Magnetic structure determination of rare-earth based, high moment, 2D parent magnet

Daniel Potashnikov (IAEC, Technion)

Under supervision of Prof. Amit Keren and Dr. Oleg Rivin

Technion seminar 2021

2D materials

<table>
<tr><td>Graphene family</td><td>Graphene</td><td>hBN
'white graphene'</td><td>BCN</td><td>Fluorographene</td><td>Graphene oxide</td></tr>
<tr><td rowspan="2">2D chalcogenides</td><td rowspan="2">MoS_2, WS_2, $MoSe_2$, WSe_2</td><td rowspan="2">Semiconducting dichalcogenides:
$MoTe_2$, WTe_2,
ZrS_2, $ZrSe_2$ and so on</td><td colspan="3">Metallic dichalcogenides:
$NbSe_2$, NbS_2, TaS_2, TiS_2, $NiSe_2$ and so on</td></tr>
<tr><td colspan="3">Layered semiconductors:
GaSe, GaTe, InSe, Bi_2Se_3 and so on</td></tr>
<tr><td rowspan="2">2D oxides</td><td>Micas,
BSCCO</td><td>MoO_3, WO_3</td><td rowspan="2">Perovskite-type:
$LaNb_2O_7$, $(Ca,Sr)_2Nb_3O_{10}$,
$Bi_4Ti_3O_{12}$, $Ca_2Ta_2TiO_{10}$ and so on</td><td colspan="2">Hydroxides:
$Ni(OH)_2$, $Eu(OH)_2$ and so on</td></tr>
<tr><td>Layered
Cu oxides</td><td>TiO_2, MnO_2, V_2O_5,
TaO_3, RuO_2 and so on</td><td colspan="2">Others</td></tr>
</table>

A.K. Geim and I.V. Grigorieva, Nature **499**, 419 (2013)

Importance of 2D materials

REVIEW ARTICLE
https://doi.org/10.1038/s41565-019-0438-6

nature nanotechnology

Magnetic 2D materials and heterostructures

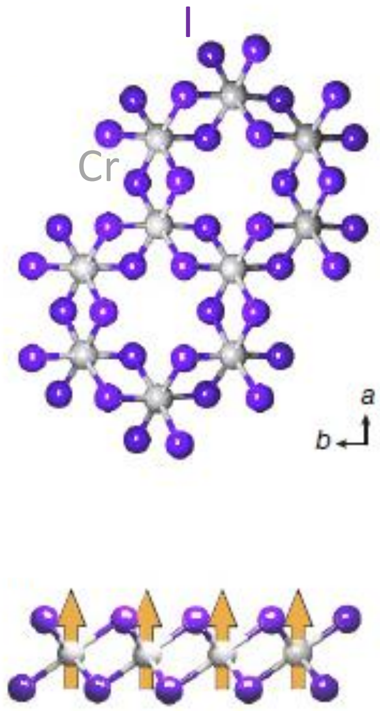
M. Gibertini[1,2], M. Koperski[3,4], A. F. Morpurgo[1,5] and K. S. Novoselov[3,4]*

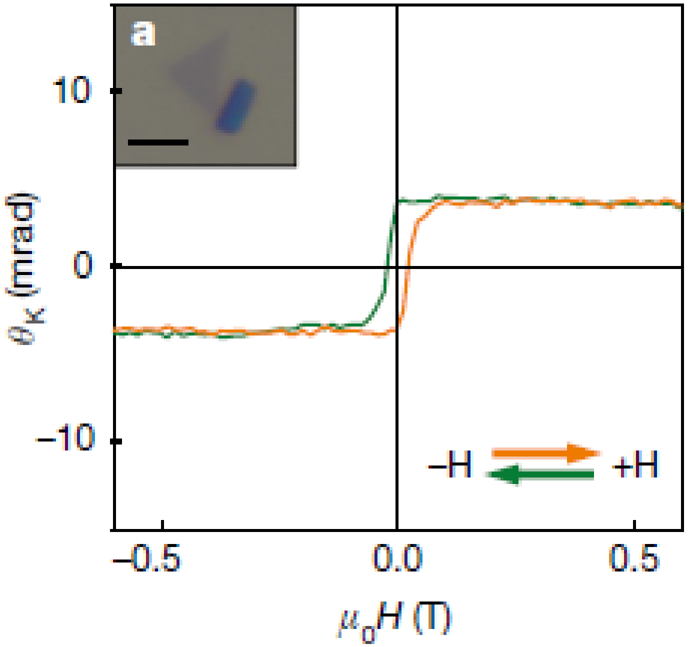
The family of two-dimensional (2D) materials grows day by day, hugely expanding the scope of possible phenomena to be explored in two dimensions, as well as the possible van der Waals (vdW) heterostructures that one can create. Such 2D materials currently cover a vast range of properties. Until recently, this family has been missing one crucial member: 2D magnets. The situation has changed over the past 2 years with the introduction of a variety of atomically thin magnetic crystals. Here we will discuss the difference between magnetic states in 2D materials and in bulk crystals and present an overview of the 2D magnets that have been explored recently. We will focus on the case of the two most studied systems—semiconducting CrI_3 and metallic Fe_3GeTe_2—and illustrate the physical phenomena that have been observed. Special attention will be given to the range of new van der Waals heterostructures that became possible with the appearance of 2D magnets, offering new perspectives in this rapidly expanding field.

M. Gibertini, M. Koperski, A. F. Morpurgo and K. S. Novoselov, Nature Nanotechnology **14**, 408 (2019)

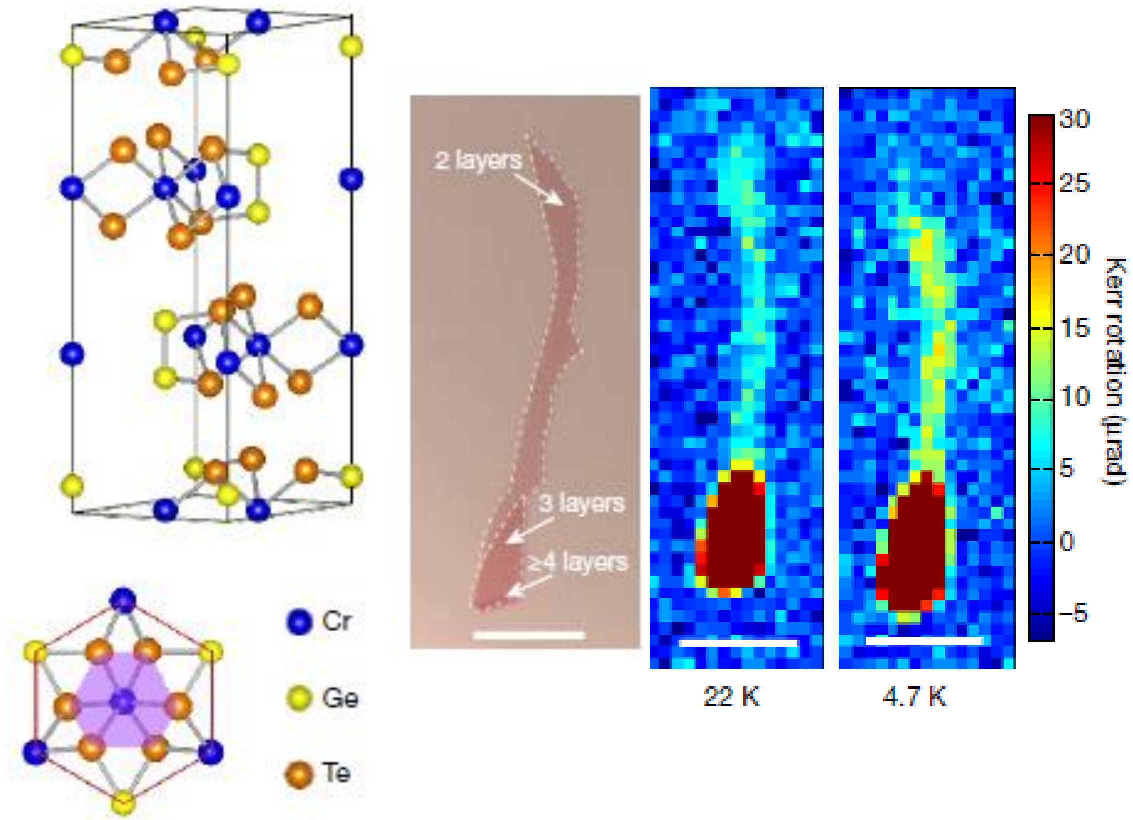
Examples of 2D magnets

CrI_3 – Huang *et al*. Nature **546**, 270 (2017)





$Cr_2Ge_2Te_6$ – Gong *et al*. Nature **546,** 265 (2017)



Nano laminated quaternary compounds – <u>*i*</u>-MAX phases

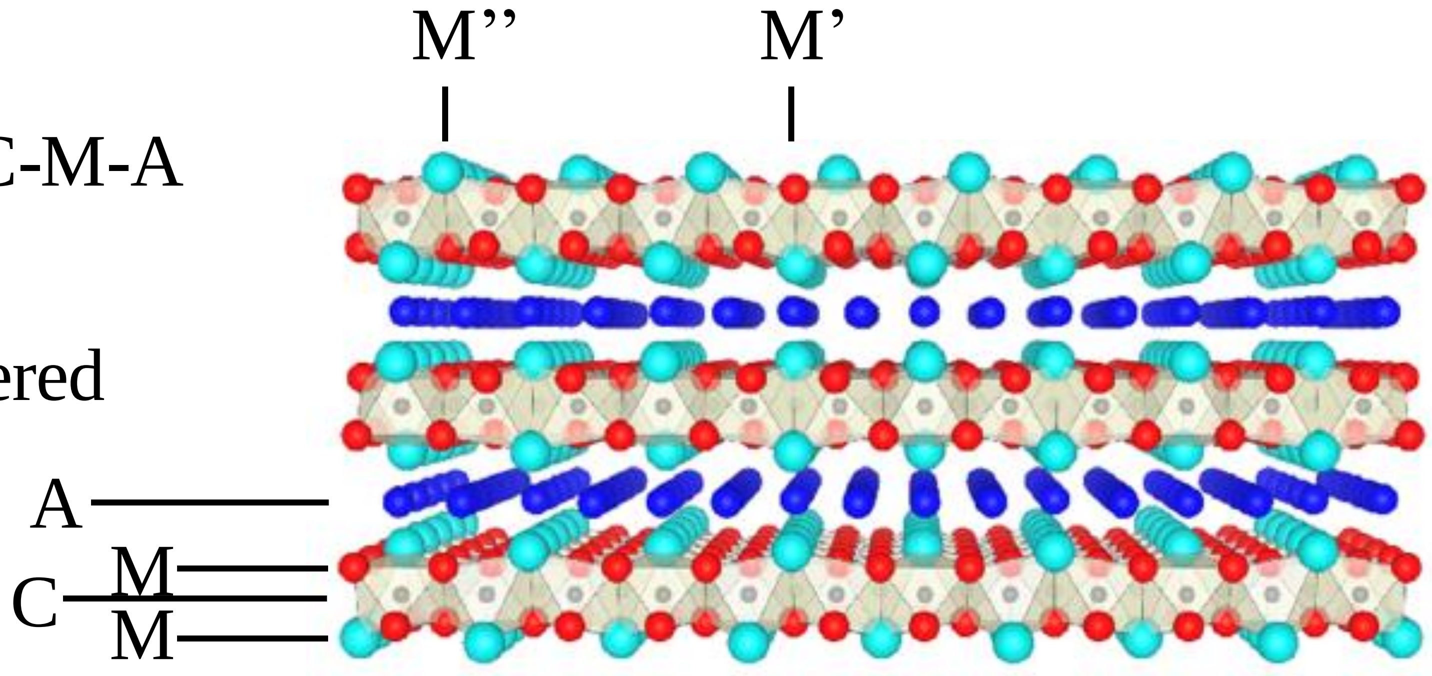
- Chemical formula: $(M'_{2/3}M''_{1/3})_2AlC$

- Monoclinic unit cell ($C2/c$) with $a \approx 9.5$ Å, $b \approx 5.5$ Å, $c \approx 14.1$ Å, $\beta \approx 103.5°$

