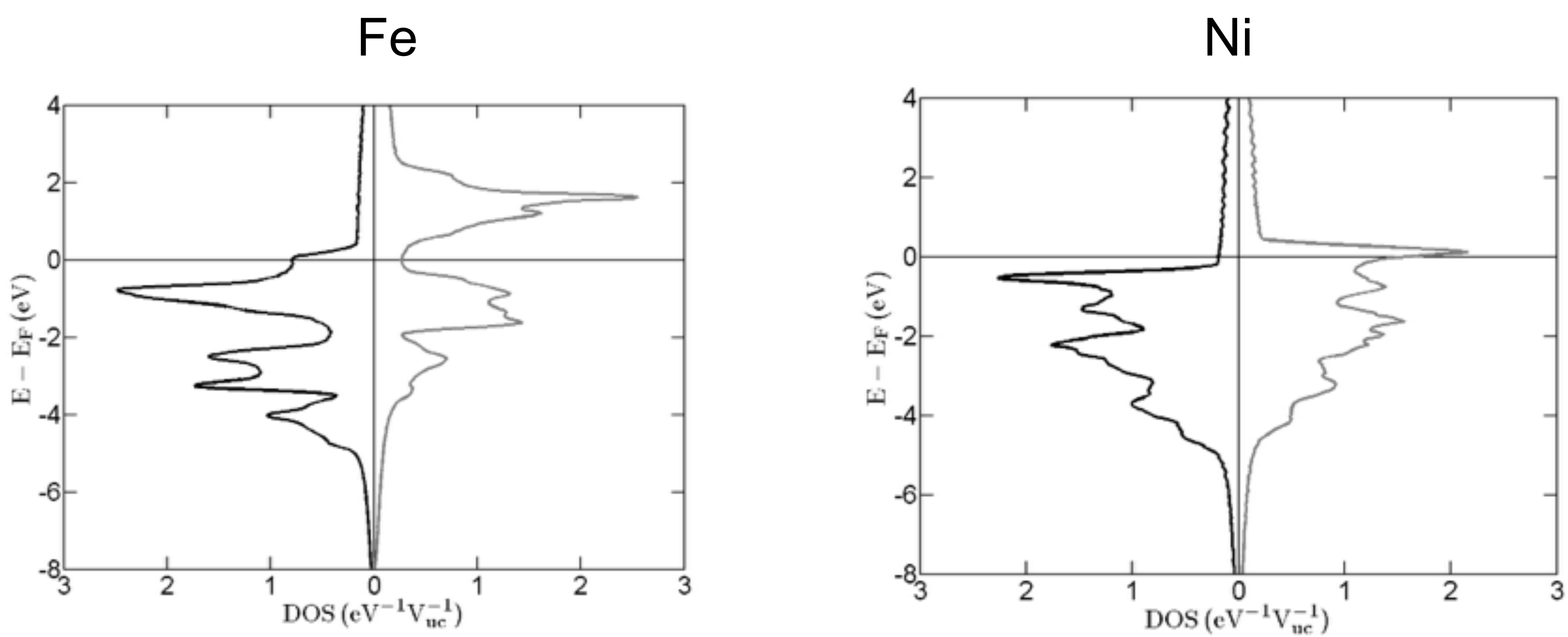
- GW calculations predict essentially results from random-k model (DOS!)
- T-matrix yields only small differences





Zhukov, Chulkov, Echenique, Phys. Rev. Lett. 93, 096401 (2004); Phys. Rev. B 73, 125105 (2006)

