DFT calculations of dichroic effect in transmission electron microscope

— ChiralTEM project —

Ján Rusz, Pavel Novák

Institute of Physics
Academy of Sciences of Czech Republic

DFTEM, ChiralTEM Workshop, Vienna, April 2006

Outline

Outline

Dynamical diffraction theory

- Electron in beam - $|\mathbf{k}\rangle$-state
- Electron in crystal - superposition of Bloch waves
- Assuming crystal periodicity, boundary conditions lead to

$$\begin{aligned}\frac{d^2\sigma}{d\Omega dE} &= \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J'_z} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \times \\ &\times \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}\end{aligned}$$

- Summation - a problem of geometry of experiment
- Mixed Dynamic Formfactor (MDFF) - a key quantity

MDFF properties

Symmetries

- $S(\mathbf{q}, \mathbf{q}', E) = \sum_{i,f} \langle i | e^{-i\mathbf{q}\cdot\mathbf{R}} | f \rangle \langle f | e^{i\mathbf{q}'\cdot\mathbf{R}} | i \rangle \delta(E + E_i - E_f)$
- Clearly $S(\mathbf{q}, \mathbf{q}', E) = S^\star(\mathbf{q}', \mathbf{q}, E)$
- In non-magnetic systems: $S(\mathbf{q}, \mathbf{q}', E) = S(-\mathbf{q}', -\mathbf{q}, E)$
- Centrosymmetric systems: $S(\mathbf{q}, \mathbf{q}', E) = S(-\mathbf{q}, -\mathbf{q}', E)$

- i.e., in non-magnetic centrosymmetric crystals MDFF is real
- But to observe dichroism, we need nonzero imaginary part of MDFF

Outline

Electronic Structure - WIEN2k program package

Self-consistency cycle

`lapw0`	Poisson equation ... $\Delta V = \rho$
`lapw1`	scal. rel. eigv. problem ... $HC^{(\nu)} = E^{(\nu)} SC^{(\nu)}$
`lapwso`	2nd variational step ... $H_{SO} C_{SO}^{(\nu)} = E_{SO}^{(\nu)} C_{SO}^{(\nu)}$
`lapw2`	val. density ... $\rho(\mathbf{r}) = \sum_{\mathbf{k}\nu} \Theta(E_F - E_{\mathbf{k}\nu}) \left\|\psi_{\mathbf{k}\nu}(\mathbf{r})\right\|^2$
`lcore`	Dirac equation for core states
`mixer`	mixing old and new $\rho(\mathbf{r})$

Needed WIEN2k outputs

- core wavefunctions and energies
- bandstructure - Bloch functions $\psi_{\mathbf{k}\nu}(\mathbf{r})$ and energies $\epsilon_{\mathbf{k}\nu}$

Initial and final states in APW

Initial state

- Localized (core) state
- Nonzero only inside the atomic sphere

$$\langle \mathbf{r}, s|i\rangle \rightarrow \langle \mathbf{r}, s|jj_z\rangle = \sum_m C^{jj_z}_{lm\frac{1}{2}s} R_{js}(r) Y_l^m(\mathbf{r}/r)$$

Final state

- Itinerant Bloch state
- Defined in the whole unit cell; inside at. sphere we have

$$\langle \mathbf{r}, s|f\rangle \rightarrow \langle \mathbf{r}, s|\mathbf{k}\nu\rangle = \sum_{LM} D^{\mathbf{k}\nu}_{LMS} u^{E_{\mathbf{k}\nu}}_{LS}(r) Y_L^M(\mathbf{r}/r)$$

Mixed Dynamic Formfactor

$$
\begin{aligned}
S(\mathbf{q},\mathbf{q}',E) &= \sum_{mm'}\sum_{LMS}\sum_{L'M'S'}\sum_{\lambda\mu}\sum_{\lambda'\mu'} 4\pi i^{\lambda-\lambda'}(2l+1)\sqrt{[\lambda,\lambda',L,L']} \\
&\times\ Y^{\lambda}_{\mu}(\mathbf{q}/q)^{*}Y^{\lambda'}_{\mu'}(\mathbf{q}'/q')\langle j_{\lambda}(q)\rangle_{ELSj}\langle j_{\lambda'}(q')\rangle_{EL'S'j} \\
&\times\ \begin{pmatrix} l & \lambda & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l & \lambda' & L' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l & \lambda & L \\ -m & \mu & M \end{pmatrix}\begin{pmatrix} l & \lambda' & L' \\ -m' & \mu' & M' \end{pmatrix} \\
&\times\ \sum_{j_z}(-1)^{m+m'}(2j+1)\begin{pmatrix} l & \frac{1}{2} & j \\ m & S & -j_z \end{pmatrix}\begin{pmatrix} l & \frac{1}{2} & j \\ m' & S' & -j_z \end{pmatrix} \\
&\times\ \underbrace{\sum_{\nu\mathbf{k}} D_{LMS}(\nu\mathbf{k})D_{L'M'S'}(\nu\mathbf{k})^{*}\delta(E+E_{nl\kappa}-E_{\nu\mathbf{k}})}_{\text{cross-DOS}}
\end{aligned}
$$

Partial charges - QTL code

Altered `QTL` code replaces `LAPW2 -qtl`

- Proper symmetrization of Bloch states → full-BZ k-mesh no more necessary
- Spin-orbit interaction properly introduced
- Gives all 1056 independent components of $\langle lms|l'm's'\rangle_{\mathbf{k}\nu}$
- Improved accuracy of I/O operations

Running `QTL`

- Perl script `initqtl.pl` prepares input and definition files
- Executing `qtl qtl.def` leads to `case.qtl1` file containing cross-charges $D_{lms}(\mathbf{k}\nu)D^{\star}_{l'm's'}(\mathbf{k}\nu)$

Integration over Brillouin zone - TETRA program

Changes introduced to original `TETRA` code

- Improved accuracy of internal and I/O operations
- Output of all cross-DOS components goes to a single file

Running `TETRA`

- Requires `case.insel` file
- Perl script `initmdff.pl` prepares input and definition files for both `TETRA` and `MDFFSO` codes
- Executing `tetra tetra.def` leads to `case.crossdos` file - cross-DOS components

Cross-DOS components

Matrix 32x32 of complex numbers $\langle lms | l'm's' \rangle$ with $l_{max} = 3$:

$$\left(\begin{array}{cccc|cccc}
\langle 00|00\rangle & \langle 00|1\bar{1}\rangle & \cdots & \langle 00|33\rangle & \langle 00|00\rangle & \langle 00|1\bar{1}\rangle & \cdots & \langle 00|33\rangle \\
\langle 1\bar{1}|00\rangle & \langle 1\bar{1}|1\bar{1}\rangle & \cdots & \langle 1\bar{1}|33\rangle & \langle 1\bar{1}|00\rangle & \langle 1\bar{1}|1\bar{1}\rangle & \cdots & \langle 1\bar{1}|33\rangle \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\langle 33|00\rangle & \langle 33|1\bar{1}\rangle & \cdots & \langle 33|33\rangle & \langle 33|00\rangle & \langle 33|1\bar{1}\rangle & \cdots & \langle 33|33\rangle \\
\hline
\langle 00|00\rangle & \langle 00|1\bar{1}\rangle & \cdots & \langle 00|33\rangle & \langle 00|00\rangle & \langle 00|1\bar{1}\rangle & \cdots & \langle 00|33\rangle \\
\langle 1\bar{1}|00\rangle & \langle 1\bar{1}|1\bar{1}\rangle & \cdots & \langle 1\bar{1}|33\rangle & \langle 1\bar{1}|00\rangle & \langle 1\bar{1}|1\bar{1}\rangle & \cdots & \langle 1\bar{1}|33\rangle \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\langle 33|00\rangle & \langle 33|1\bar{1}\rangle & \cdots & \langle 33|33\rangle & \langle 33|00\rangle & \langle 33|1\bar{1}\rangle & \cdots & \langle 33|33\rangle
\end{array}\right)$$

Spin blocks: $\left(\begin{array}{c|c} \uparrow\uparrow & \uparrow\downarrow \\ \hline \downarrow\uparrow & \downarrow\downarrow \end{array}\right)$