- Has a layered structure: M-C-M-A

- M' and M'' are <u>i</u>n-plane ordered

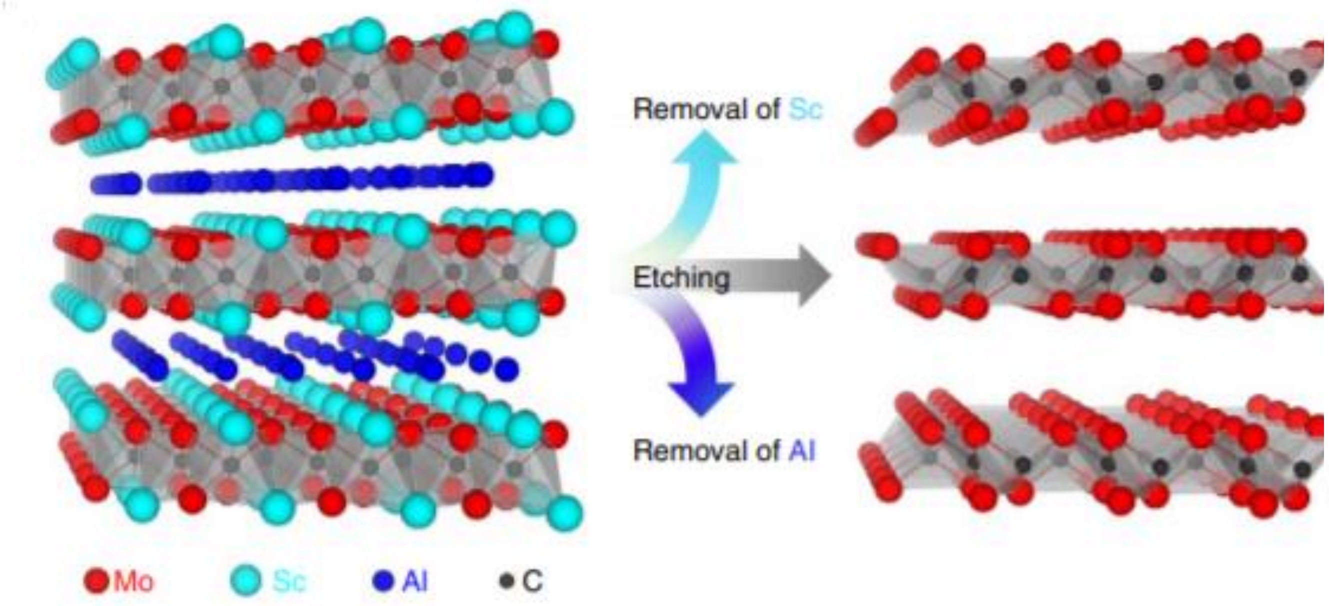
- Example: $(Mo_{2/3}Sc_{1/3})_2AlC$

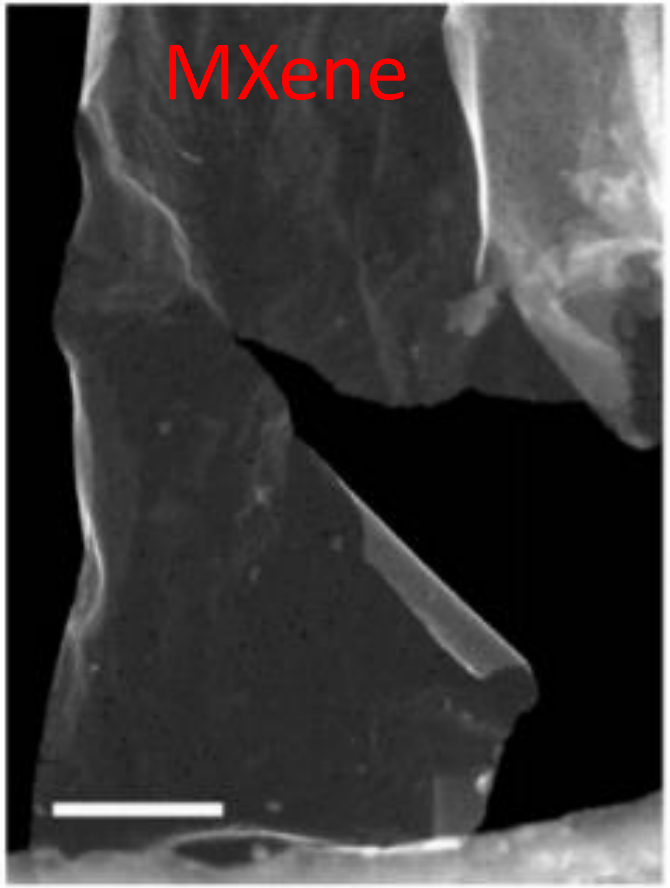


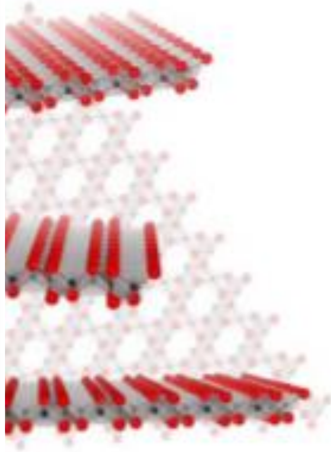
Creation of two-dimensional layers: Example $(Mo_{2/3}Sc_{1/3})_2AlC$

- Chemical etching with HF + TBAOH

- Delamination in water



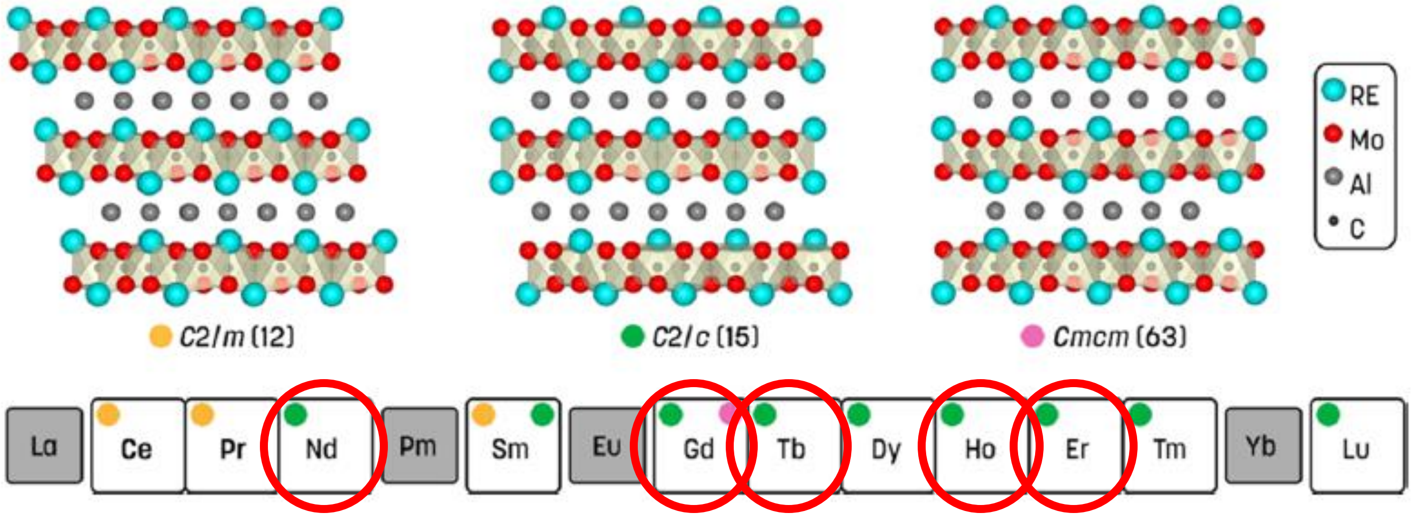




Q. Tao *et al*, Nature communications **8**, 14949 (2017)

Magnetic 2D sheets?

- The possibility to replace Sc with rare earths (RE) [1] ⇒ RE-*i*-MAX
- Addition of RE gives rise to complex magnetic interactions
- Objective: Investigate the magnetic structure of these new compounds

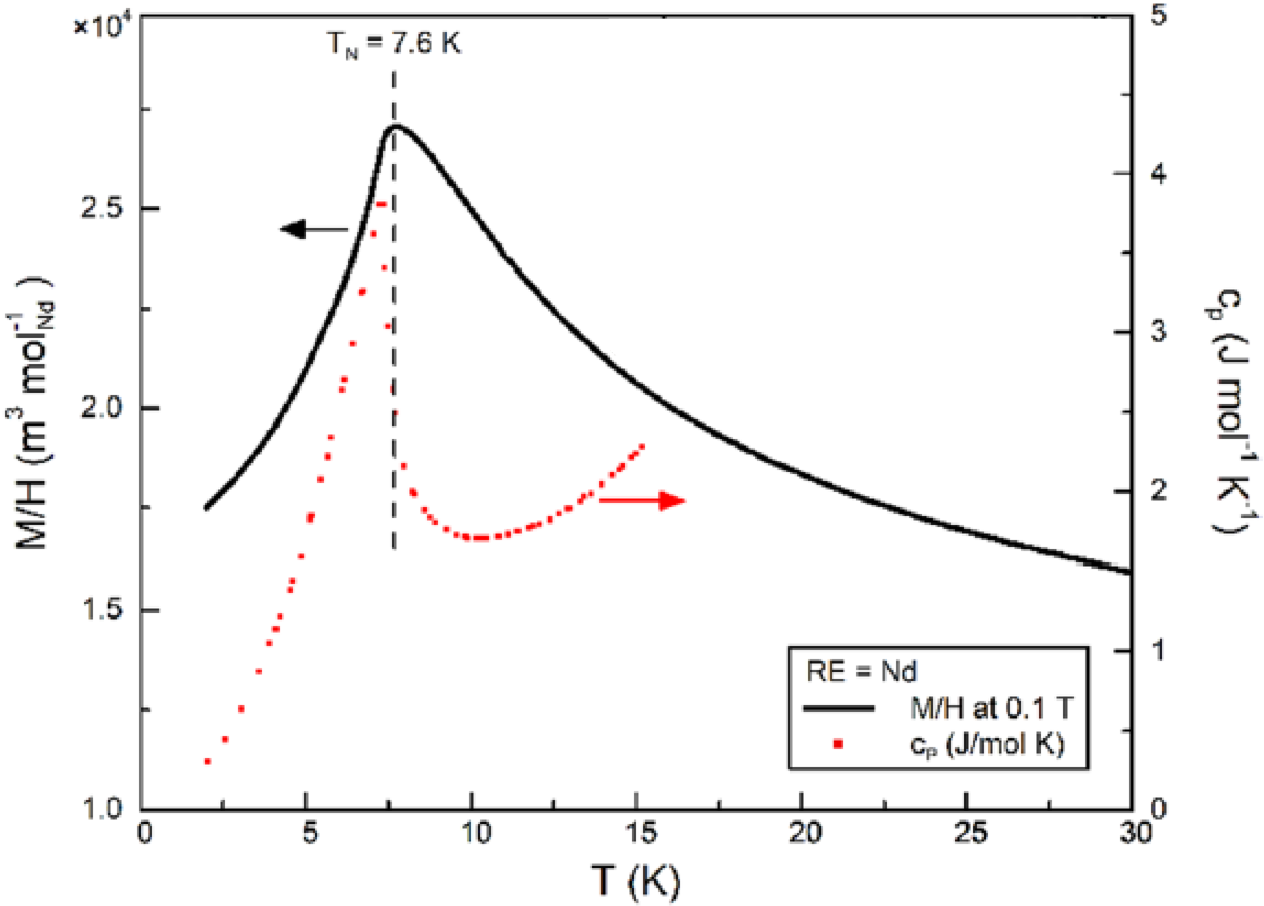


[1] Q. Tao, J. Lu, M. Dahlqvist, … , O. Rivin, D. Potashnikov, … Chem. Mater. **31,** 2019