Iron vs. Nickel: DOS/random-k

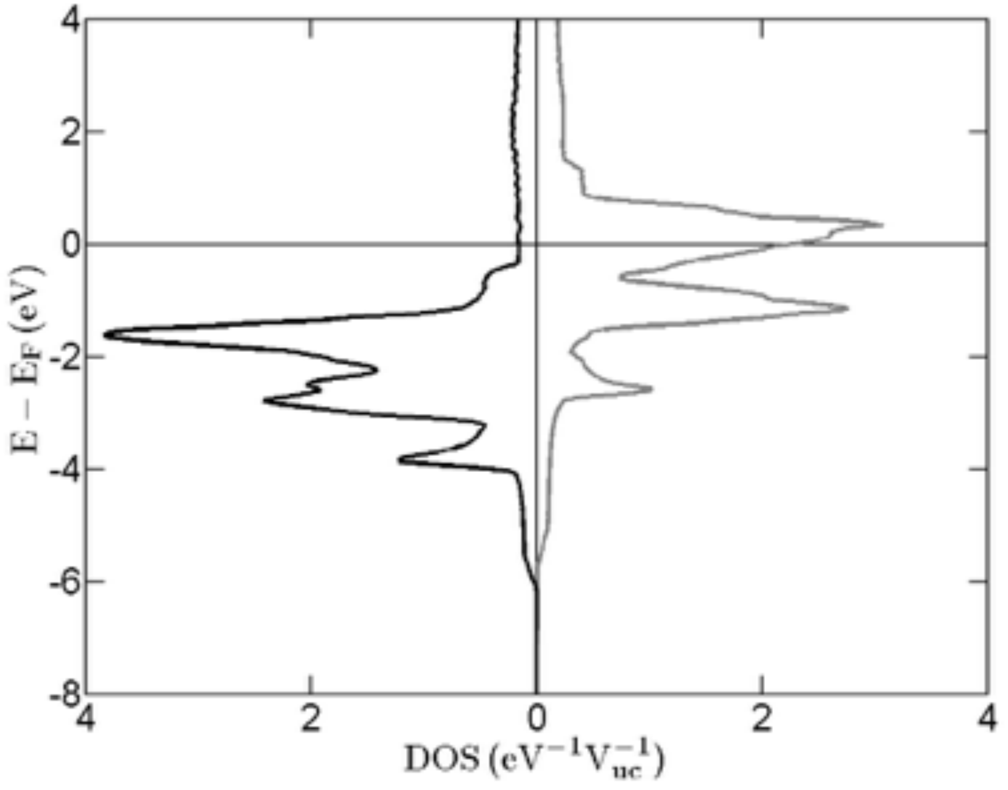


- Very different DOS at Fermi energy for Fe and Ni
- High spin polarisation at Fermi energy: very different scattering phase space in the different spin channels
- Random-k model: spin-dependent DOS determines lifetimes

Cobalt DOS

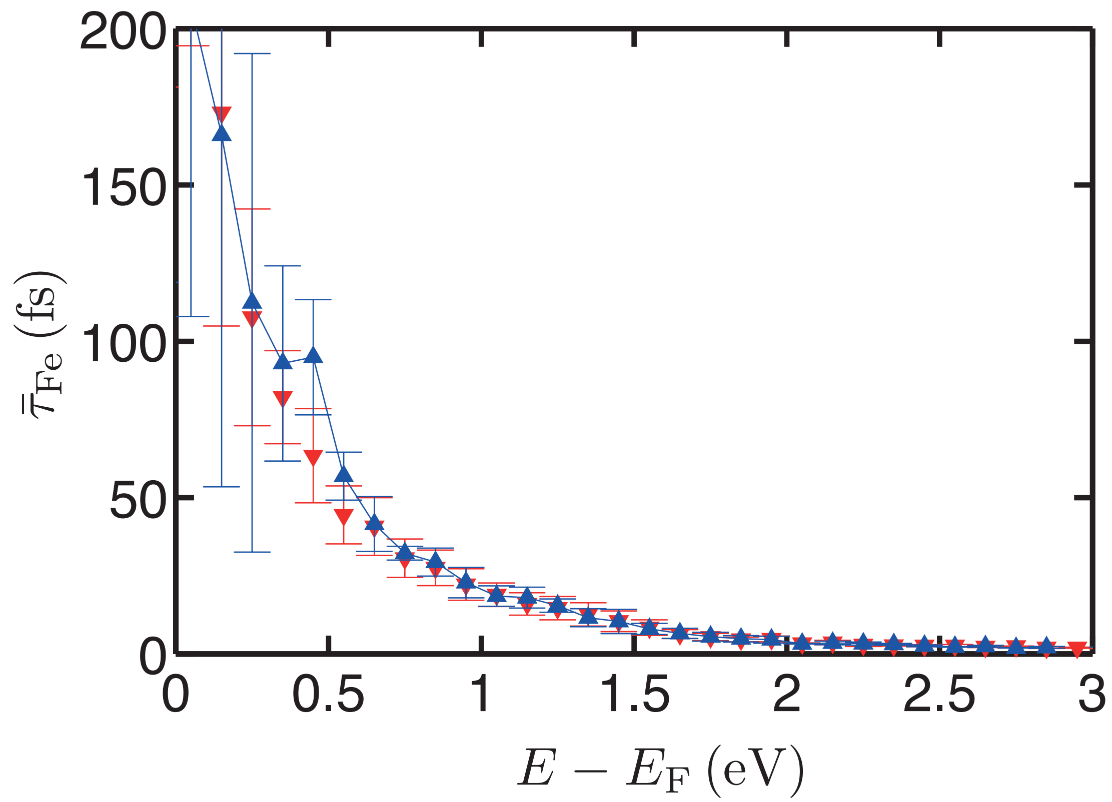
- Pronounced spin polarisation at Fermi energy