Calculation of S(q,q',E) - MDFFSO program

Changes introduced to original `MDFF` code

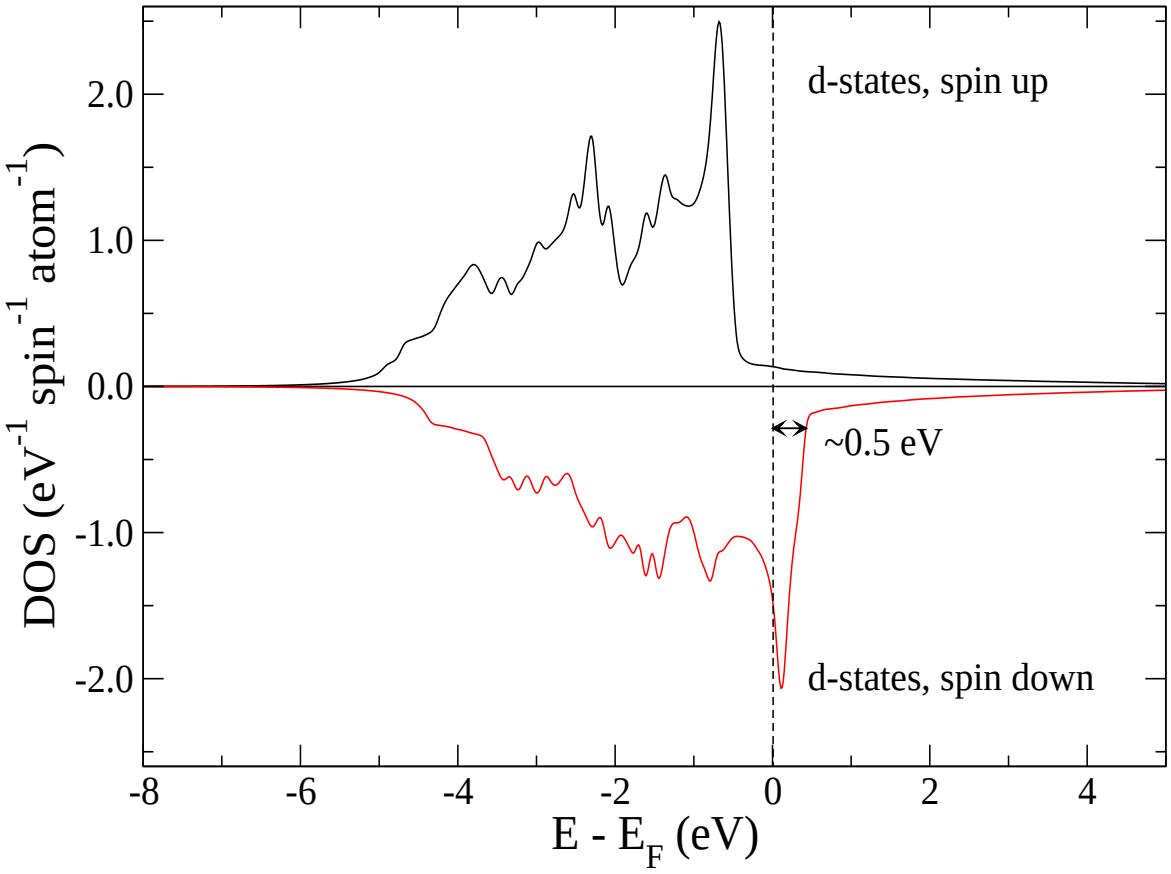
- Relativistic treatment of initial (core) states
- Extended to include spin-up/down cross-terms
- Calculation speed optimizations
- Improved accuracy of I/O operations (reading `case.crossdos` file)

Running `MDFFSO`

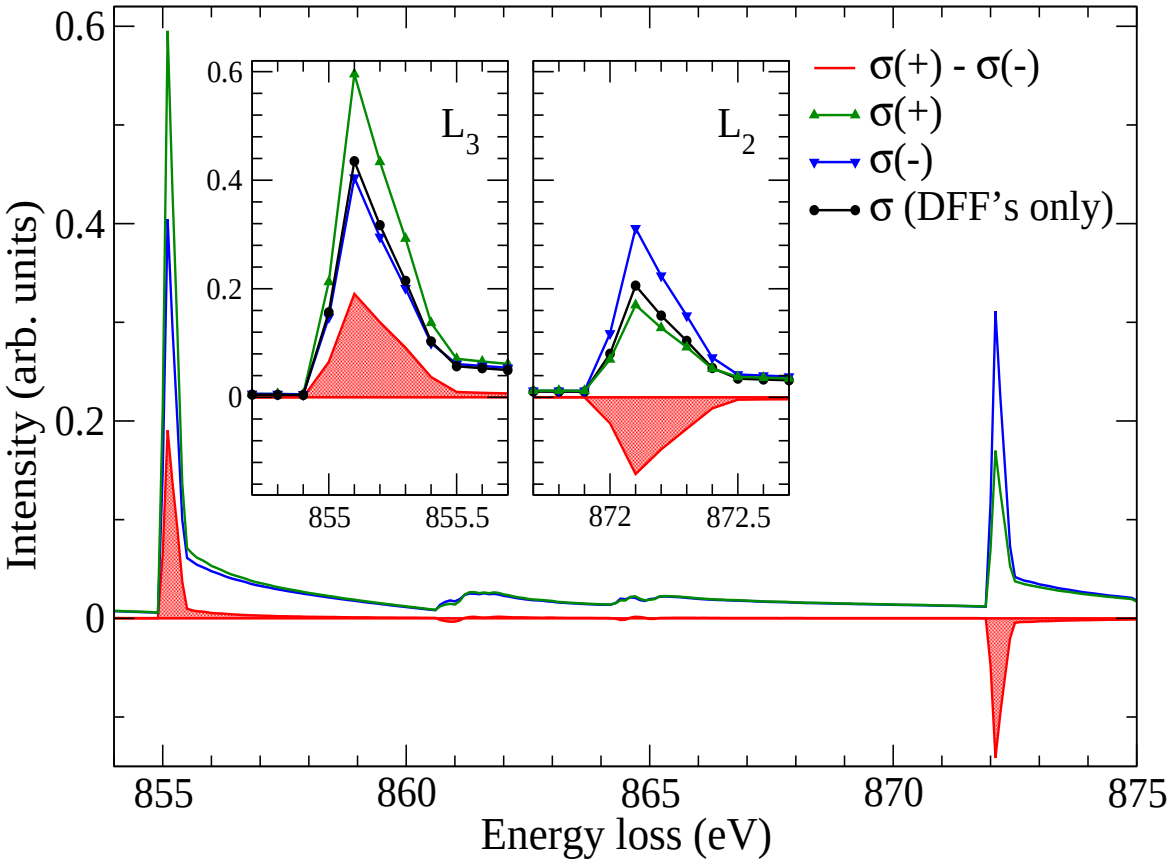
- Requires `case.insel` file
- Executing `mdffso mdffso.def` leads to `case.mdffso` file - ready for summation with `ilX` codes

Outline

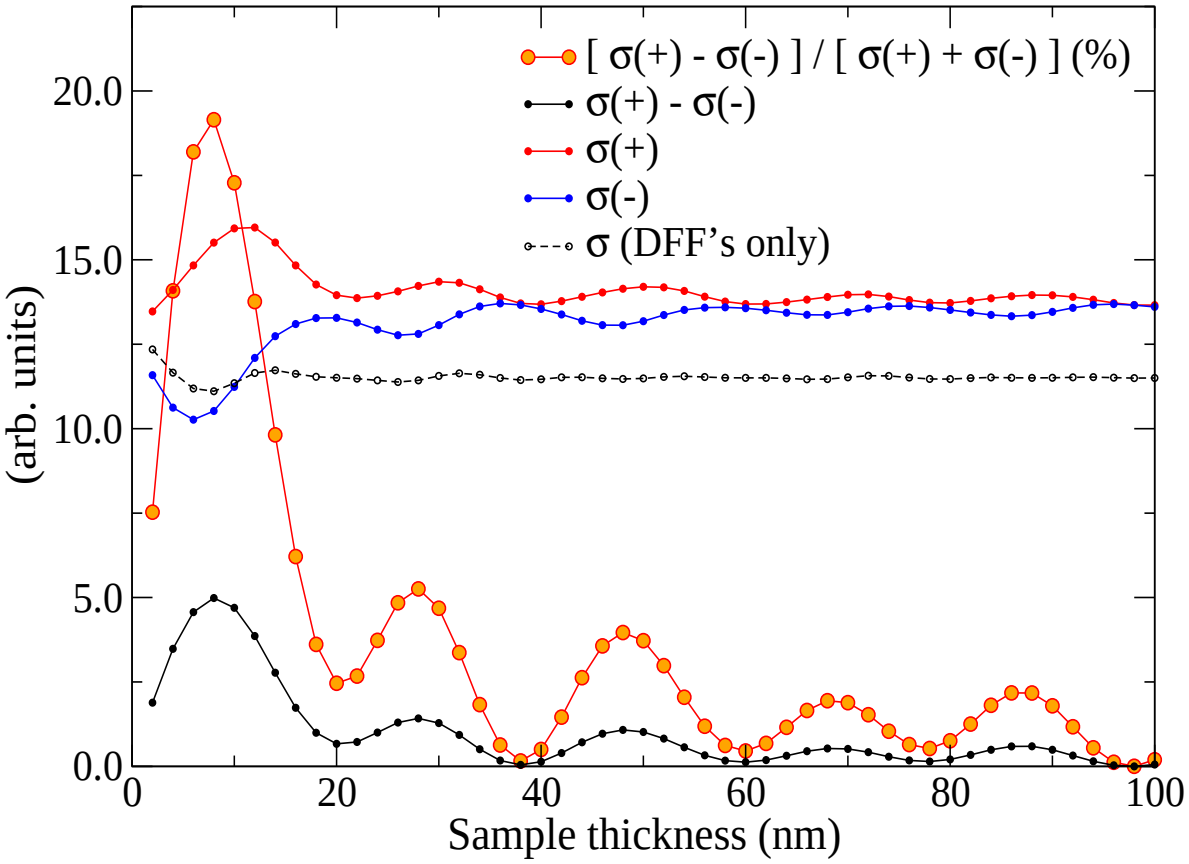
fccNi: density of states - 3d projections