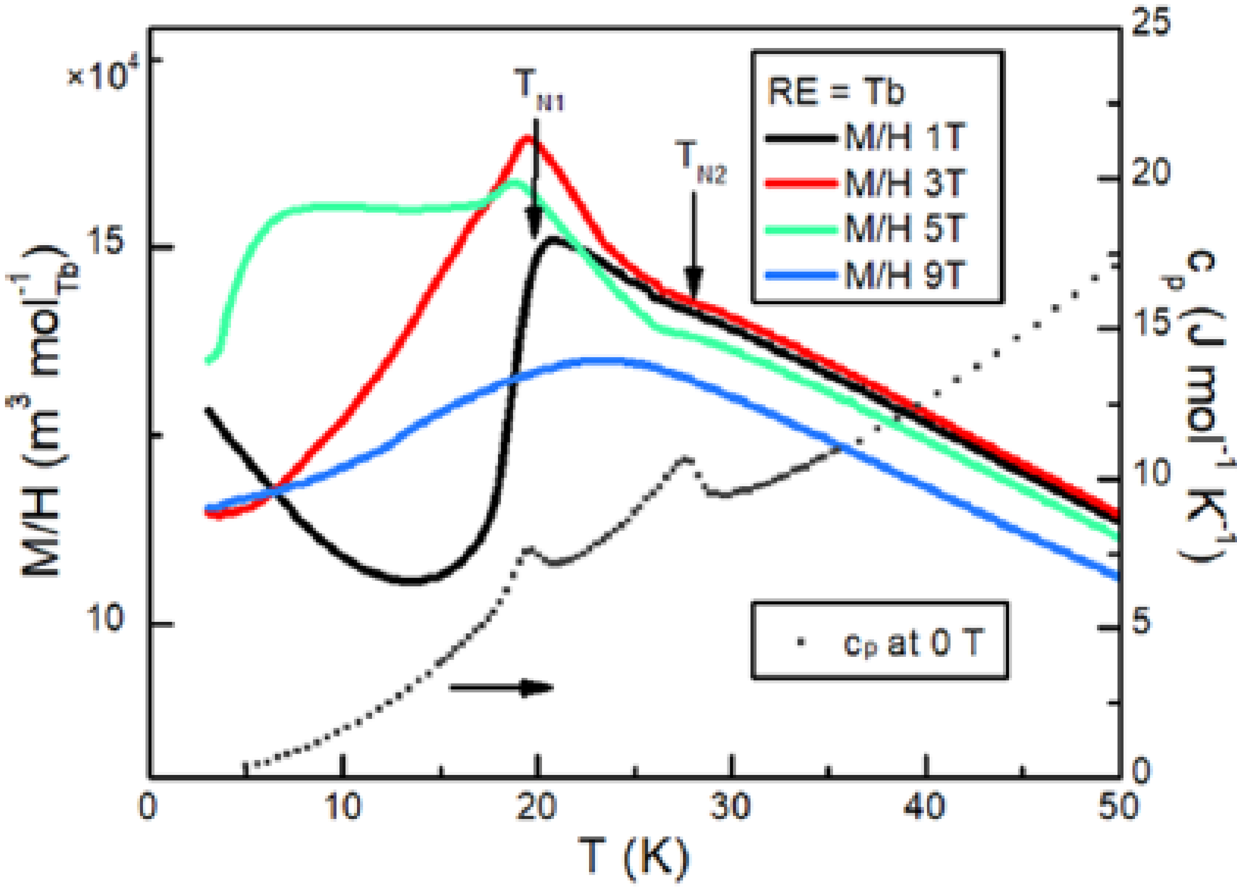
Preliminary measurements

Preliminary measurements

RE = Nd



RE = Tb

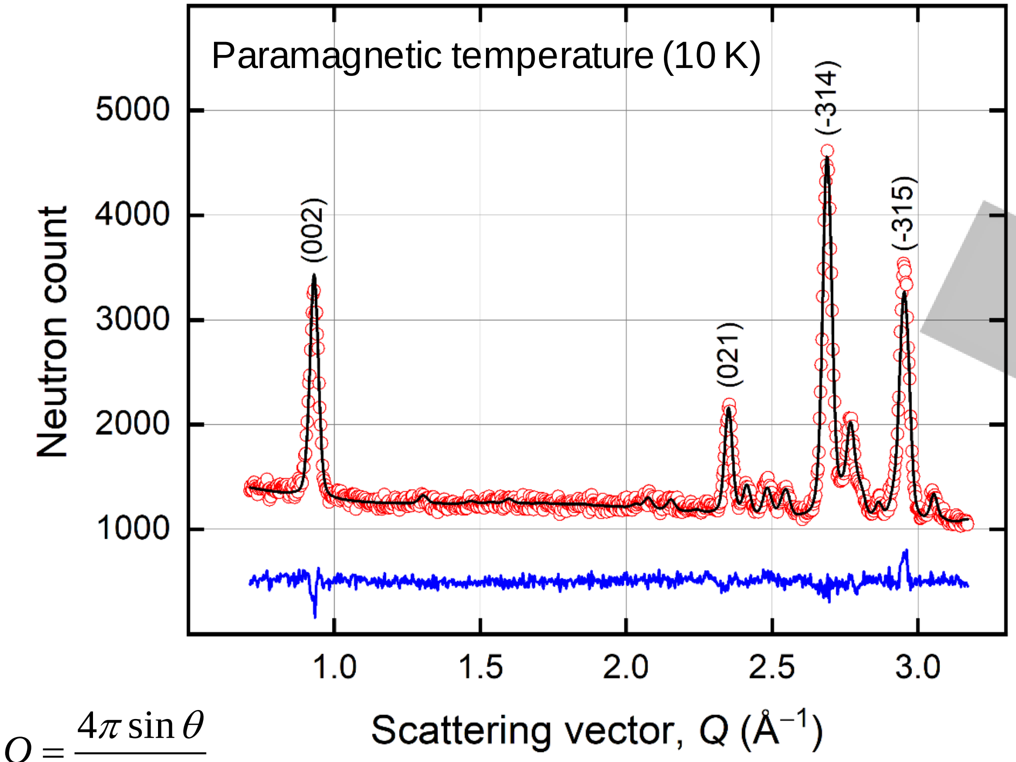


[1] Q. Tao, J. Lu, M. Dahlqvist, … , O. Rivin, **D. Potashnikov**, … Chem. Mater. **31,** 2019

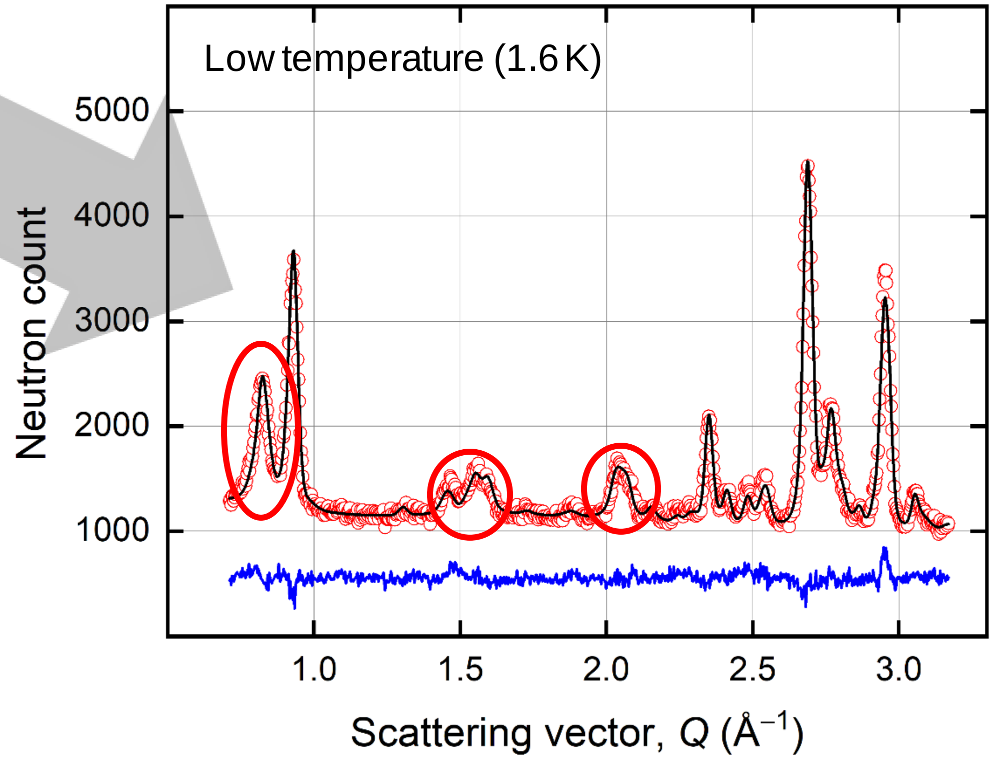
Neutron diffraction

Neutron diffraction measurements

RE = Er



New reflections appear =
Onset of magnetic ordering



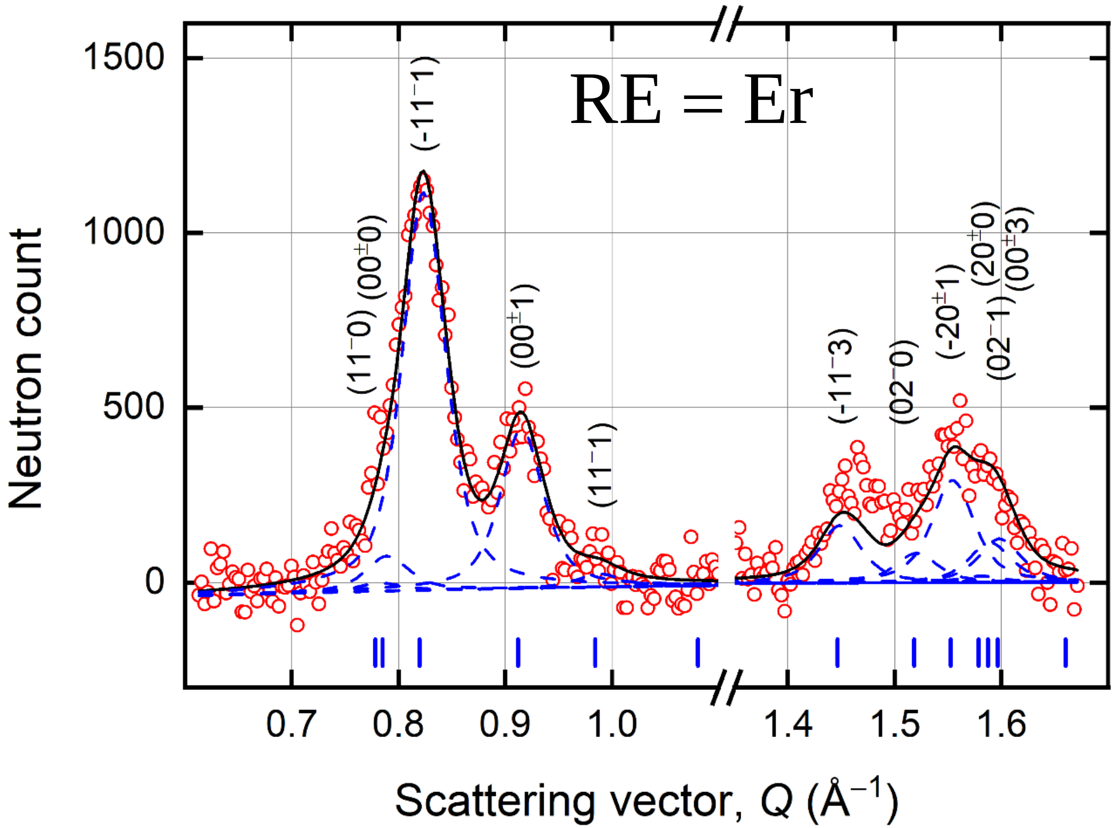
Theory

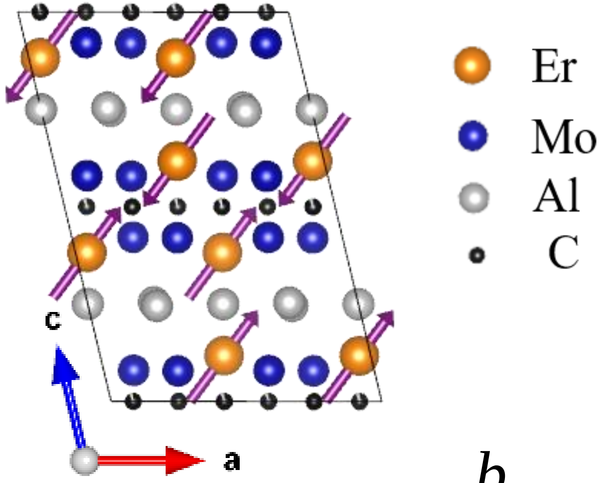
$$Q = \frac{4\pi \sin\theta}{\lambda}$$

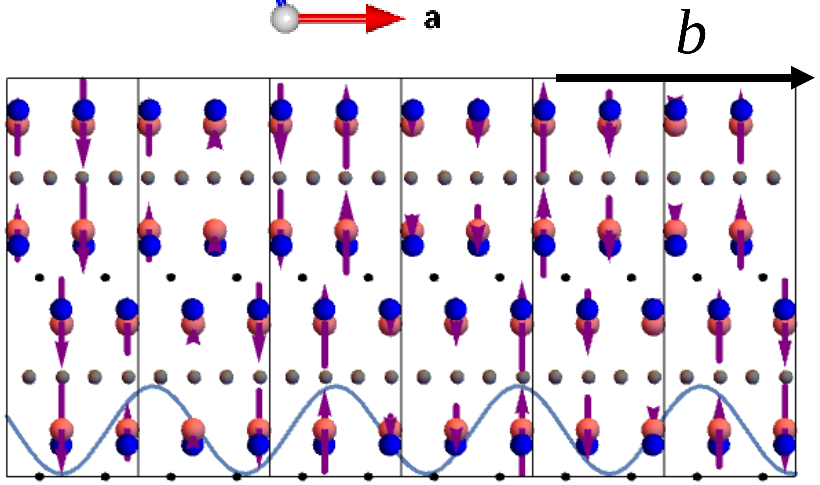
Q – Momentum transfer
λ – Neutron wavelength
θ – Bragg angle