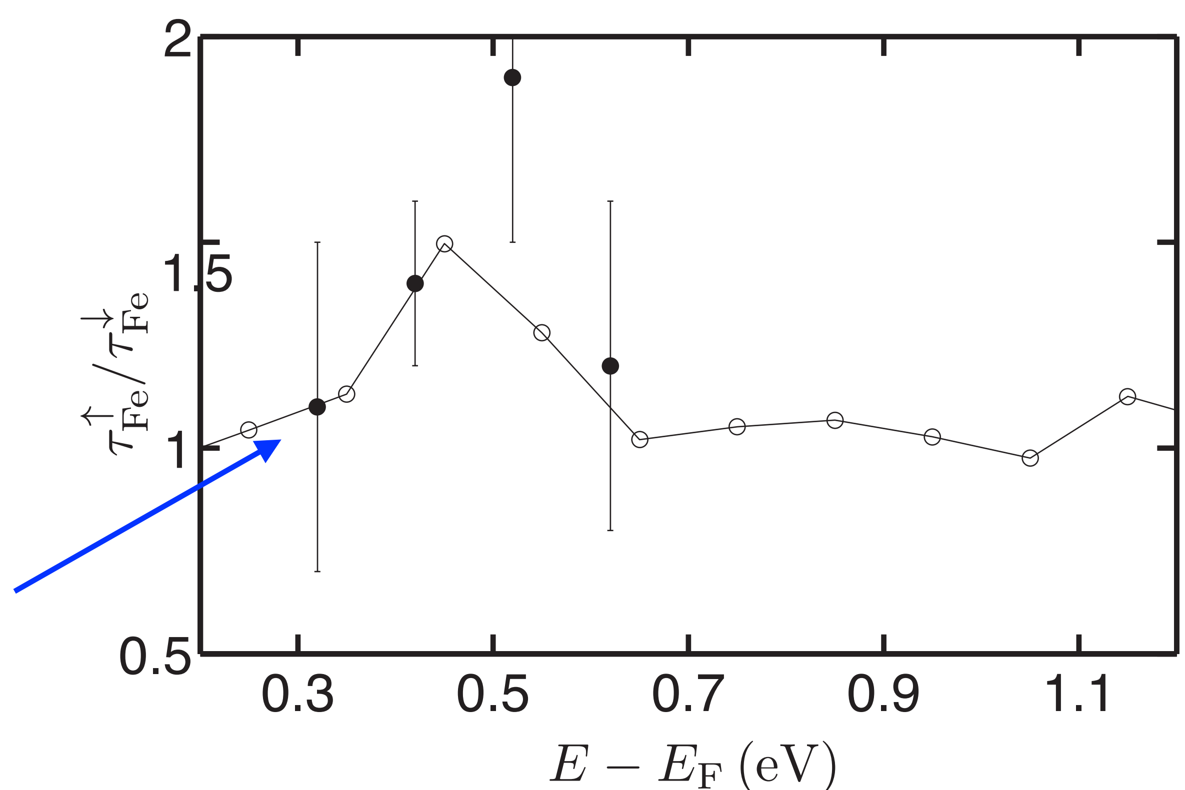
Co



Lifetimes in Iron

- Compute k- and band resolved lifetimes
- Average lifetimes in energy "bins"
- Use scatter in *k* as "error bar"
- Small error bar: Only few bands intersect Fermi energy
- Good agreement for "spin asymmetry"
- Results essentially in agreement with earlier ab-initio calculations
- "Spin-integrated" lifetimes also in agreement with experiment*