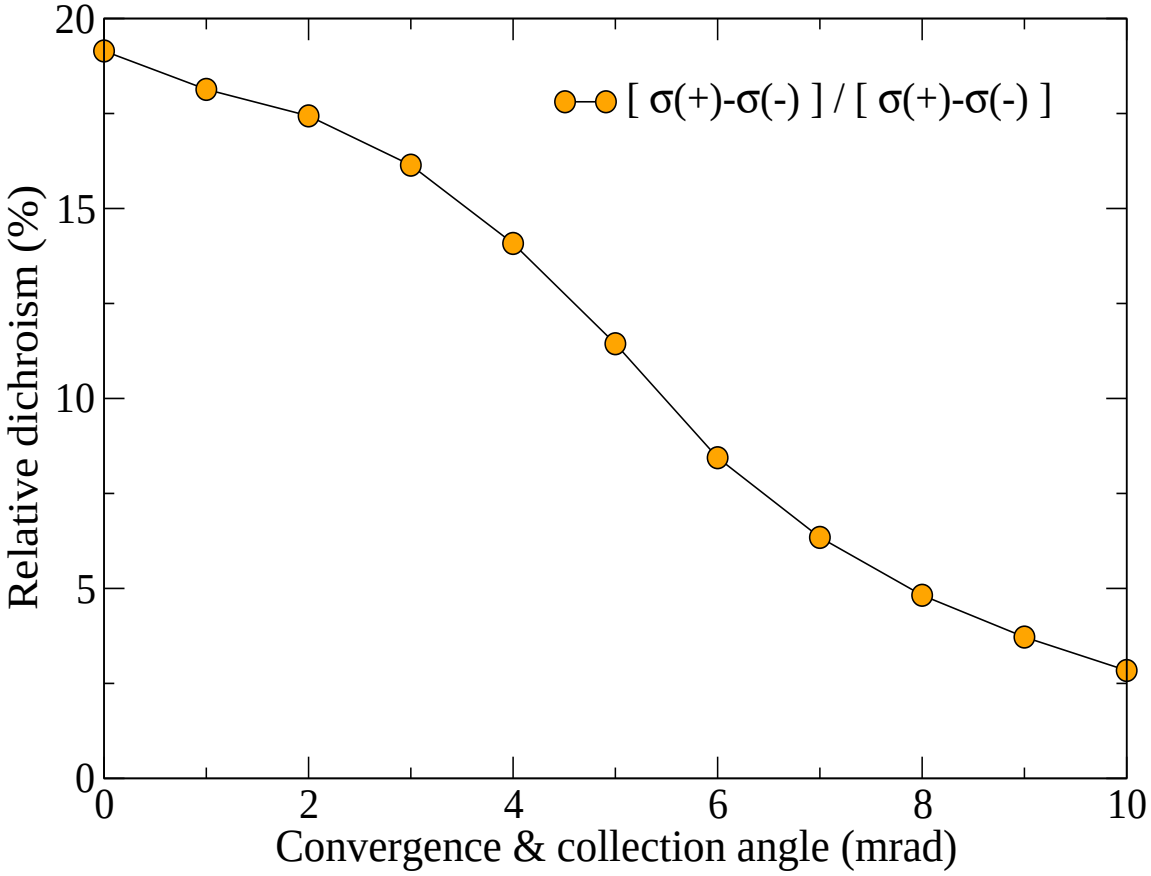
fccNi: dichroism



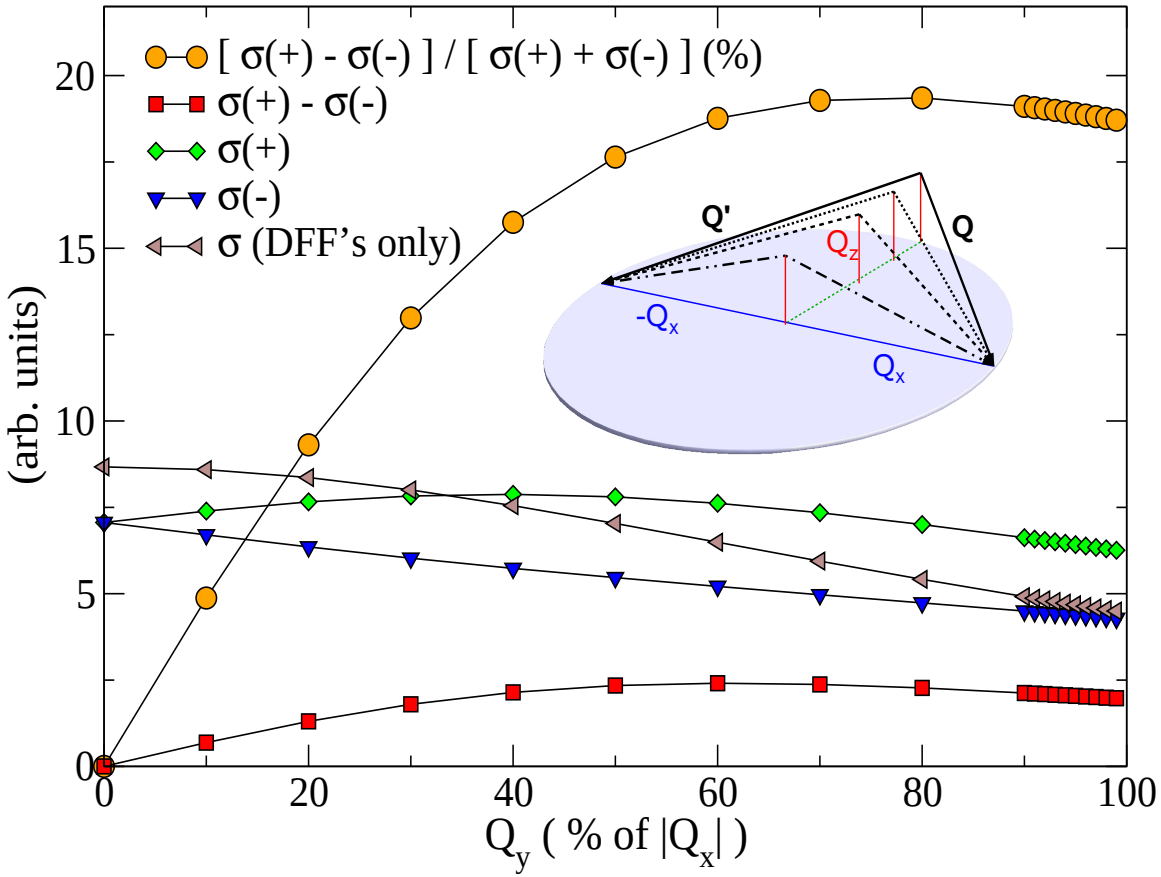
fccNi: thickness profile



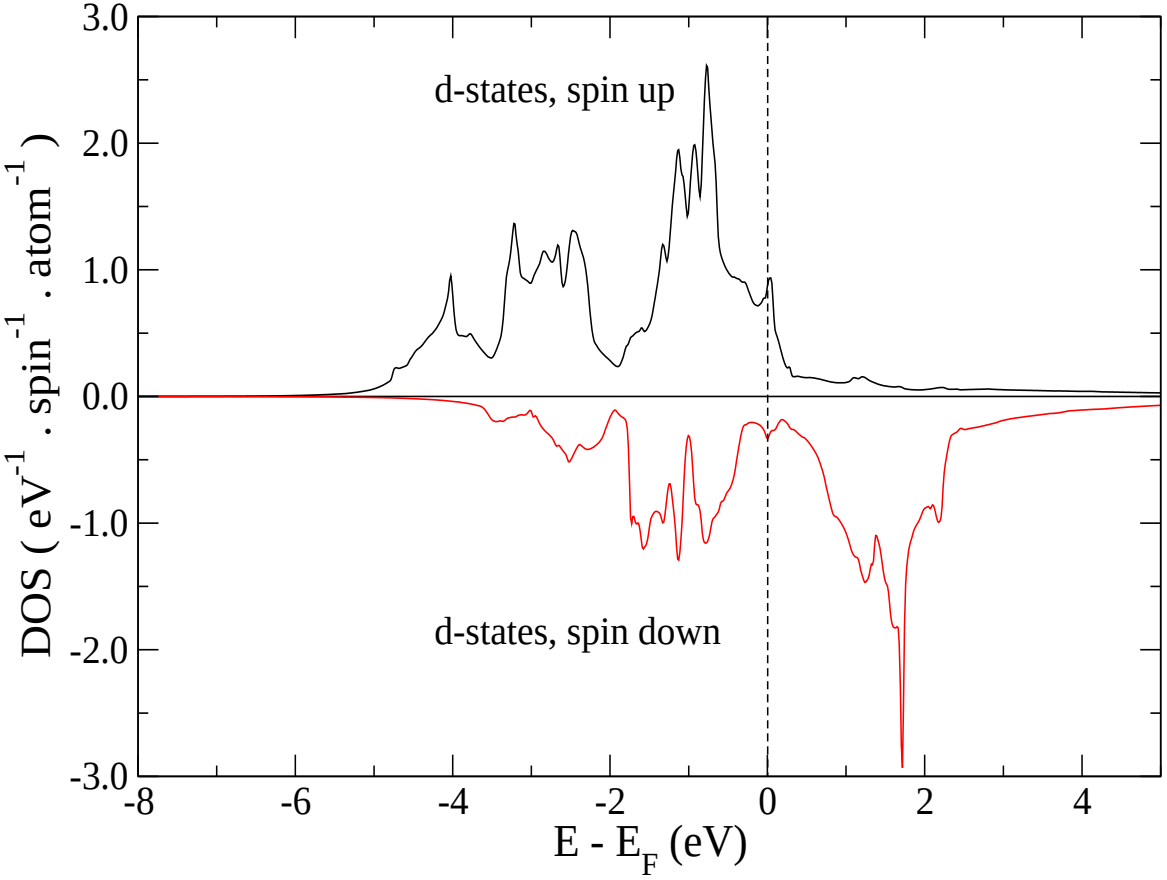