Magnetic structure determination

- Refinement of the magnetic reflections gives the magnetic structure

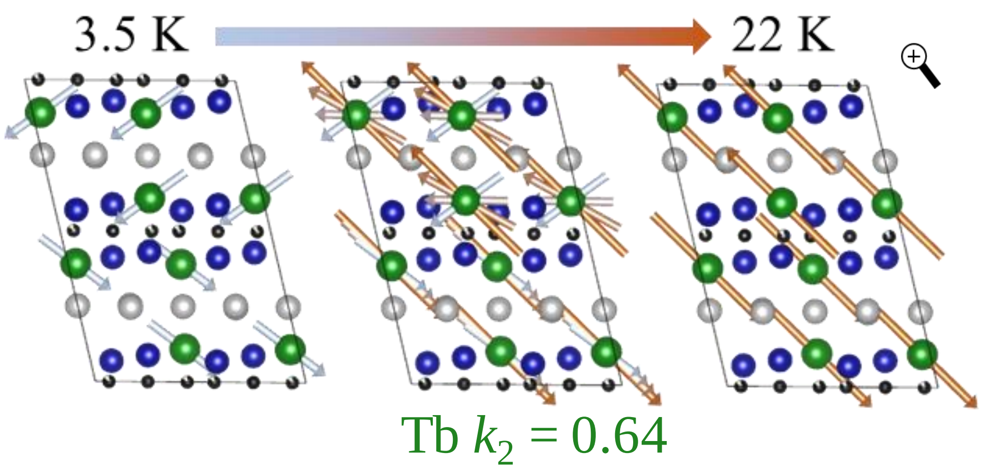


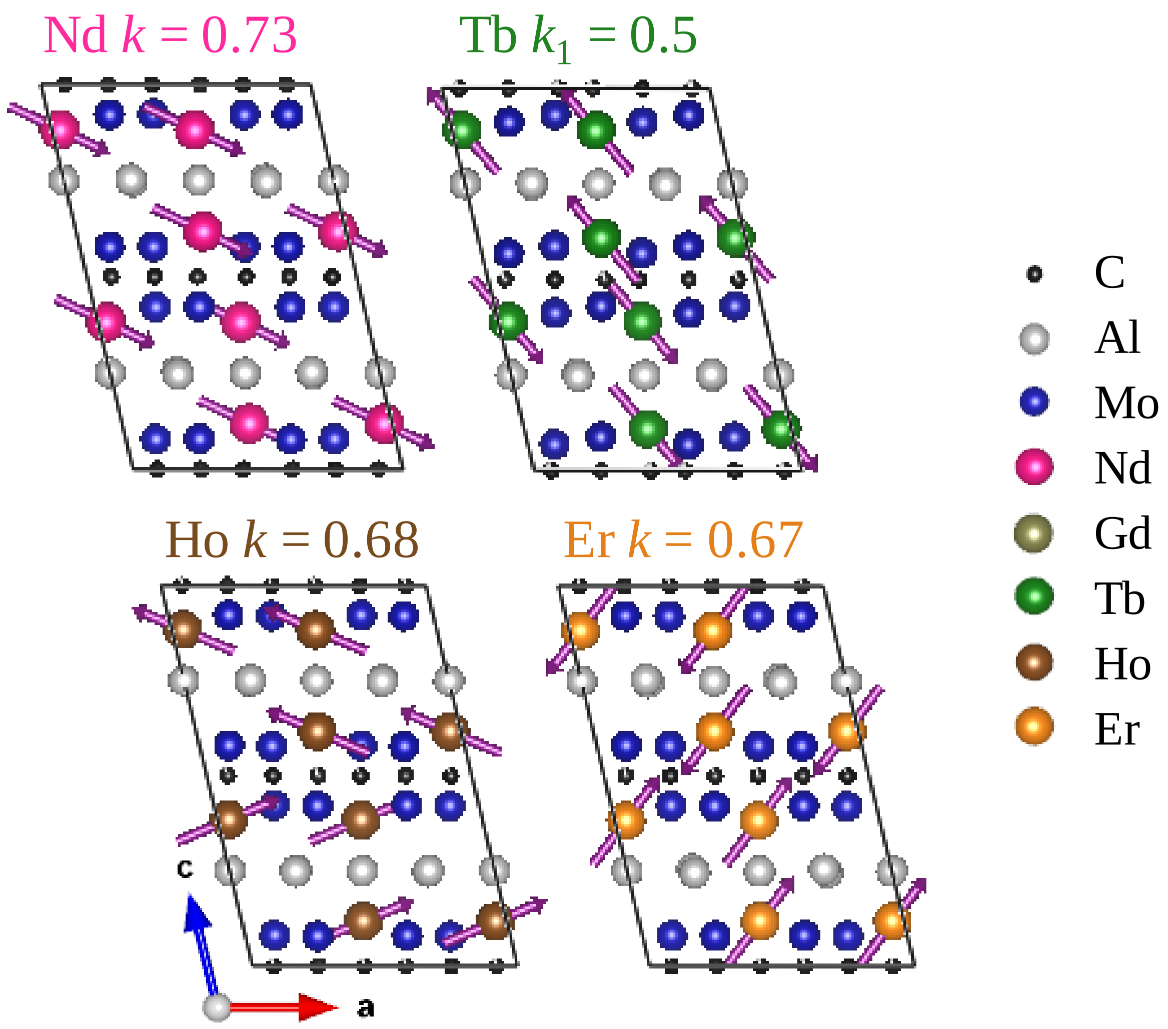




Observed magnetic structures from NPD

- All structures are SDWs with **k** P**b**
- Moments are oriented in the *a*-*c* plane
- Tb *i*-MAX contains two structures





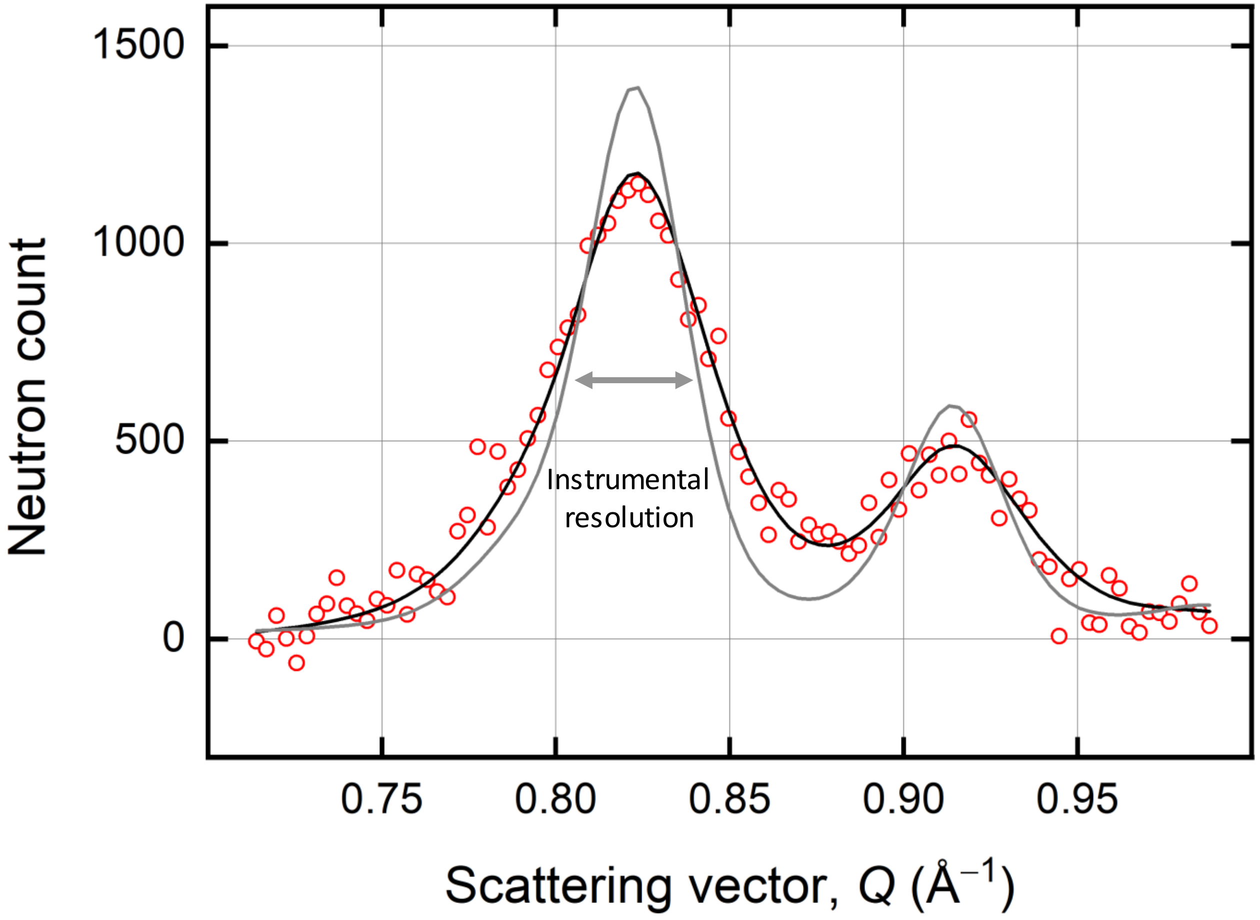
Observation of short-range ordering (SRO)

- Magnetic reflections in Ho and Er *i*-MAX show broadening
- Presence of SRO together with long-range order
- Correlation length is estimated using Scherrer's formula

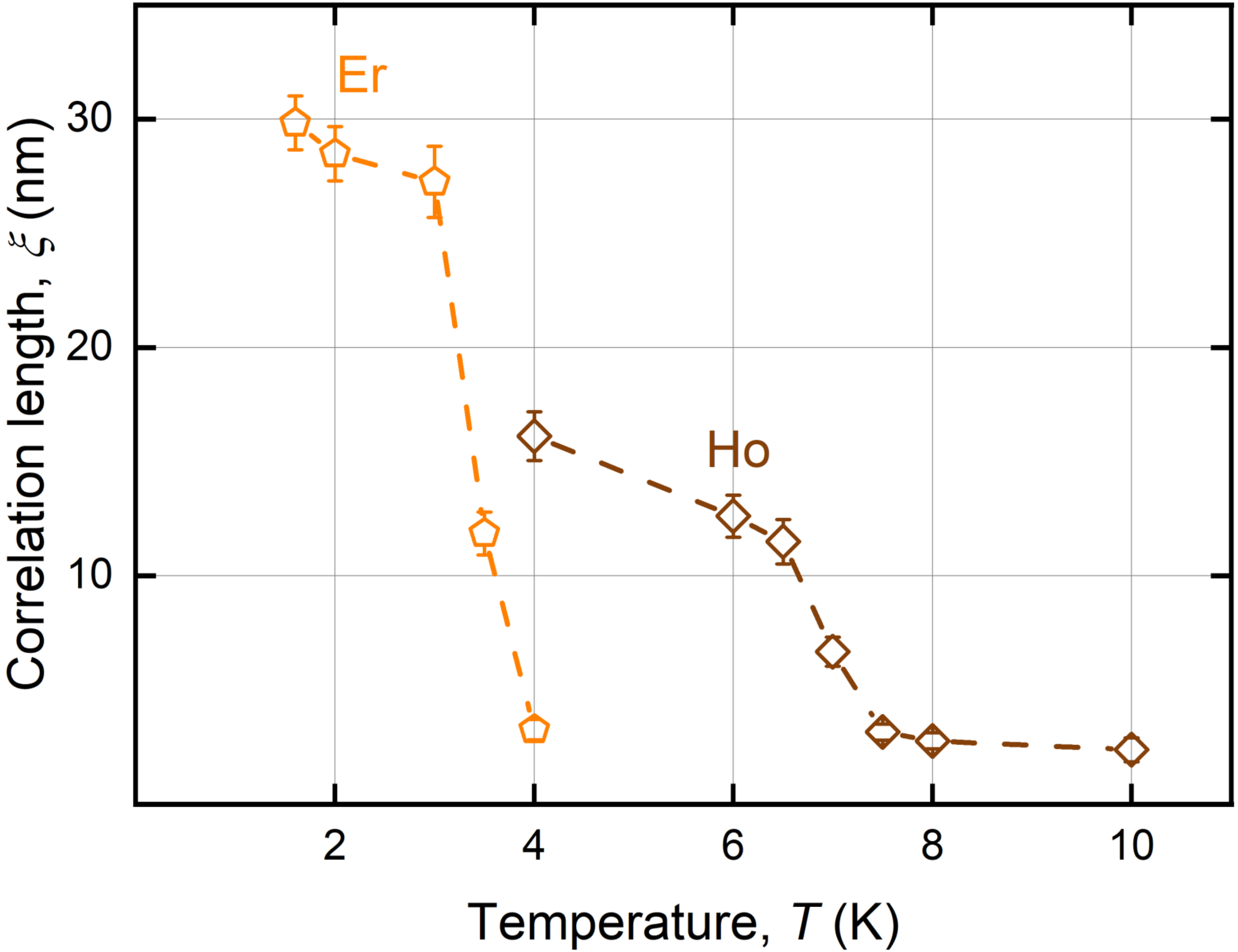
$$\xi = \frac{0.89\lambda}{\beta \cos\theta}$$

λ – Neutron wavelength
β – FWHM of line broadening
θ – Bragg angle

RE = Er



Temperature evolution – correlation length

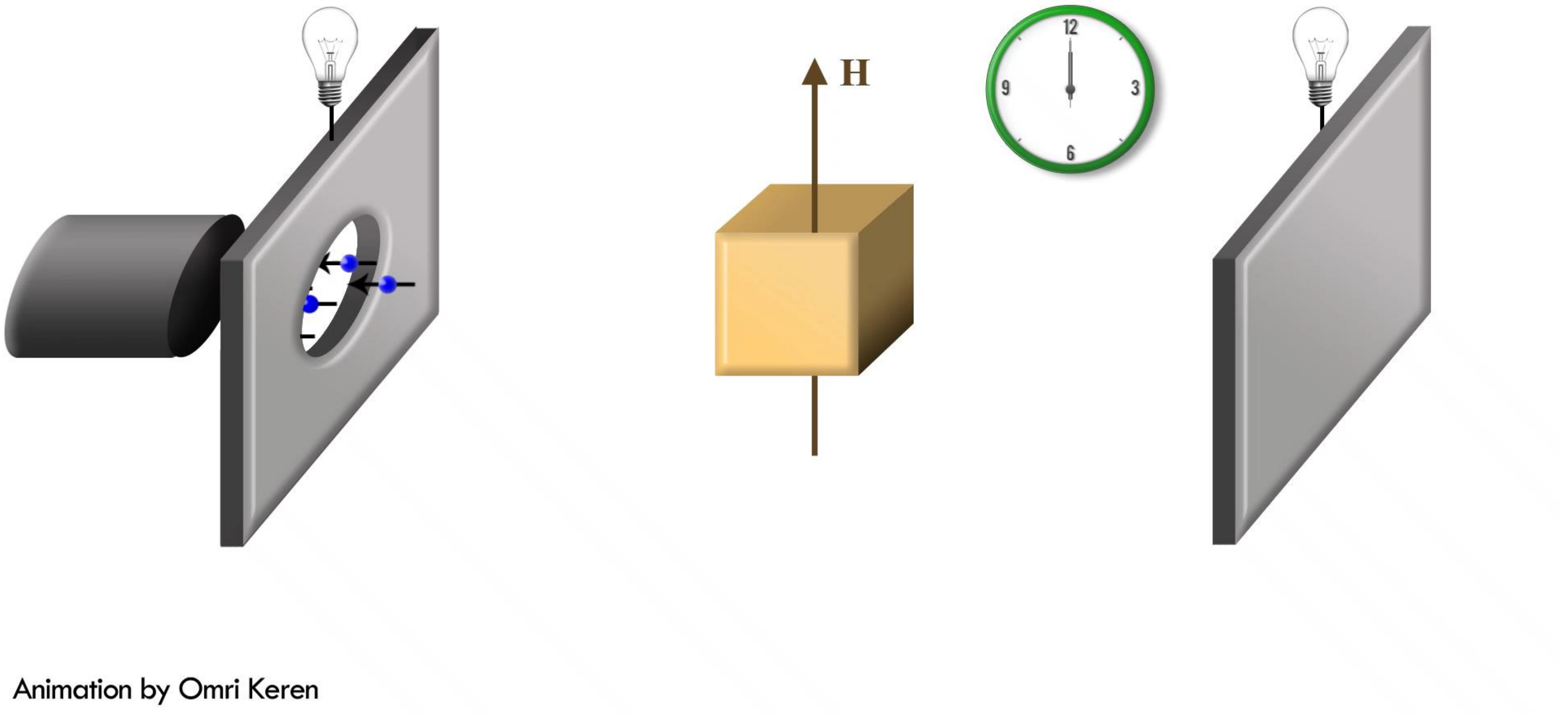


Gd *i*-MAX

- Gd is a strong neutron absorber and therefore cannot be easily measured with NPD
- However, the Gd *i*-MAX had the highest sample quality with single crystals available ⇒ high potential for attempting to produce a MXene
- An alternative method to determine its magnetic structure was required