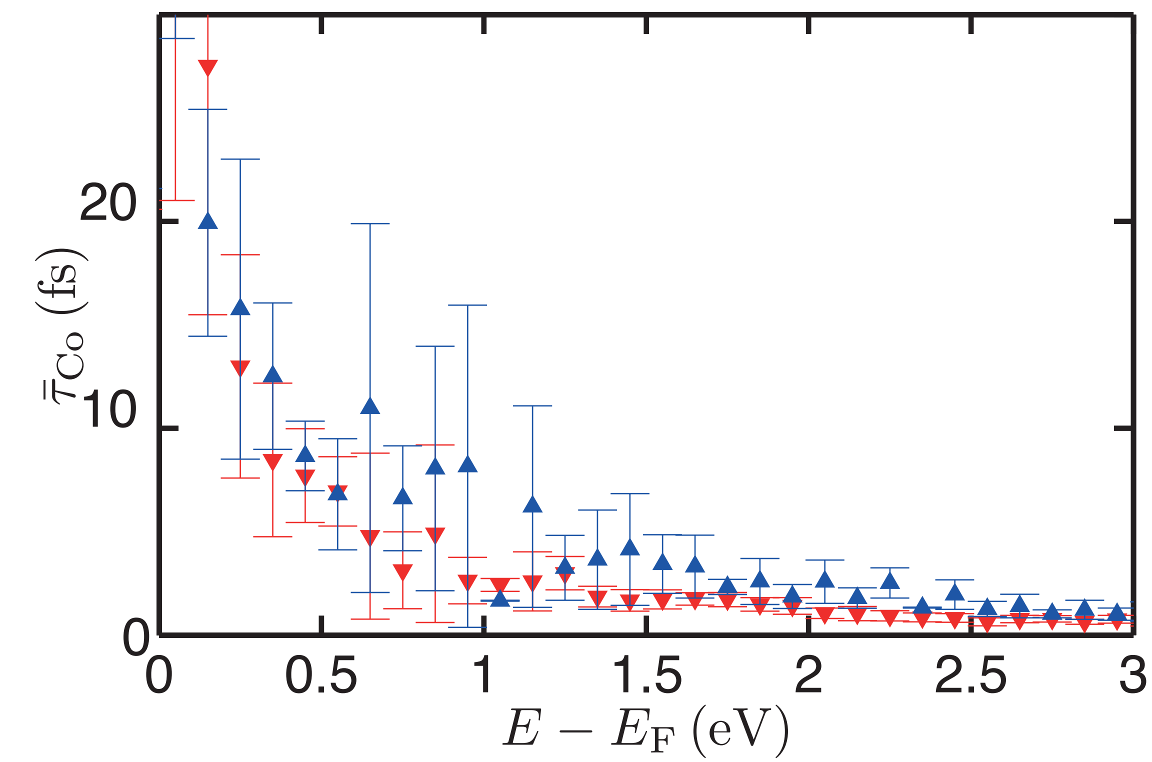


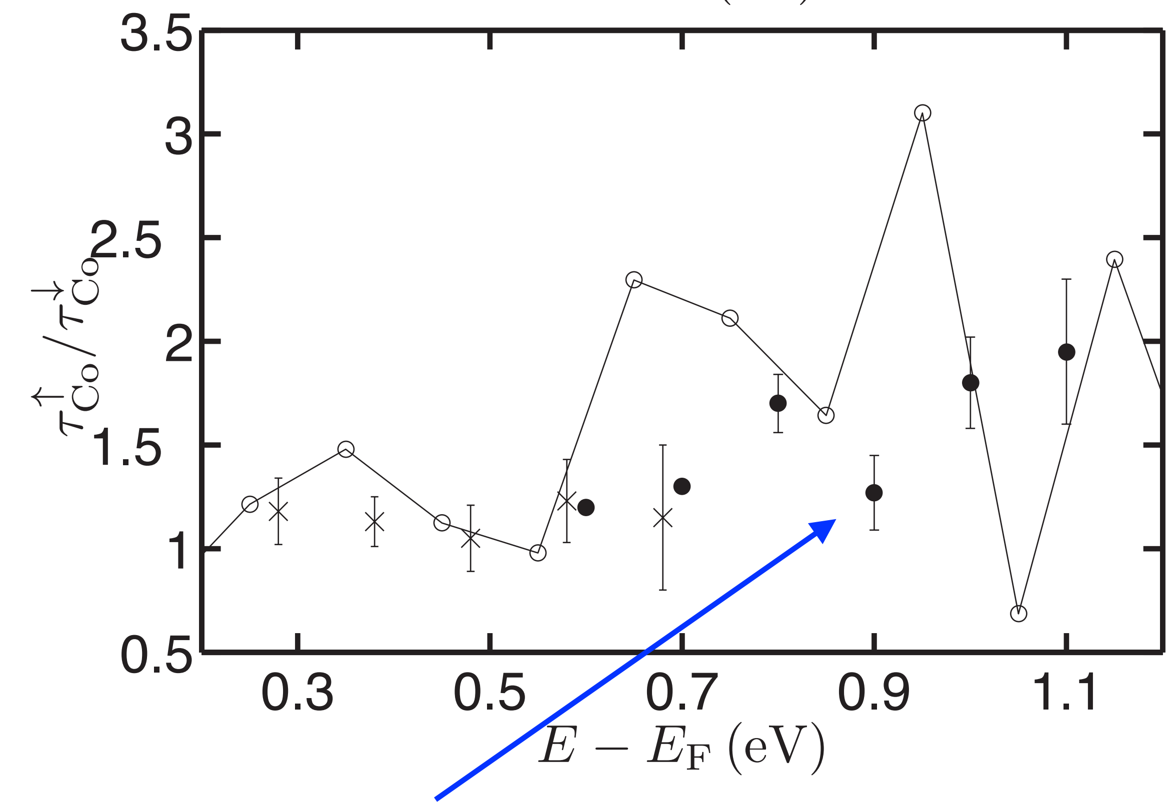
Knorren, Bennemann, Burgermeister, Aeschlimann, Phys. Rev. B 61, 9427 (2000)

Kaltenborn and Schneider, arXiv1403.4728(2014)

Spin-dependent Lifetimes in Cobalt

- Pronounced scatter
- Good agreement with experiment for "spin asymmetry"
- "Spin-integrated" lifetimes also in agreement with experiment*
- Spin-orbit coupling "flips spins"; DOS argument for separate spin channels does not apply



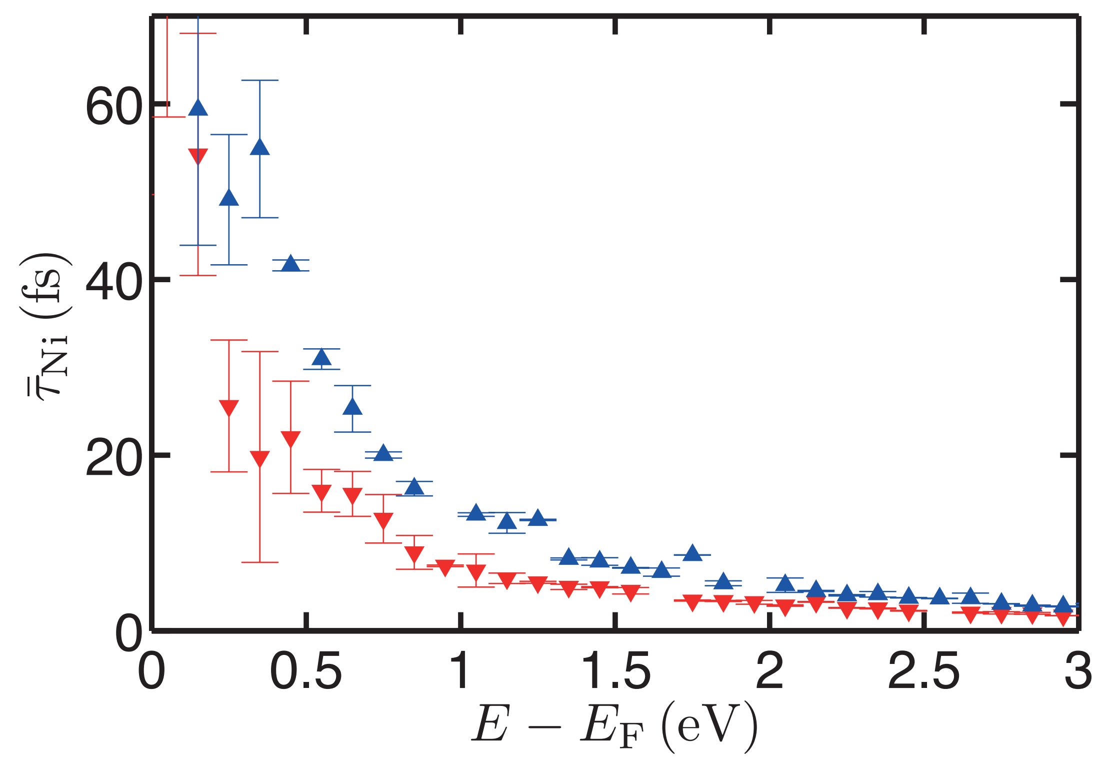


Kaltenborn and Schneider, arXiv1403.4728(2014)