fccNi: convergence & collection angle profile



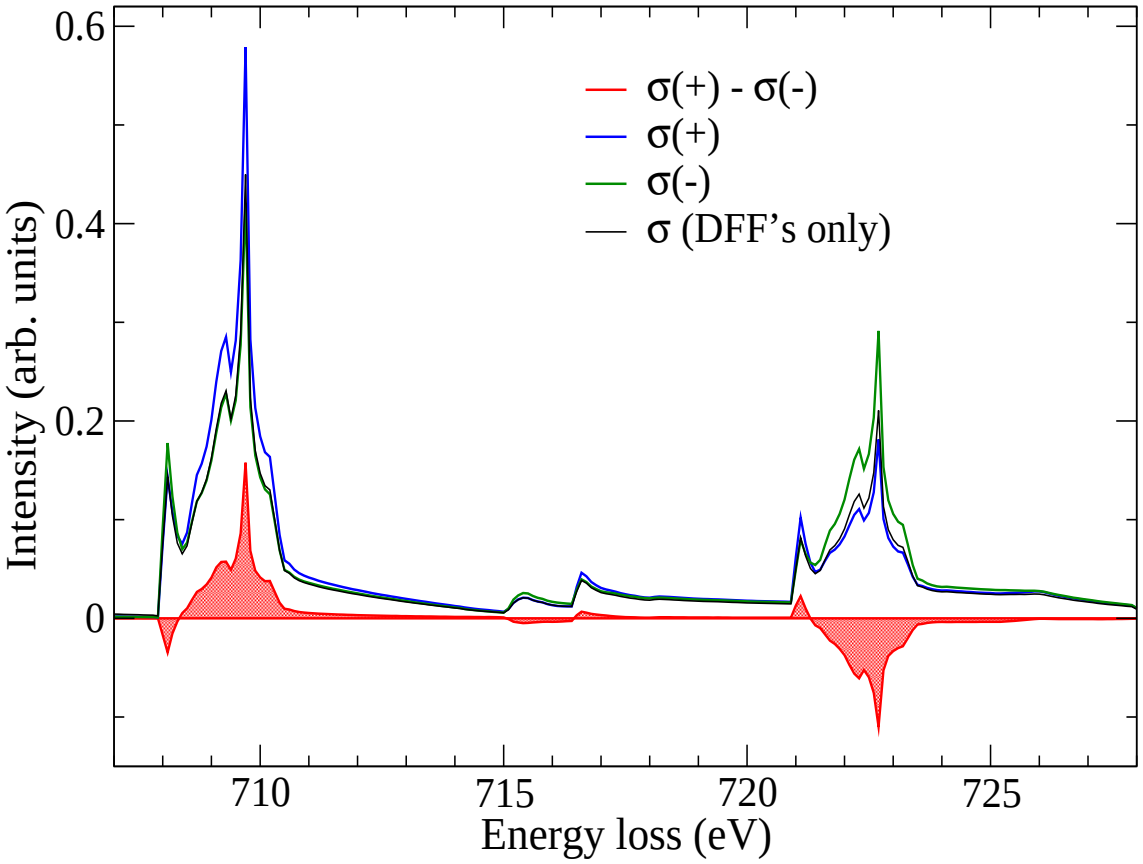
fccNi: detector placement sensitivity



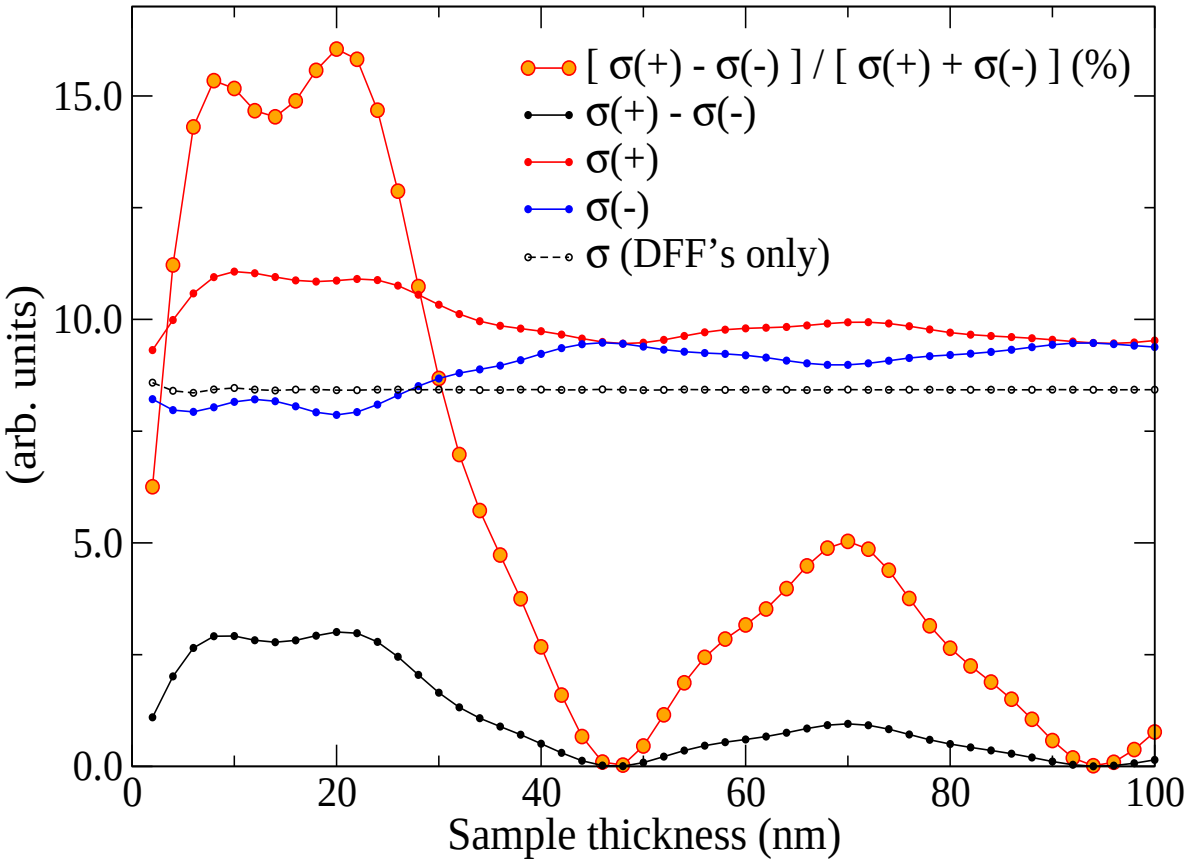
bccFe: density of states - 3d projections