Muon spin rotation

Muon spin rotation (μSR)



Animation by Omri Keren

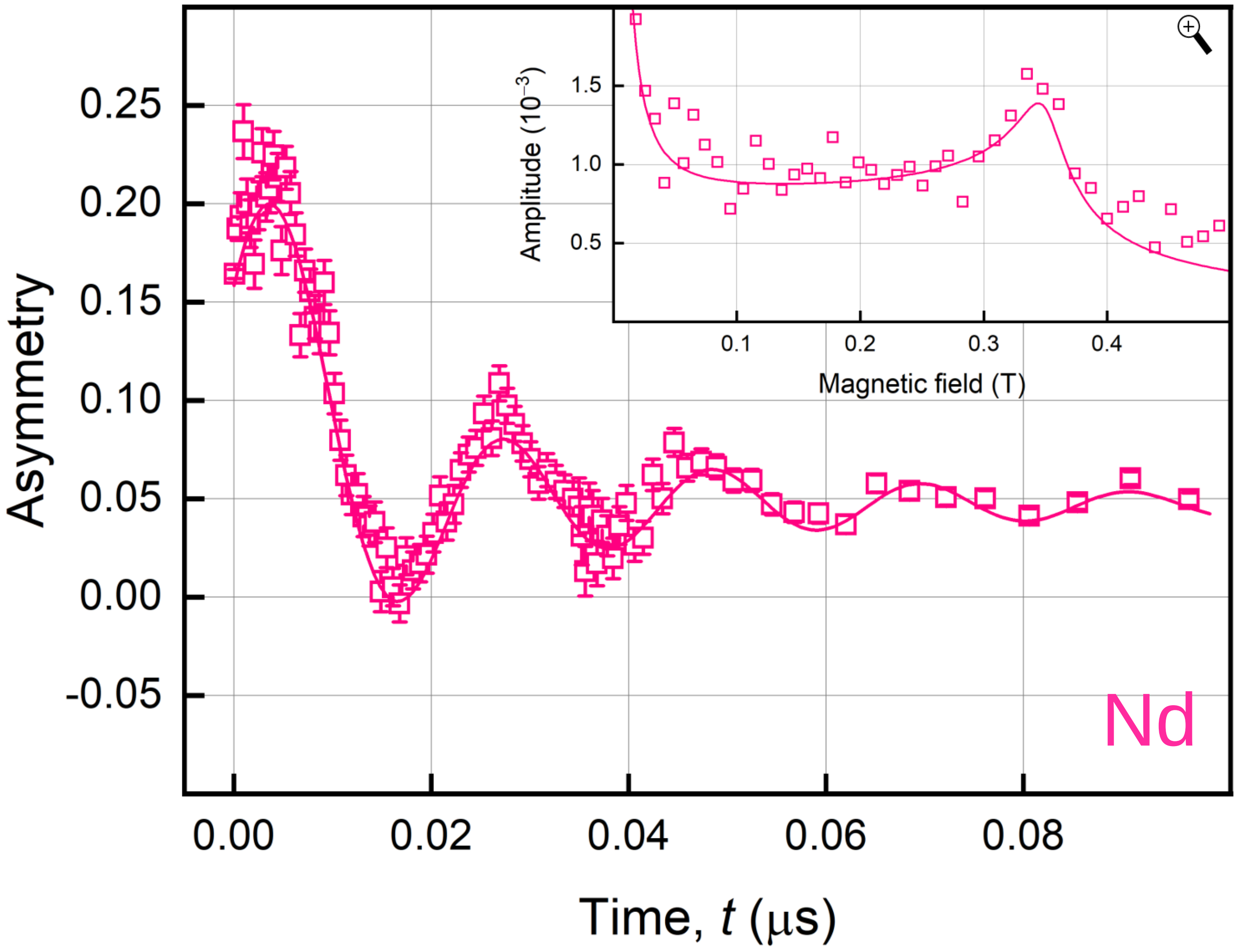
Theoretical background

Zero field μSR

- Nd *i*-MAX shows Bessel-like oscillations

- The field distribution is continuous ⇒ Incommensurate SDW

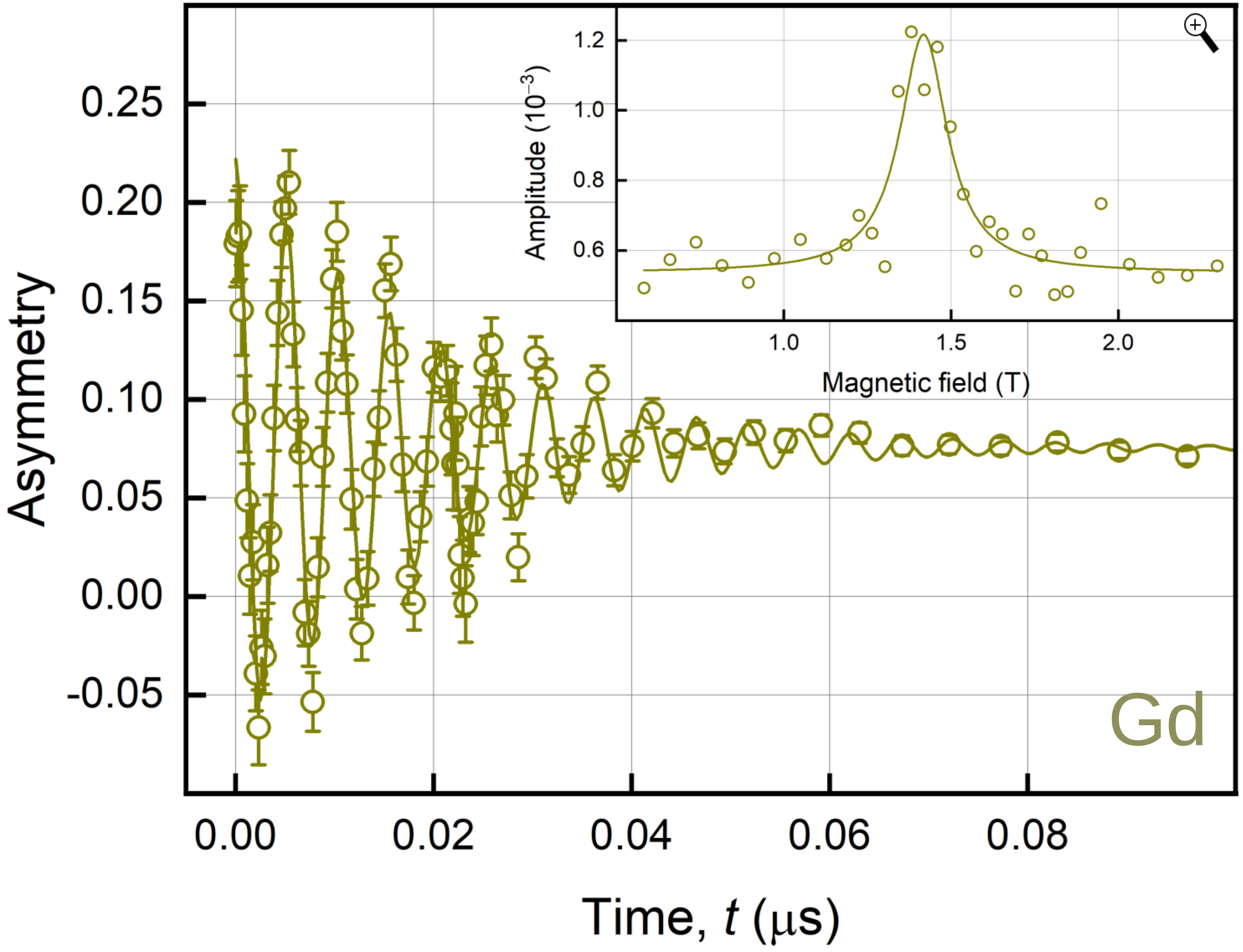
- Maximal magnetic field is 0.35 T



Zero field μSR

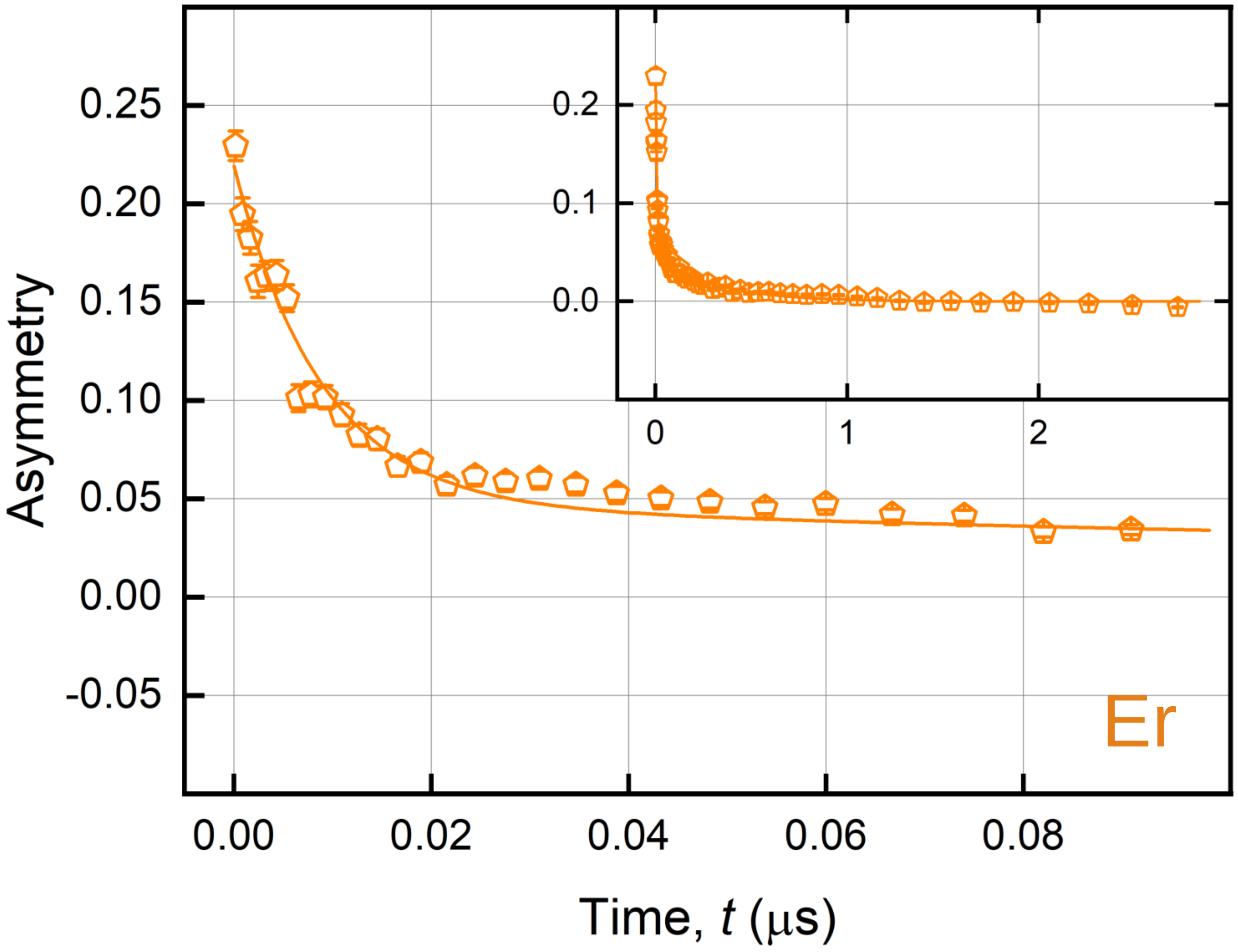
- Gd *i*-MAX shows a single frequency ⇒ FM or AFM configuration