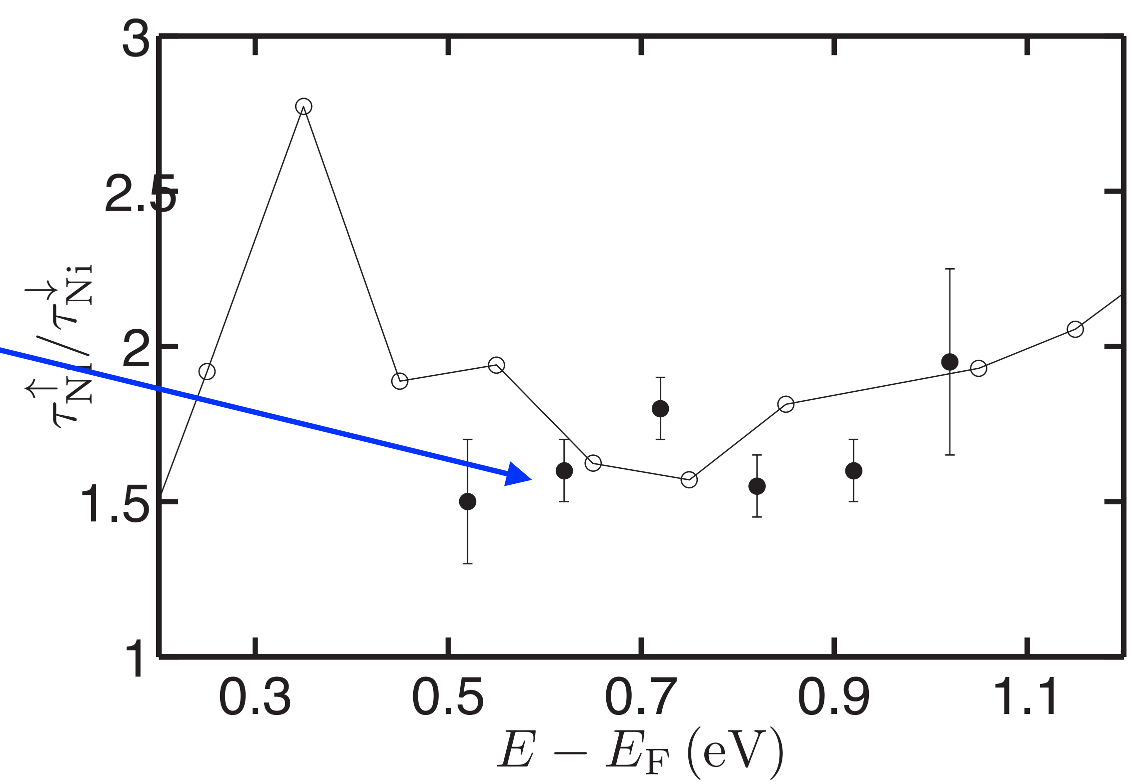
Goris *et al.*, Phys. Rev. Lett. 107, 026601 (2011)

Lifetimes in Nickel

- Small “error bar” (scatter in k)
- Good agreement with measurements
- Very different result from earlier calculations without spin-orbit coupling
- Spin-orbit coupling “flips spins”; DOS argument for separate spin channels does not apply