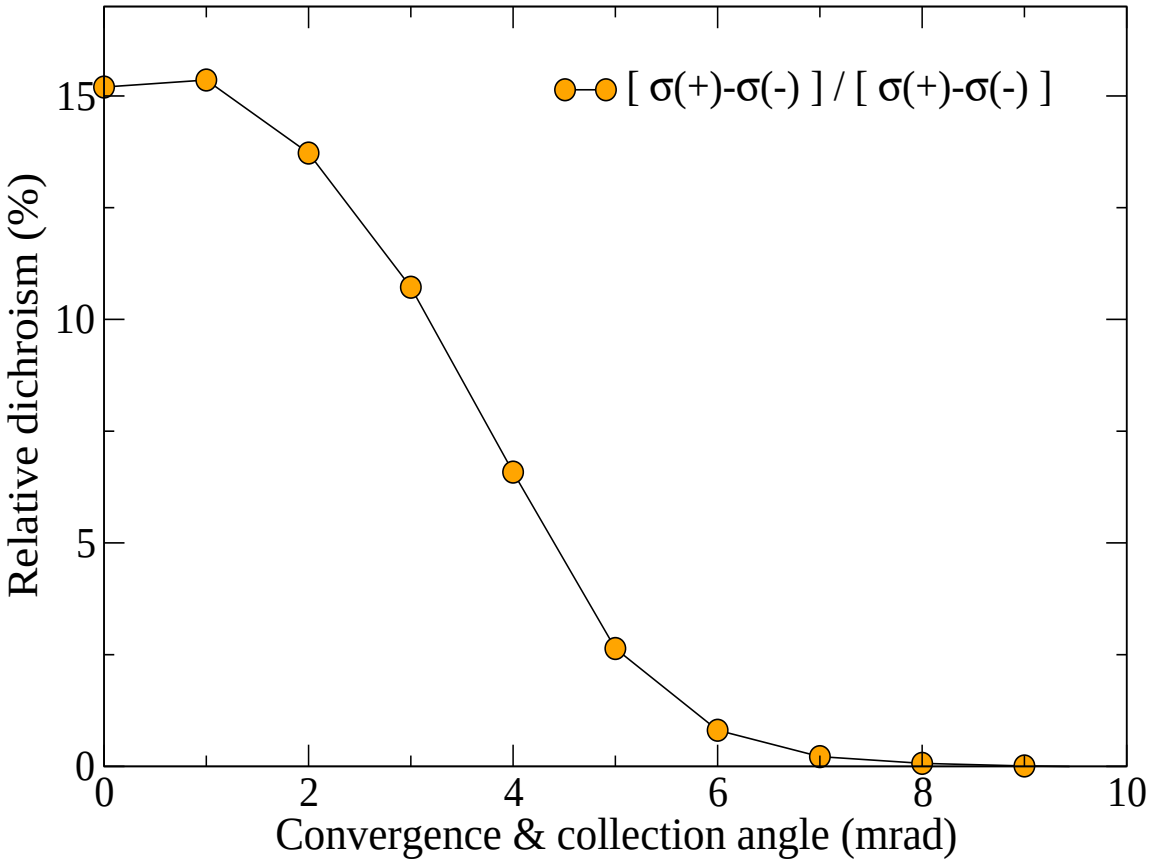
bccFe: dichroism



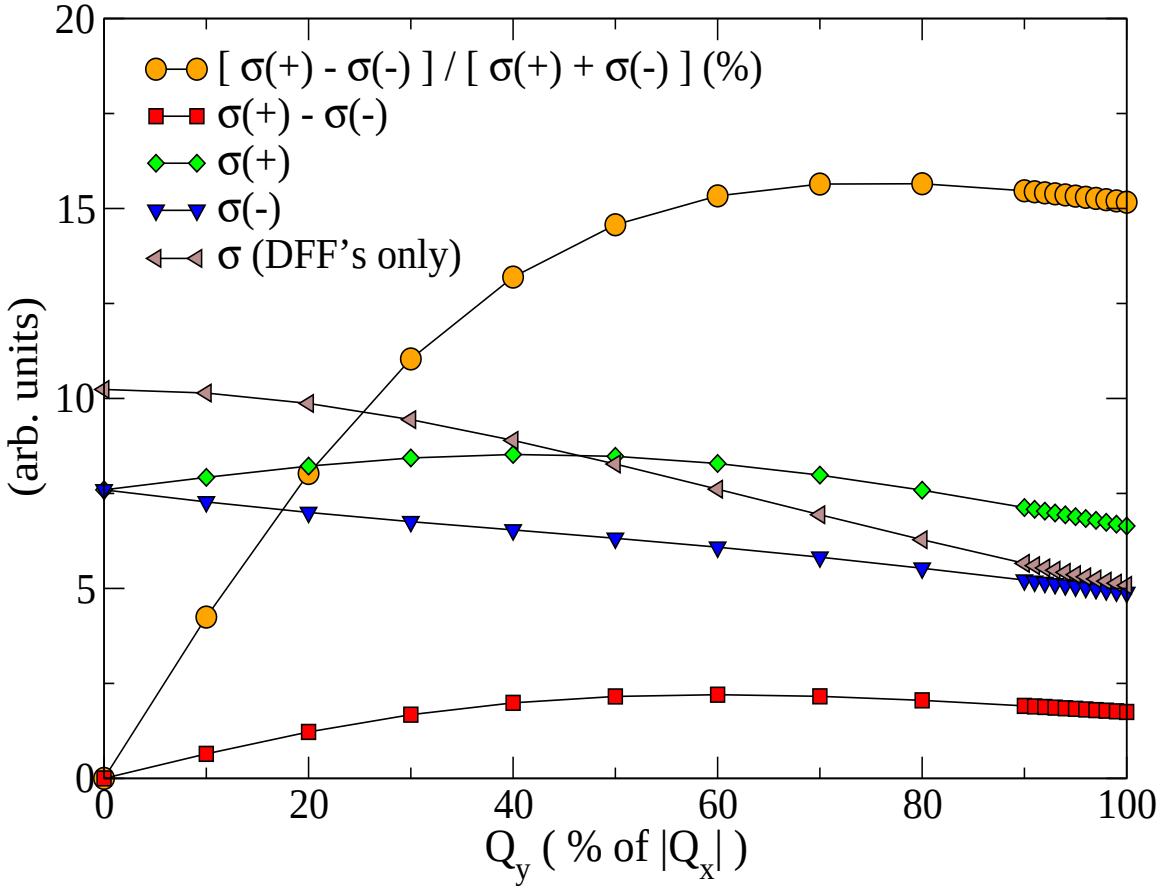
bccFe: thickness profile



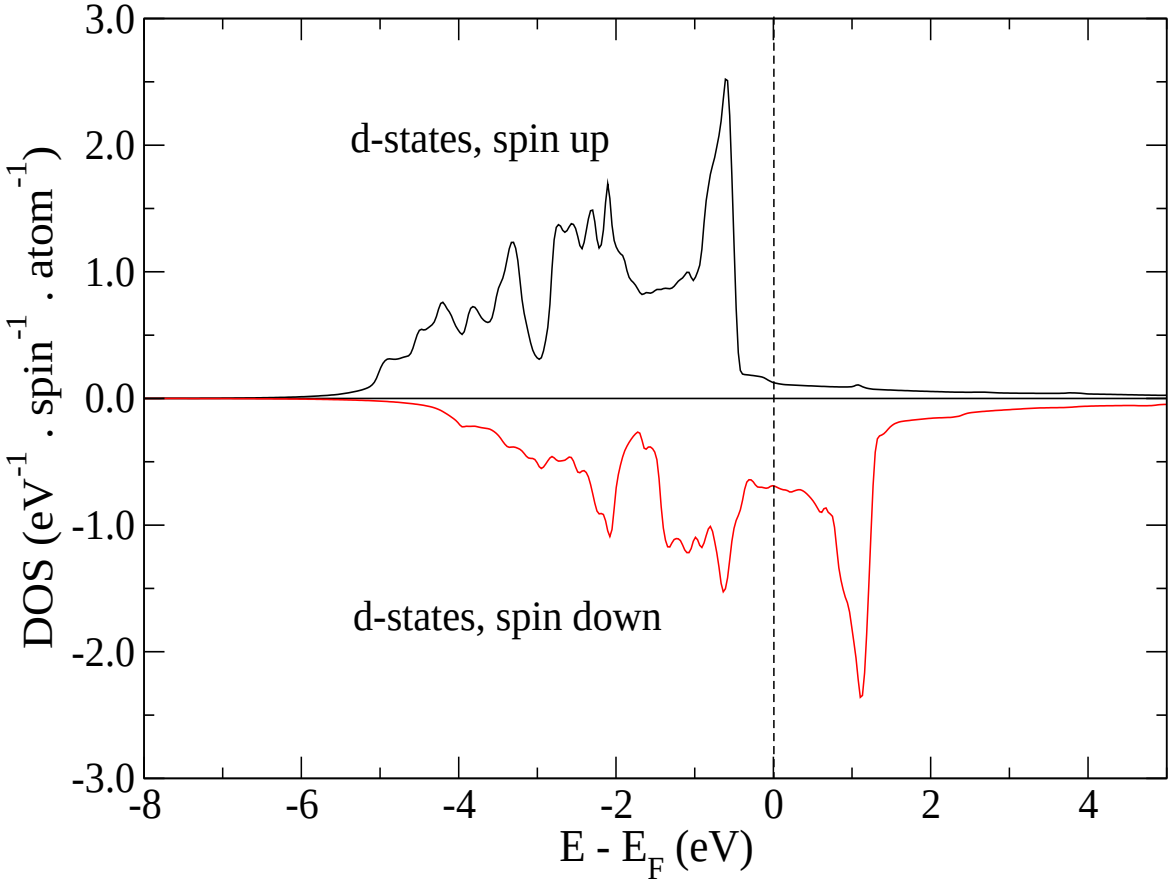
bccFe: convergence & collection angle profile