- Maximal magnetic field is 1.4 T



Zero field μSR

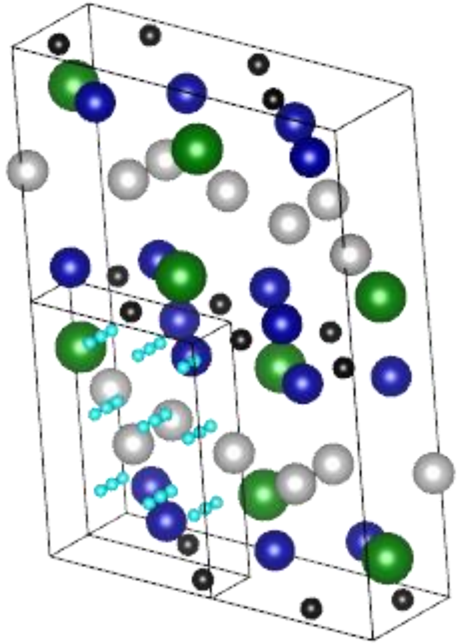
- Tb, Ho and Er *i*-MAX show a strong relaxation and decay to zero asymmetry
- Magnetic fluctuations relax the muons
- Possible connection with observed SRO in Ho and Er



Muon site determination

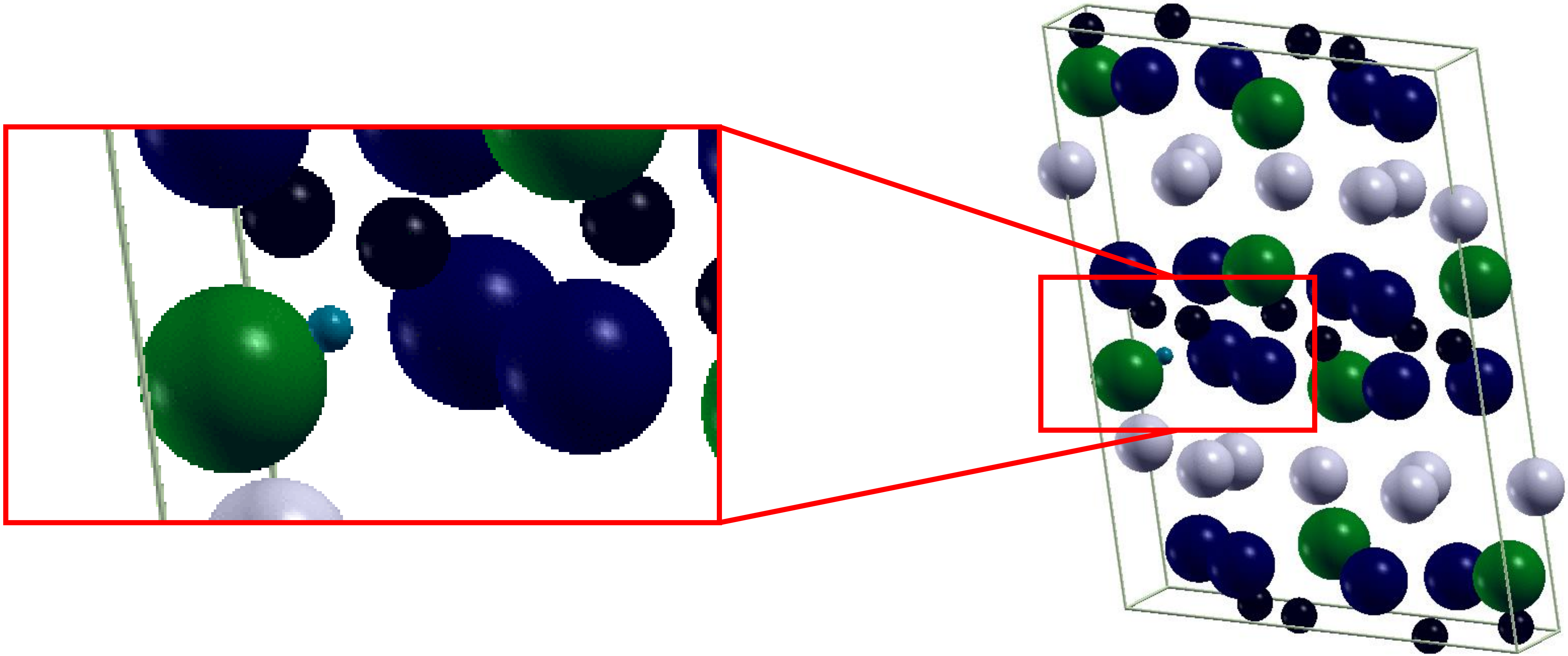
Muon site calculation - methodology

- Candidate muon sites are searched for using a structural-relaxation method [1] (calculated using density functional theory)
- Muons are approximated as hydrogen atoms and implanted in the unit cell (3 × 3 × 3 grid in the asymmetric unit)
- The unit cell is relaxed in the presence of the muon leading it to a candidate stopping site



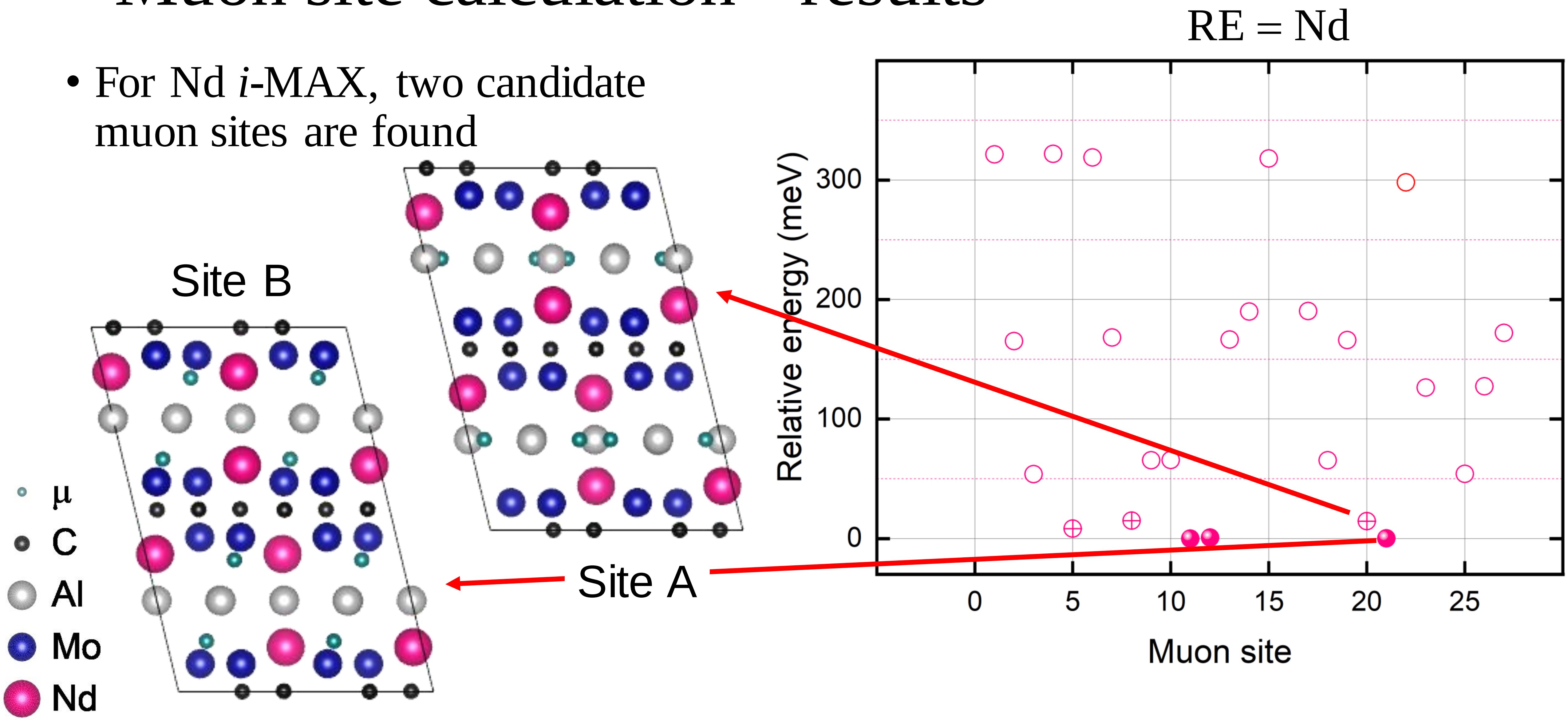
[1] P. Bonfa, F. Sartori and R. De Renzi, J. Phys. Chem. C **119**, 4278 (2015)

Example: Muon site relaxation



Muon site calculation - results

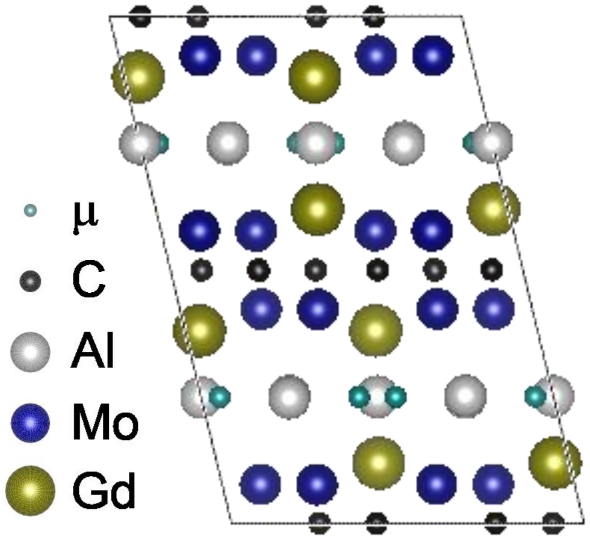
- For Nd *i*-MAX, two candidate muon sites are found