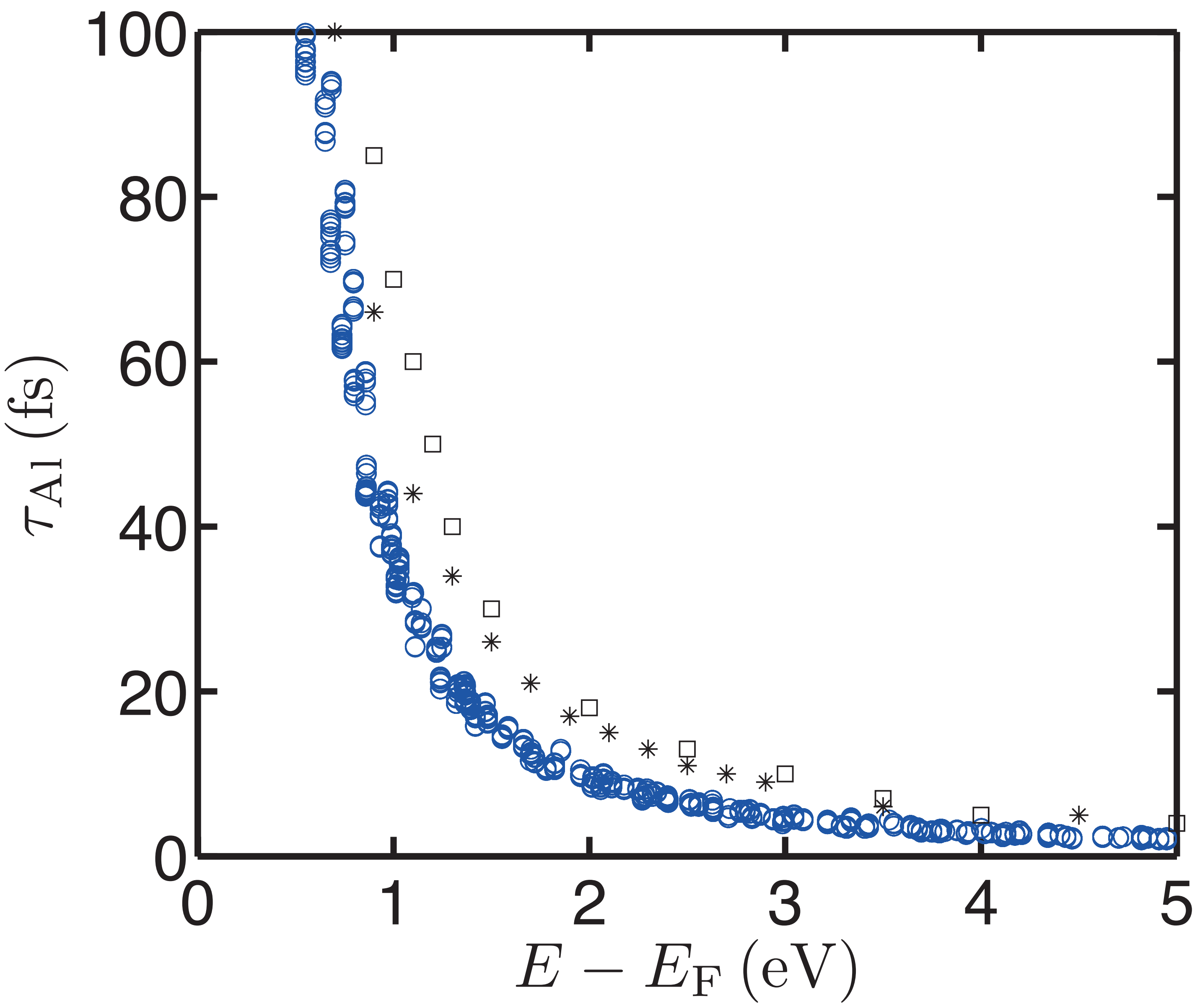


Knorren, Bennemann, Burgermeister, Aeschlimann, Phys. Rev. B 61, 9427 (2000)



Kaltenborn and Schneider, arXiv1403.4728(2014)

Electronic Lifetime in Aluminum

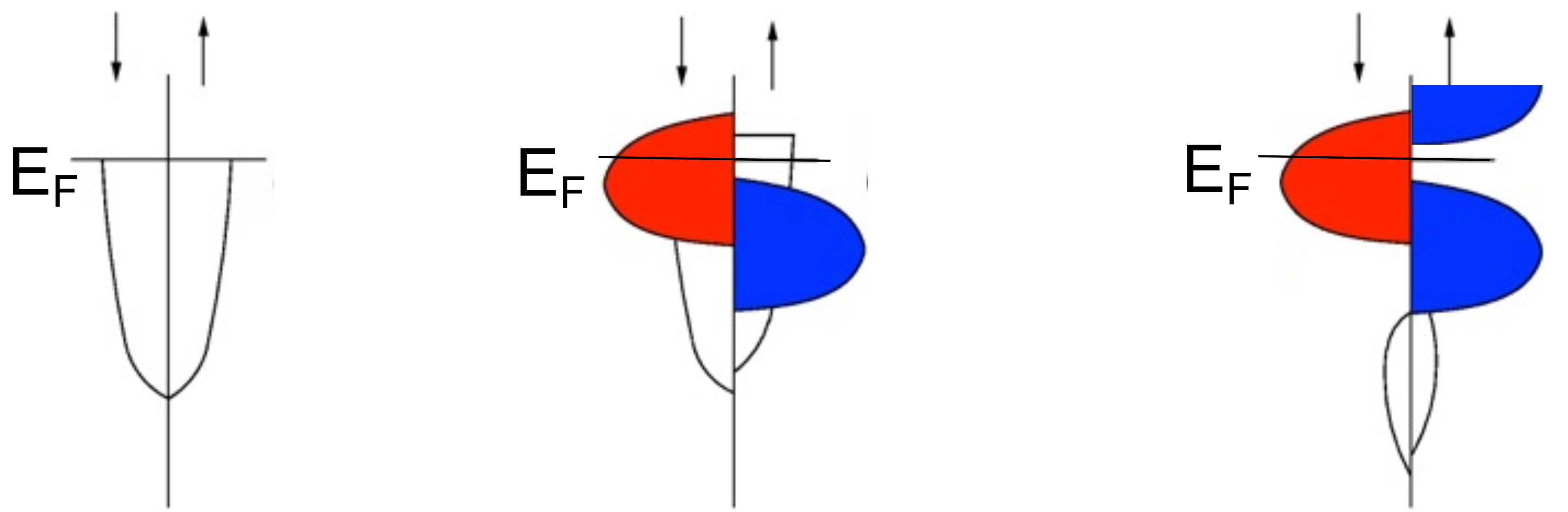


- Benchmark results for aluminium calculated with Wien97, LMTO codes without spin-orbit coupling in wave functions
- Surprisingly large effect due to inclusion of spin-orbit coupling in wave functions

Kaltenborn and Schneider, arXiv1403.4728(2014)

Heusler Alloys: Half-Metallic Ferromagnets

Spin polarization: $P(E) = \dfrac{N(E_{\uparrow}) - N(E_{\downarrow})}{N(E_{\uparrow}) + N(E_{\downarrow})}$