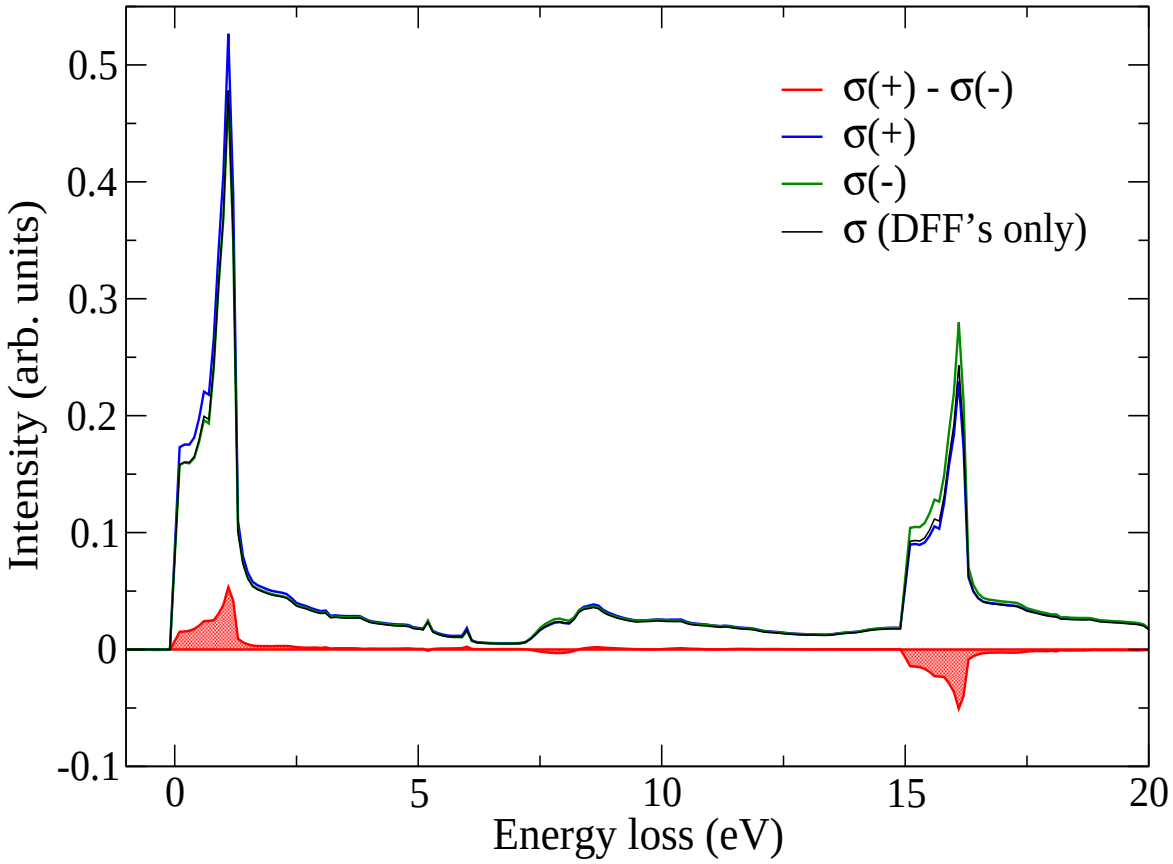
bccFe: detector placement sensitivity



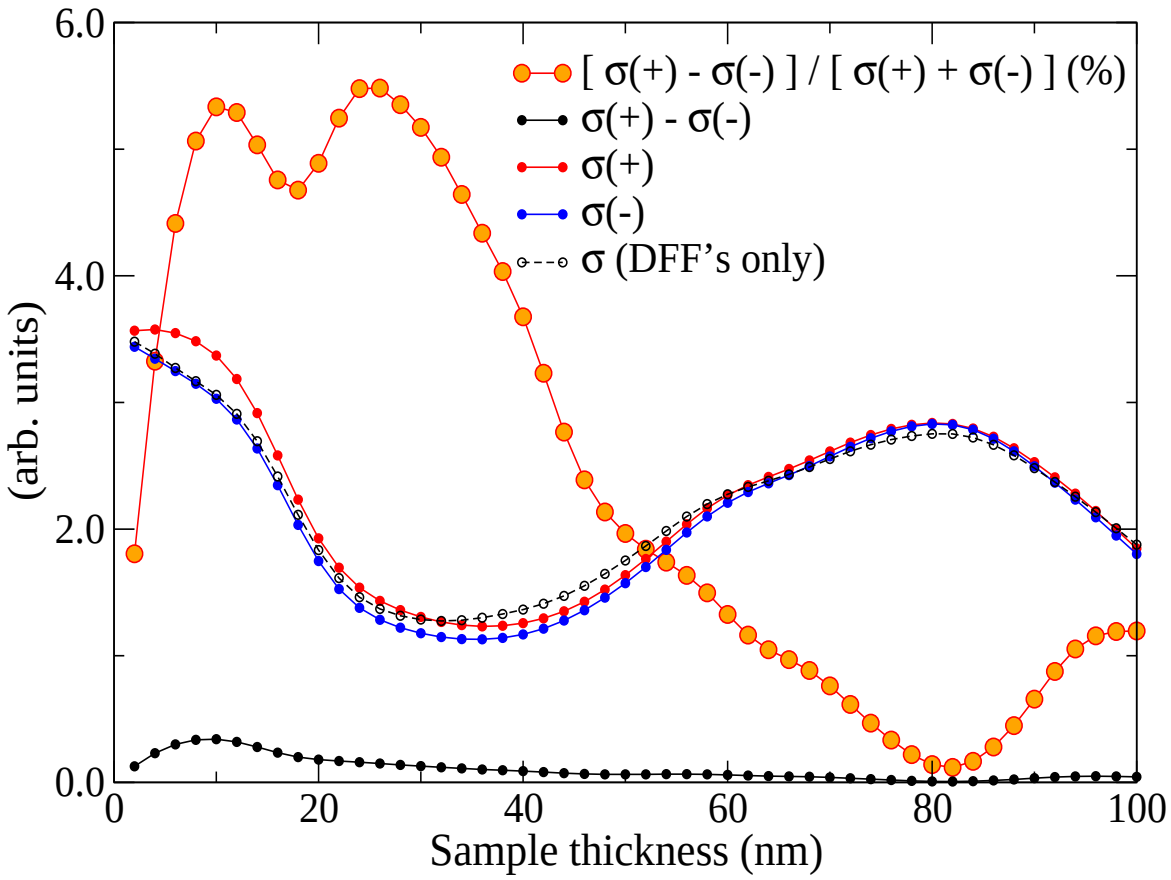
hcpCo: density of states - 3d projections