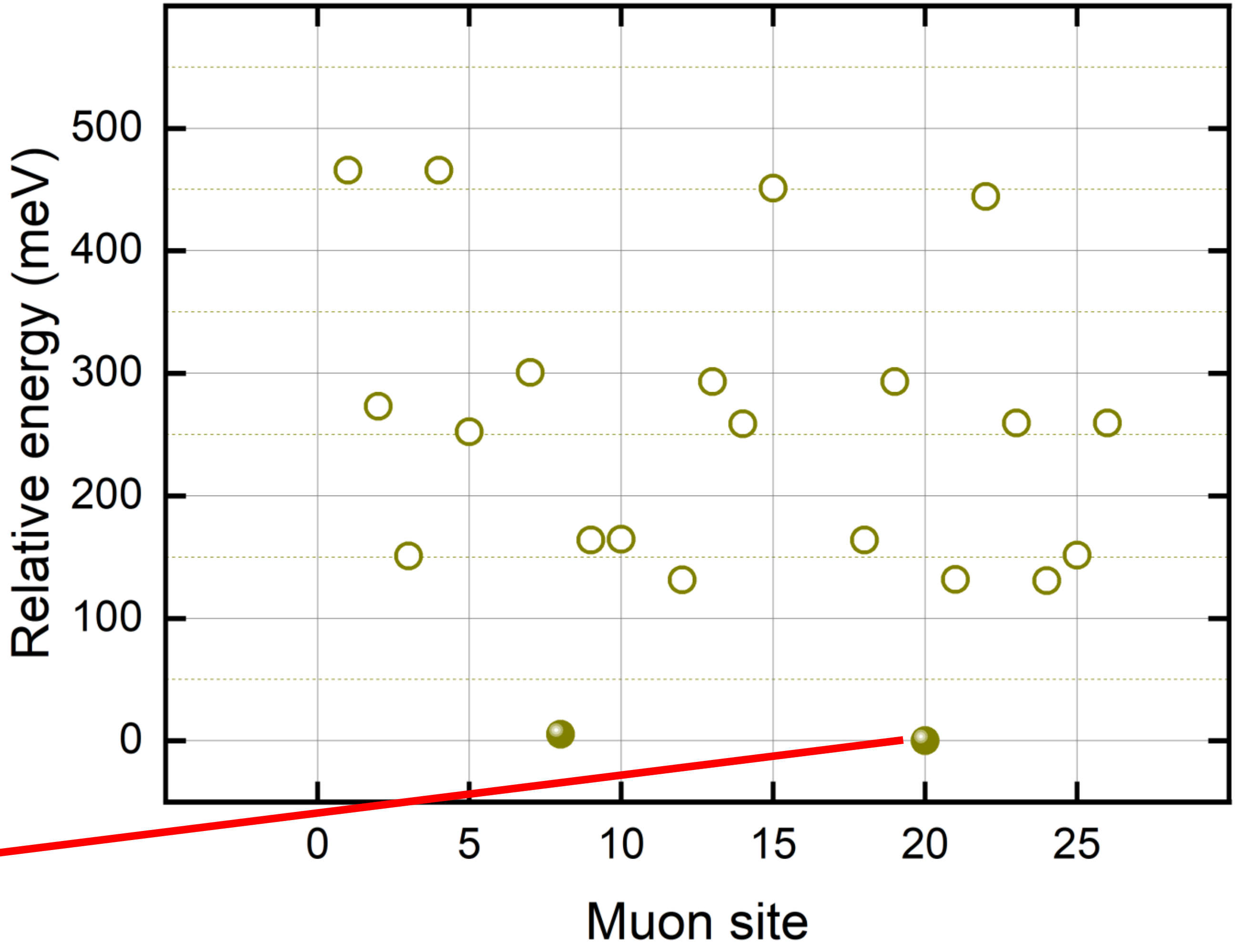
Muon site calculation - results

- For Nd *i*-MAX, two candidate muon sites are found

- For Gd *i*-MAX and heavier compounds, only site A has the lowest energy



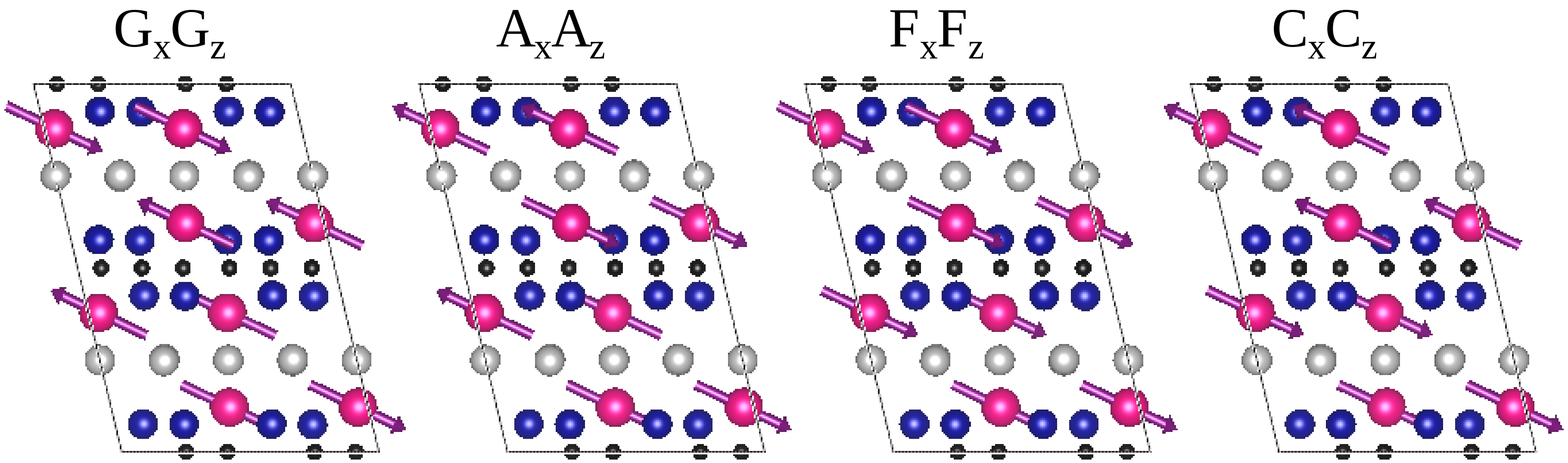
RE = Gd



Muon site calculation - verification

- To verify our muon site calculation, the magnetic structure of Nd *i*-MAX is predicted and compared with NPD results

- From symmetry analysis, four magnetic modes are compatible with the *i*-MAX symmetry



Muon site calculation - verification

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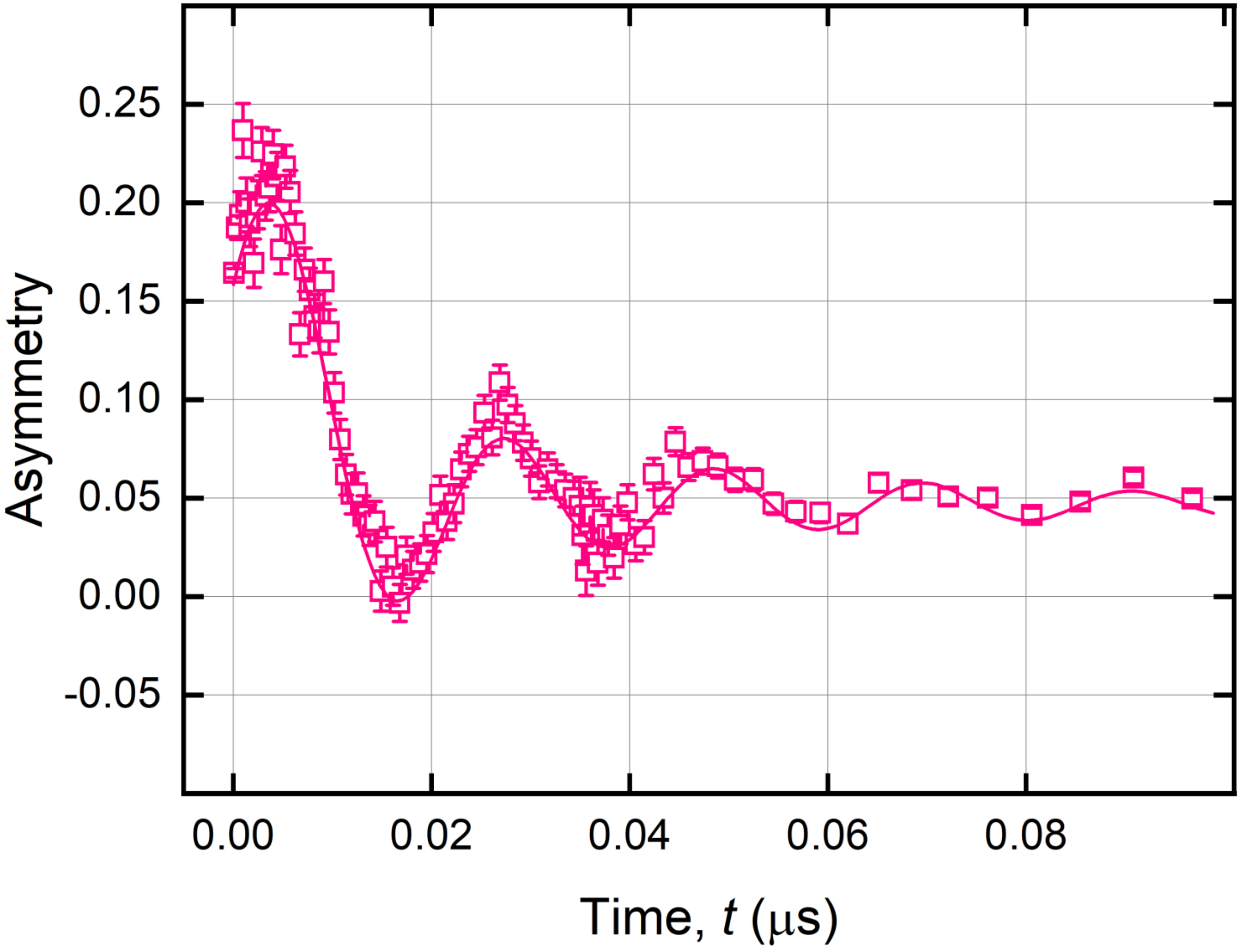

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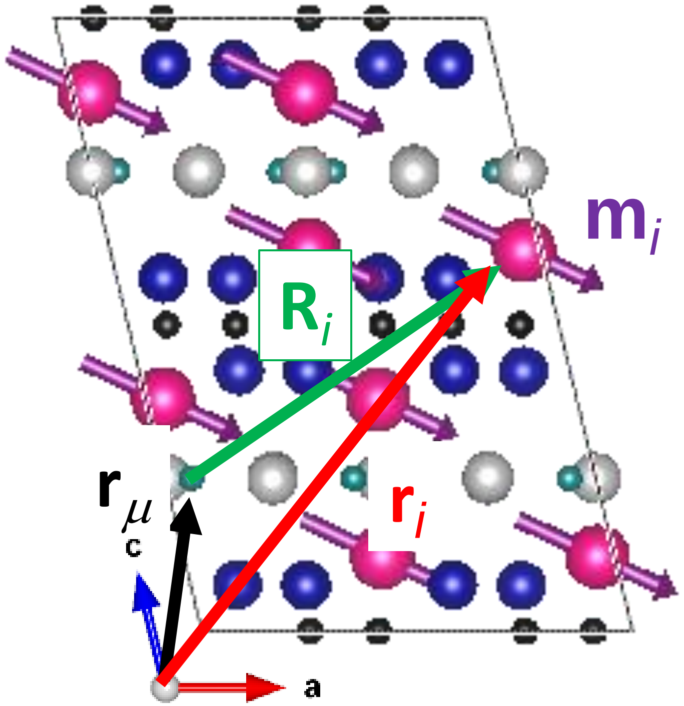
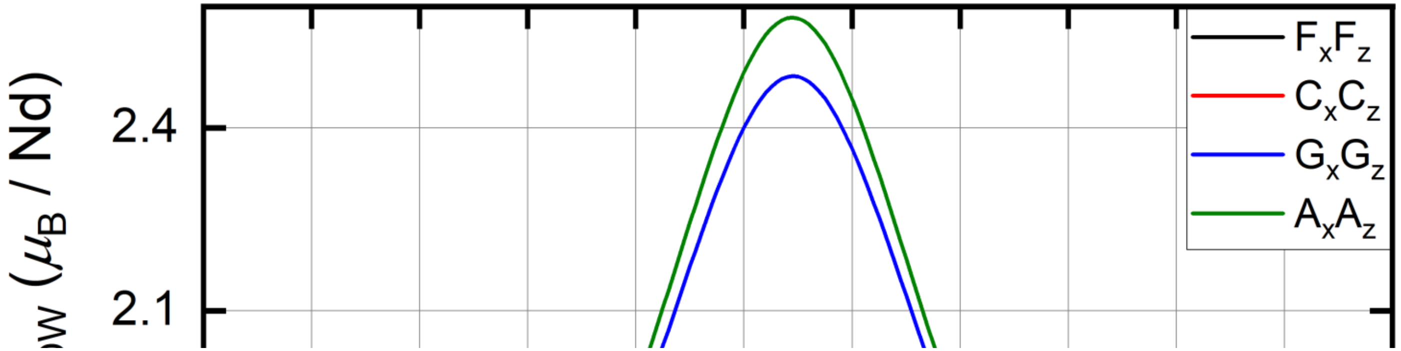
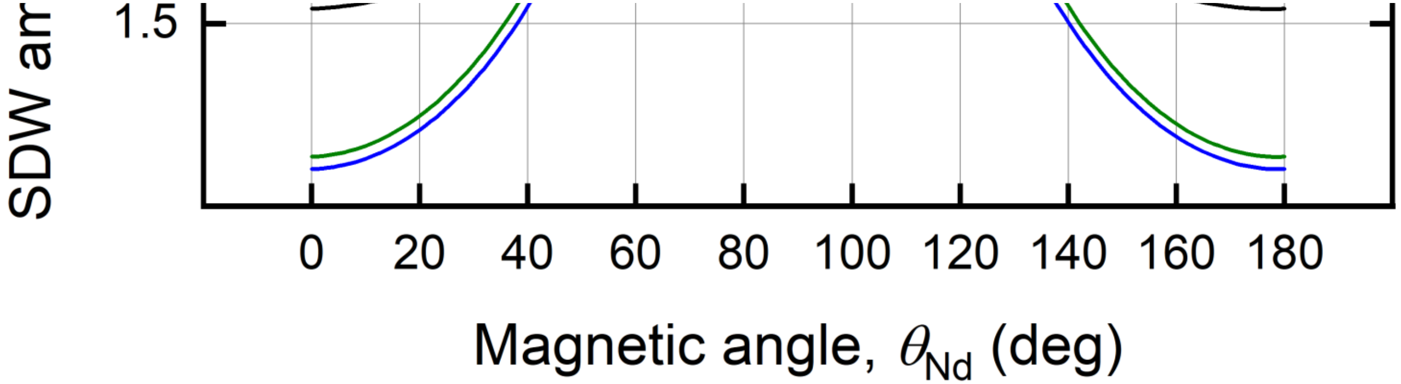


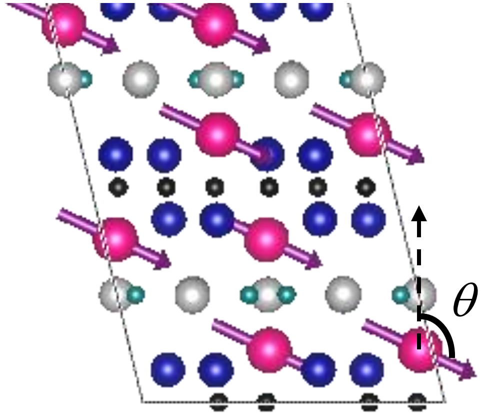
Muon site calculation – verification: site A