Gap @ Fermi energy in minority spin channel

<u>Metal</u>

$P(E_F)=0$

<u>Ferromagnetic metal</u>

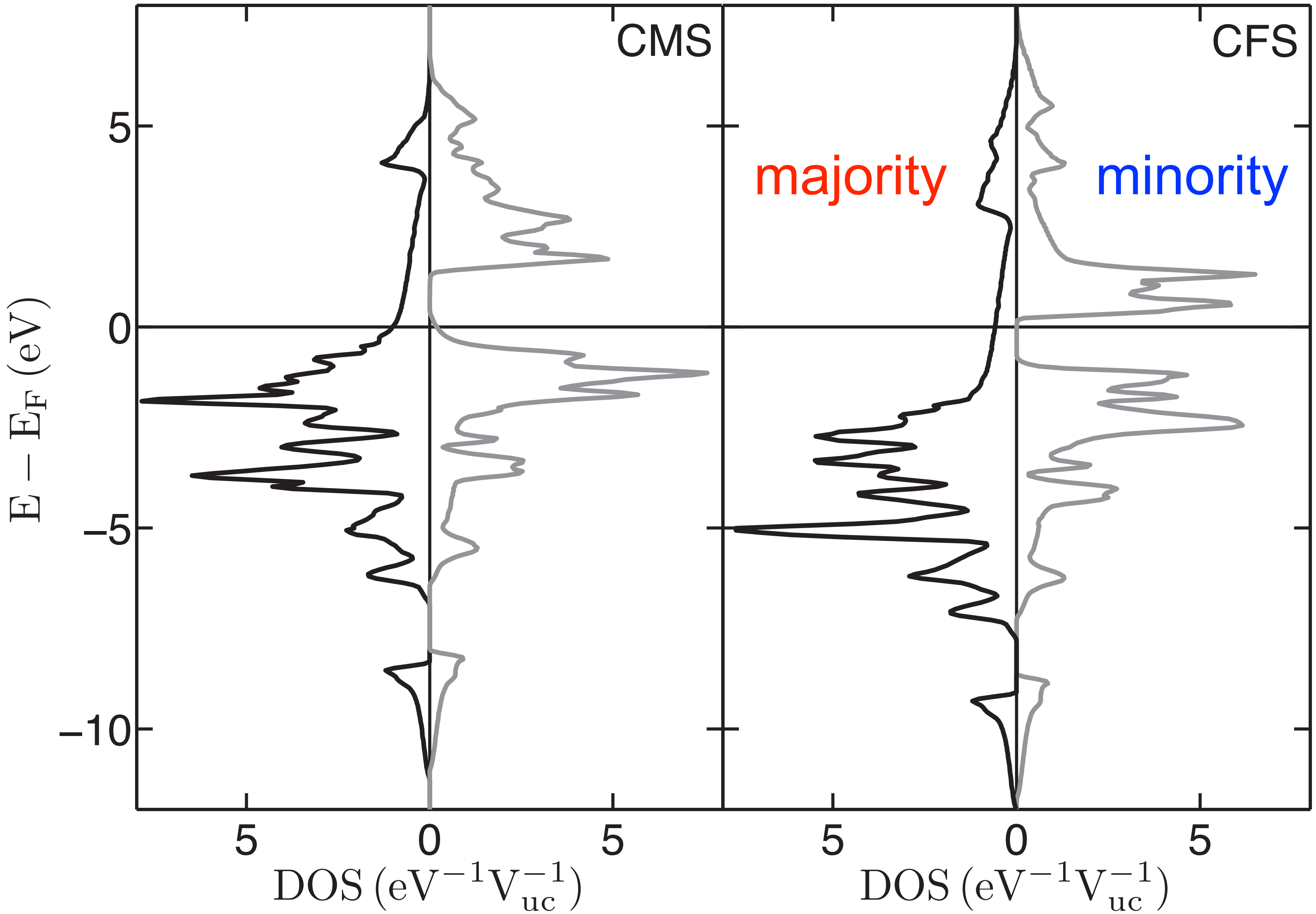
$0<P(E_F)<100\%$

<u>Half-metallic ferromagnet</u>

$P(E_F)=100\%$

Heusler alloy: X_2YZ (X,Y = transition metals; Z = main group element)