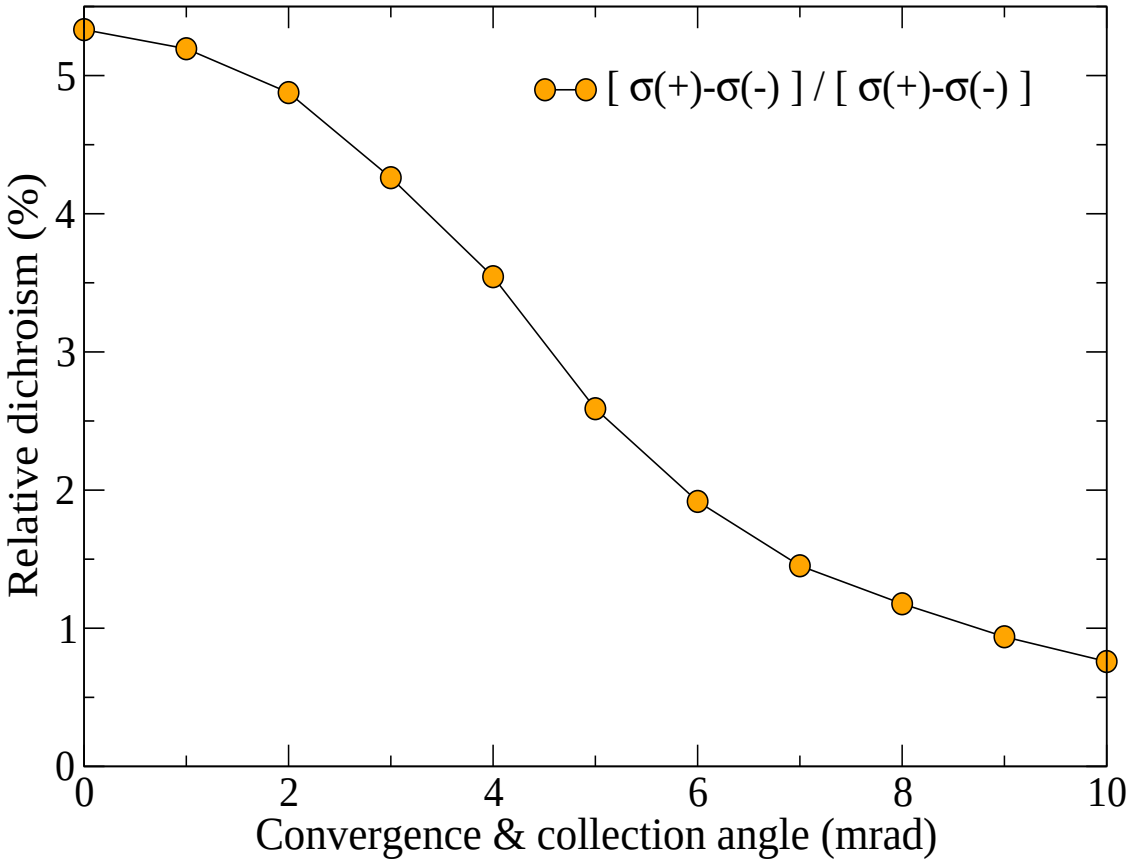
hcpCo: dichroism



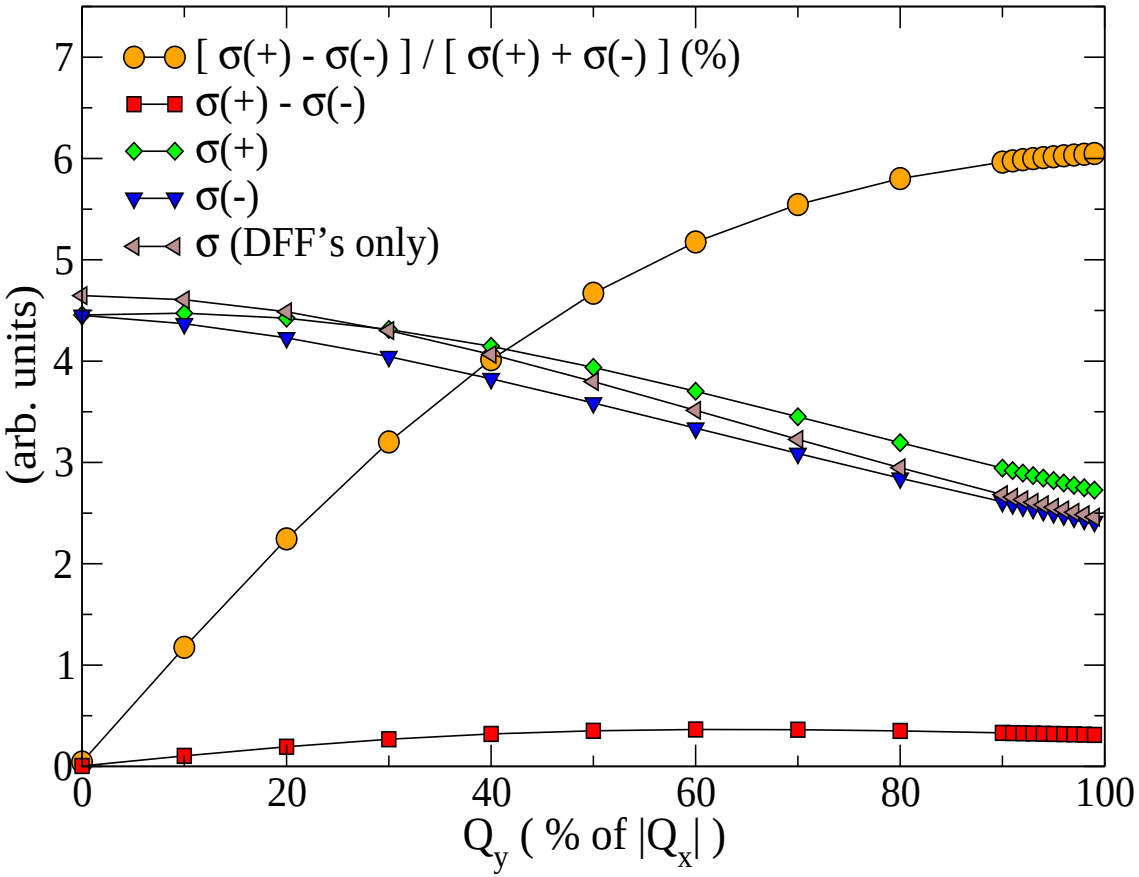
hcpCo: thickness profile



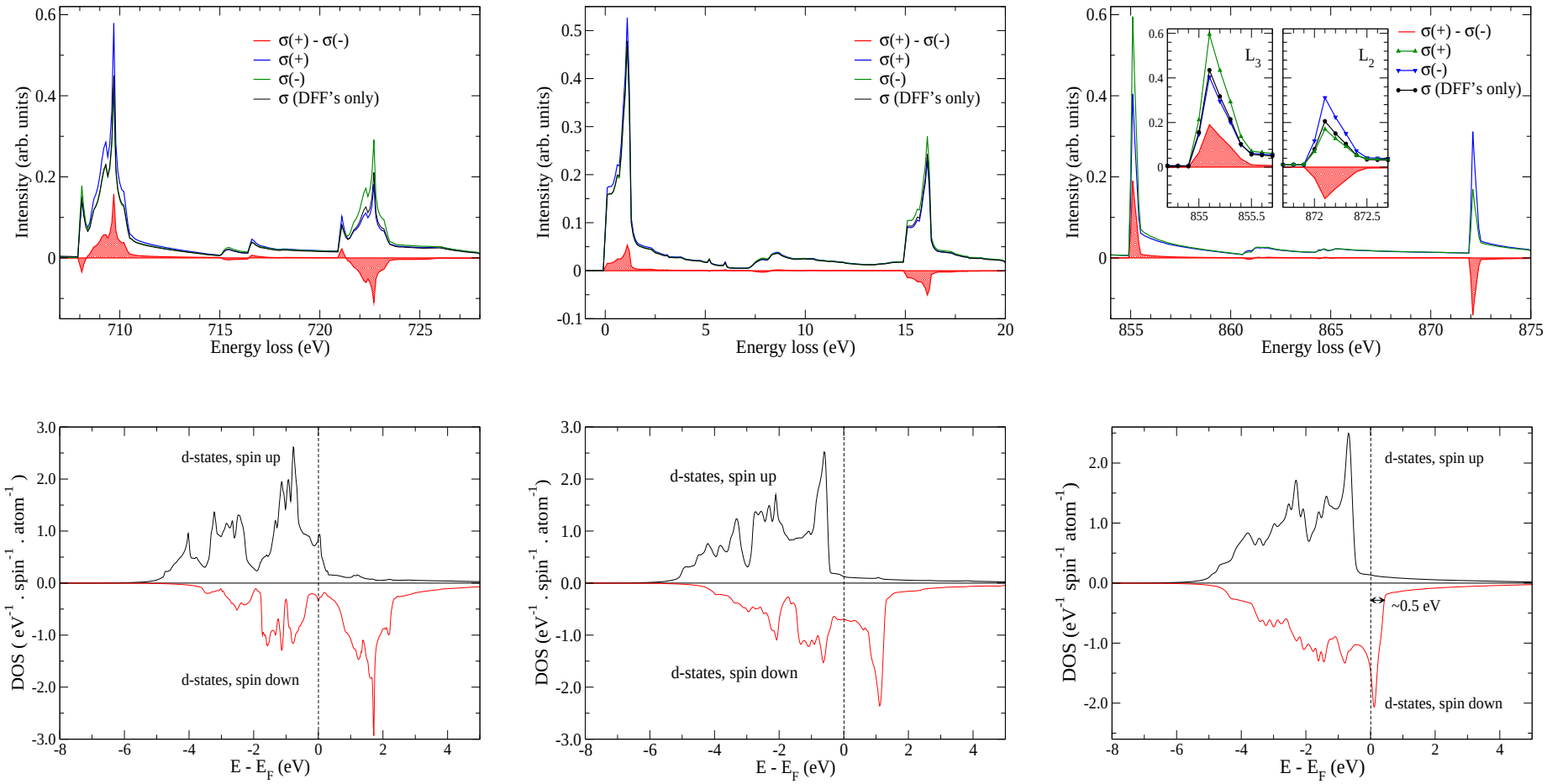
hcpCo: convergence & collection angle profile



hcpCo: detector placement sensitivity



Why so small dichroism in Co?