Heusler Compounds

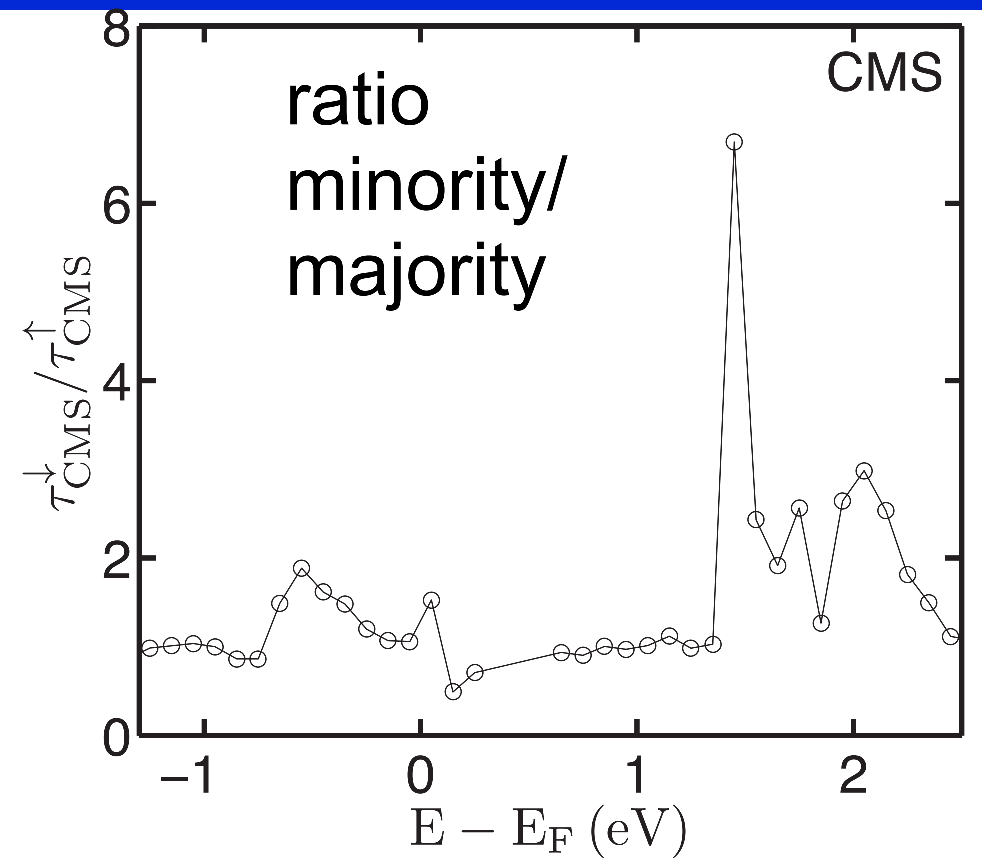


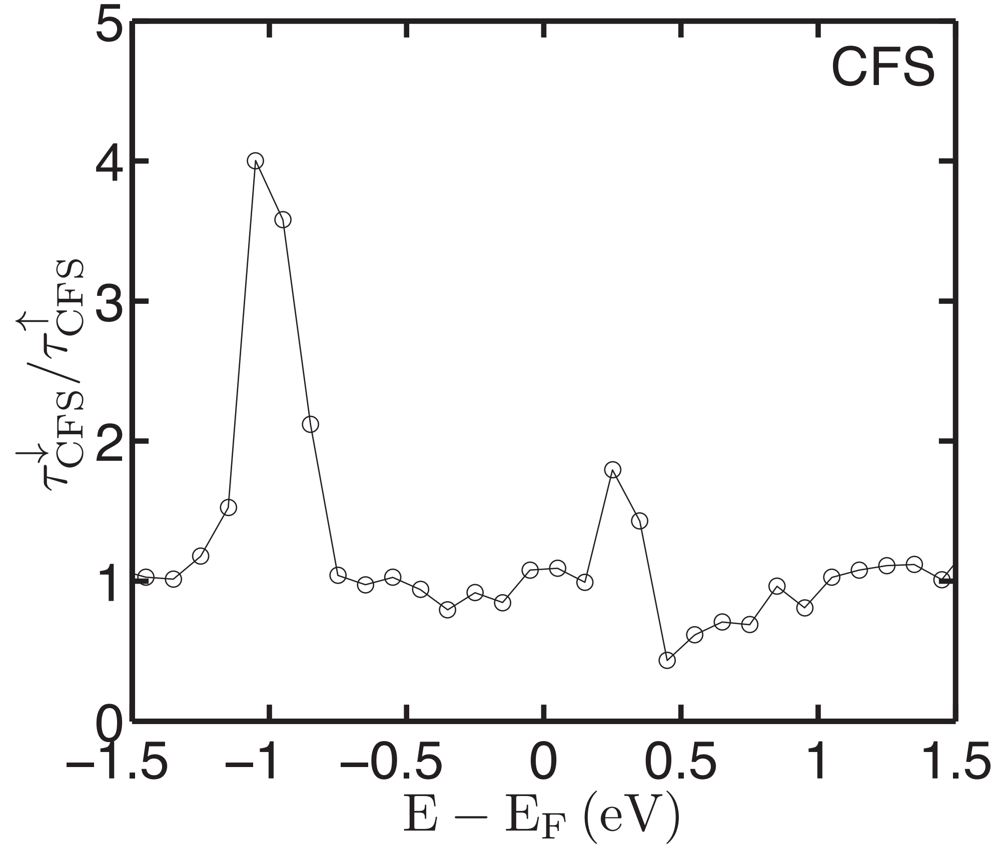
- Compare CoMnSi and CoFeSi
- Gap below and above Fermi energy for minority electrons

Band structure calculation checked against: B. Balke et al., Phys. Rev. B **74**, 104405 (2006)

Heuslers: Spin-dependent Lifetimes

- Small spin-asymmetry (minority/majority) over wide energy range
- Gap in minority DOS not visible
- Only around special energies a ratio of 4 or 5 to 1 is reached





Kaltenborn and Schneider, Phys. Rev. B 89, 115127 (2014).

Conclusions

- Ab-initio based calculation of optical excitation and “classical” Elliott-Yafet carrier-spin dynamics in ferromagnetic metals
- DFT (T = 0K) band structure and electron-phonon coupling matrix elements
- “Simple” model including dynamics of exchange splitting (magnetic order parameter) improves achievable magnetization quenching at realistic fluences
- Calculation of spin asymmetry including spin-orbit coupling in the wave functions for ferromagnets and Heusler compounds
- Spin-orbit coupling washes out differences in the scattering phase space in the spin-dependent DOS