bcc Fe hcp Co fcc Ni

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3},\frac{2}{3},\frac{1}{4}\},\{\frac{2}{3},\frac{1}{3},\frac{3}{4}\}$

  DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

  MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

  $\exp(i\mathbf{u}_1\cdot\mathbf{G}) = (-\frac{1}{2},\frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2\cdot\mathbf{G}) = (-\frac{1}{2},-\frac{\sqrt{3}}{2})$

  $\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3},\frac{2}{3},\frac{1}{4}\},\{\frac{2}{3},\frac{1}{3},\frac{3}{4}\}$

  DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

  MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

  $\exp(i\mathbf{u}_1\cdot\mathbf{G}) = (-\frac{1}{2},\frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2\cdot\mathbf{G}) = (-\frac{1}{2},-\frac{\sqrt{3}}{2})$

  $\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\}, \{\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\}$

DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

$\exp(i\mathbf{u}_1 \cdot \mathbf{G}) = (-\frac{1}{2}, \frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2 \cdot \mathbf{G}) = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$

$\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\}, \{\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\}$

  DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

  MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

  $\exp(i\mathbf{u}_1 \cdot \mathbf{G}) = (-\frac{1}{2}, \frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2 \cdot \mathbf{G}) = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$

  $\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\}, \{\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\}$

  DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

  MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

  $\exp(i\mathbf{u}_1 \cdot \mathbf{G}) = (-\frac{1}{2}, \frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2 \cdot \mathbf{G}) = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$

  $\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\}, \{\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\}$

  DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

  MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

  $\exp(i\mathbf{u}_1 \cdot \mathbf{G}) = (-\frac{1}{2}, \frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2 \cdot \mathbf{G}) = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$

  $\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Why so small dichroism in Co?

Effect of summation over atoms

$$\frac{d^2\sigma}{d\Omega dE} = \frac{4\gamma^2}{a_0^2}\frac{k_{out}}{k_{in}}\sum_{\mathbf{J}}\sum_{\mathbf{J}'} T_{J_z,J_z'} A_{\mathbf{J}} A^{\star}_{\mathbf{J}'} \frac{1}{N}\sum_{\mathbf{u}} e^{i(\mathbf{Q}_{J_{xy}}-\mathbf{Q}_{J'_{xy}})\mathbf{u}} \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$$

- Ni & Fe: $N = 1, \quad \mathbf{u} = 0 \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$
- Co: $N = 2, \quad \mathbf{u}_{1,2} = \{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\}, \{\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\}$

  DFF: $\mathbf{q} = \mathbf{q}' \quad \rightarrow \quad \frac{1}{N}\sum(\ldots) = 1 \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

  MDFF: $\mathbf{q} \perp \mathbf{q}', \quad \mathbf{q} - \mathbf{q}' = \mathbf{G}, \quad \mathbf{G} = (2,0,0)$

  $\exp(i\mathbf{u}_1 \cdot \mathbf{G}) = (-\frac{1}{2}, \frac{\sqrt{3}}{2}), \quad \exp(i\mathbf{u}_2 \cdot \mathbf{G}) = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$

  $\frac{1}{N}\sum(\ldots) = -\frac{1}{2} \times \frac{S_{\mathbf{u}}(\mathbf{Q}_{J_{xy}},\mathbf{Q}_{J'_{xy}},E)}{Q^2_{J_{xy}} Q^2_{J'_{xy}}}$

Can we do better?

Yes, let's choose a better **G**

- let $\mathbf{G} = (G_x, G_y, 0)$
- requiring $\mathbf{G} \cdot \mathbf{u}_1 = 2\pi n_1$ and $\mathbf{G} \cdot \mathbf{u}_2 = 2\pi n_2$
  we get (in (hkl) notation) $\mathbf{G} = (2n_2 - n_1, 2n_1 - n_2, 0)$
- e.g., let $n_1 = 1$ and $n_2 = 1$, then $\mathbf{G} = (110)$.

Can we do better?

Yes, let's choose a better **G**

- let $\mathbf{G} = (G_x, G_y, 0)$
- requiring $\mathbf{G} \cdot \mathbf{u}_1 = 2\pi n_1$ and $\mathbf{G} \cdot \mathbf{u}_2 = 2\pi n_2$
  we get (in (hkl) notation) $\mathbf{G} = (2n_2 - n_1, 2n_1 - n_2, 0)$
- e.g., let $n_1 = 1$ and $n_2 = 1$, then $\mathbf{G} = (110)$.

Can we do better?

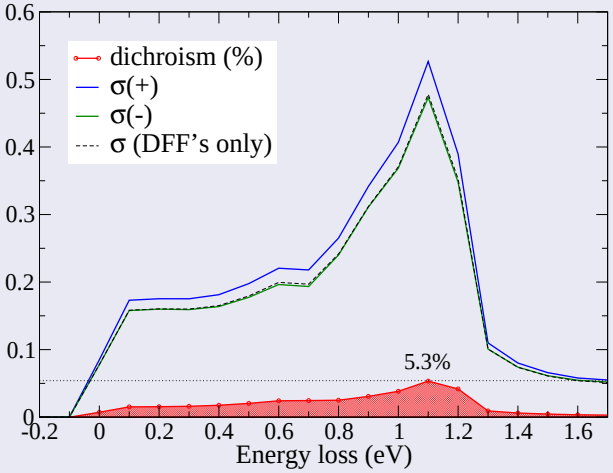
Yes, let's choose a better **G**

- let $\mathbf{G} = (G_x, G_y, 0)$
- requiring $\mathbf{G} \cdot \mathbf{u}_1 = 2\pi n_1$ and $\mathbf{G} \cdot \mathbf{u}_2 = 2\pi n_2$
  we get (in (hkl) notation) $\mathbf{G} = (2n_2 - n_1, 2n_1 - n_2, 0)$
- e.g., let $n_1 = 1$ and $n_2 = 1$, then $\mathbf{G} = (110)$.

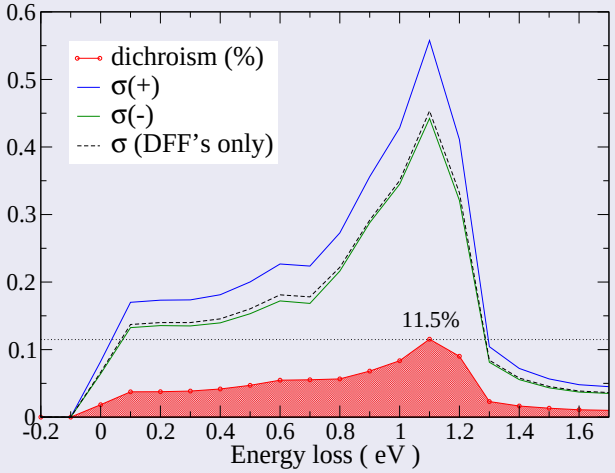
Can we do better?

Yes, let's choose a better **G**

- let $\mathbf{G} = (G_x, G_y, 0)$
- requiring $\mathbf{G} \cdot \mathbf{u}_1 = 2\pi n_1$ and $\mathbf{G} \cdot \mathbf{u}_2 = 2\pi n_2$
  we get (in (hkl) notation) $\mathbf{G} = (2n_2 - n_1, 2n_1 - n_2, 0)$
- e.g., let $n_1 = 1$ and $n_2 = 1$, then $\mathbf{G} = (110)$.



$\mathbf{G} = (200)$



$\mathbf{G} = (110)$

Outline

Conclusions and outlook

Conclusions

- A coherent set of programs for calculation of MDFF was prepared
- A dichroic effect on bccFe, hcpCo and fccNi was calculated
- Calculations indicate that dichroic effect is:
  - weakly sensitive to detector misplacements of up to 30% q_y
  - rather sensitive to sample thickness
  - sensitive to collection/convergence angle
- There is an important dependence of dichroism strength on exp. geometry - on the systematic row indices