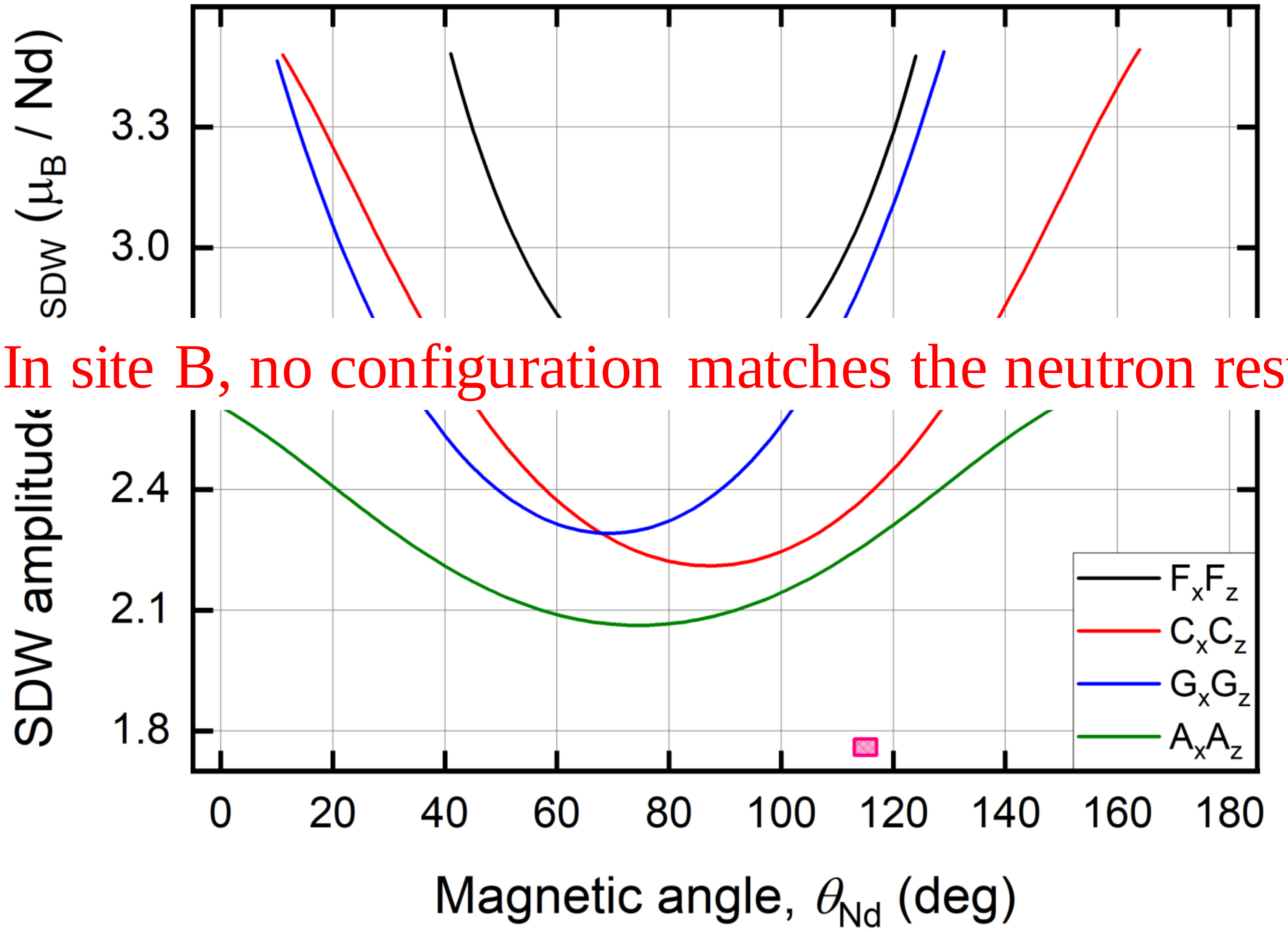
- In site A, the F_xF_z configuration is consistent with the neutron results

- It is also the configuration determined by NPD





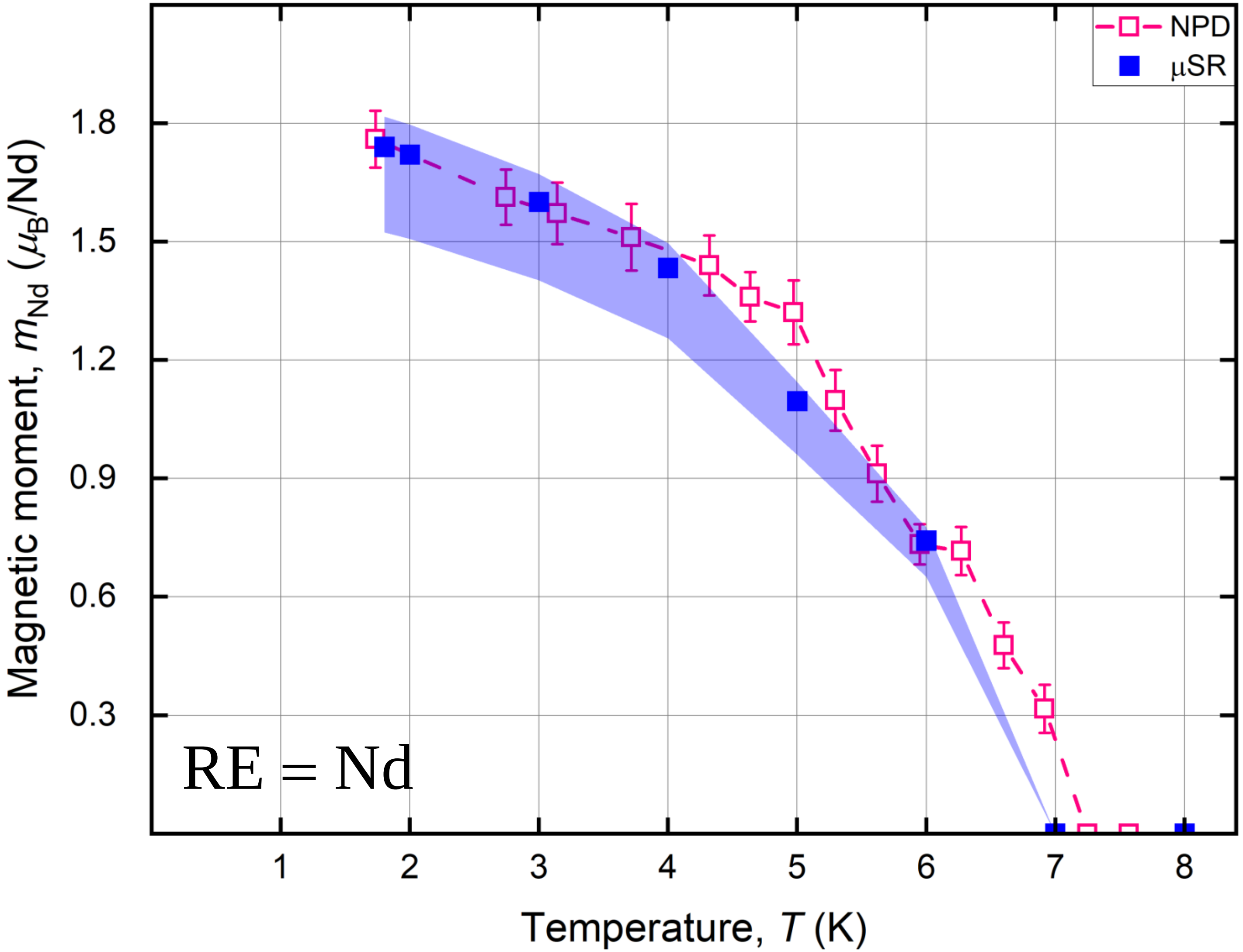
Muon site calculation – verification: site B



In site B, no configuration matches the neutron results

Muon site calculation – temperature evolution

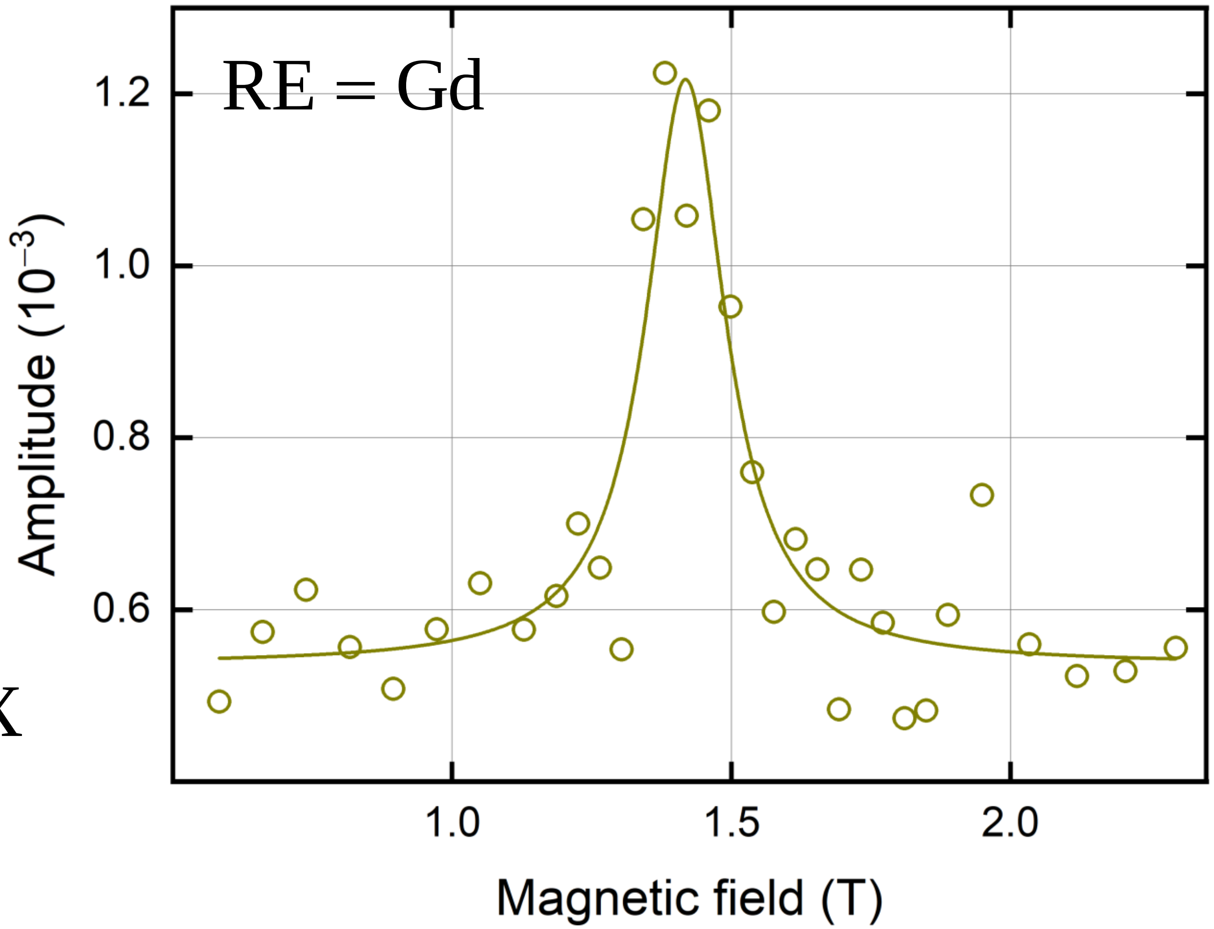
- Good agreement is observed between both techniques
- This validates our muon site and dipolar sum calculations
- The same method can now be applied to Gd *i*-MAX



Magnetic structure of Gd *i*-MAX

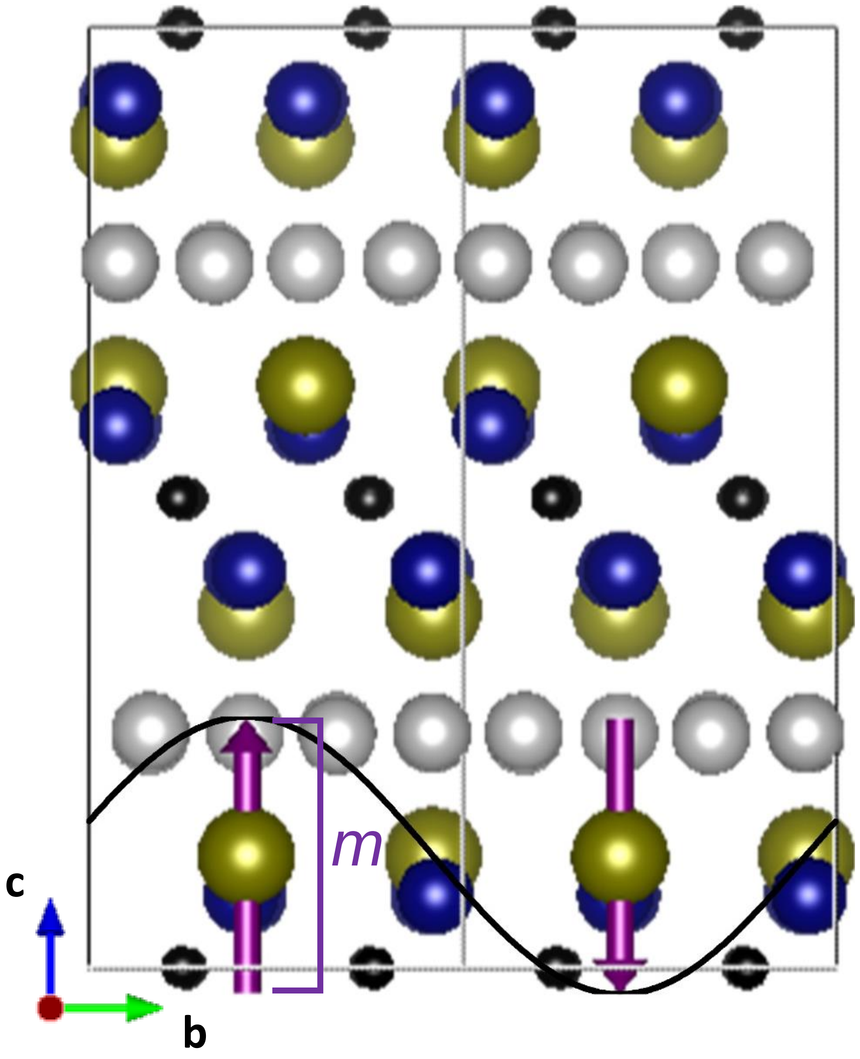
Determining the magnetic structure of Gd

- A single frequency in the field spectrum ⇒ simple FM or AFM (possible doubling of the unit cell)
- $\mathbf{k}_1$ in the Tb *i*-MAX is (0, 0.5, 0)
- Constrain search space to the four magnetic modes tested for Nd *i*-MAX



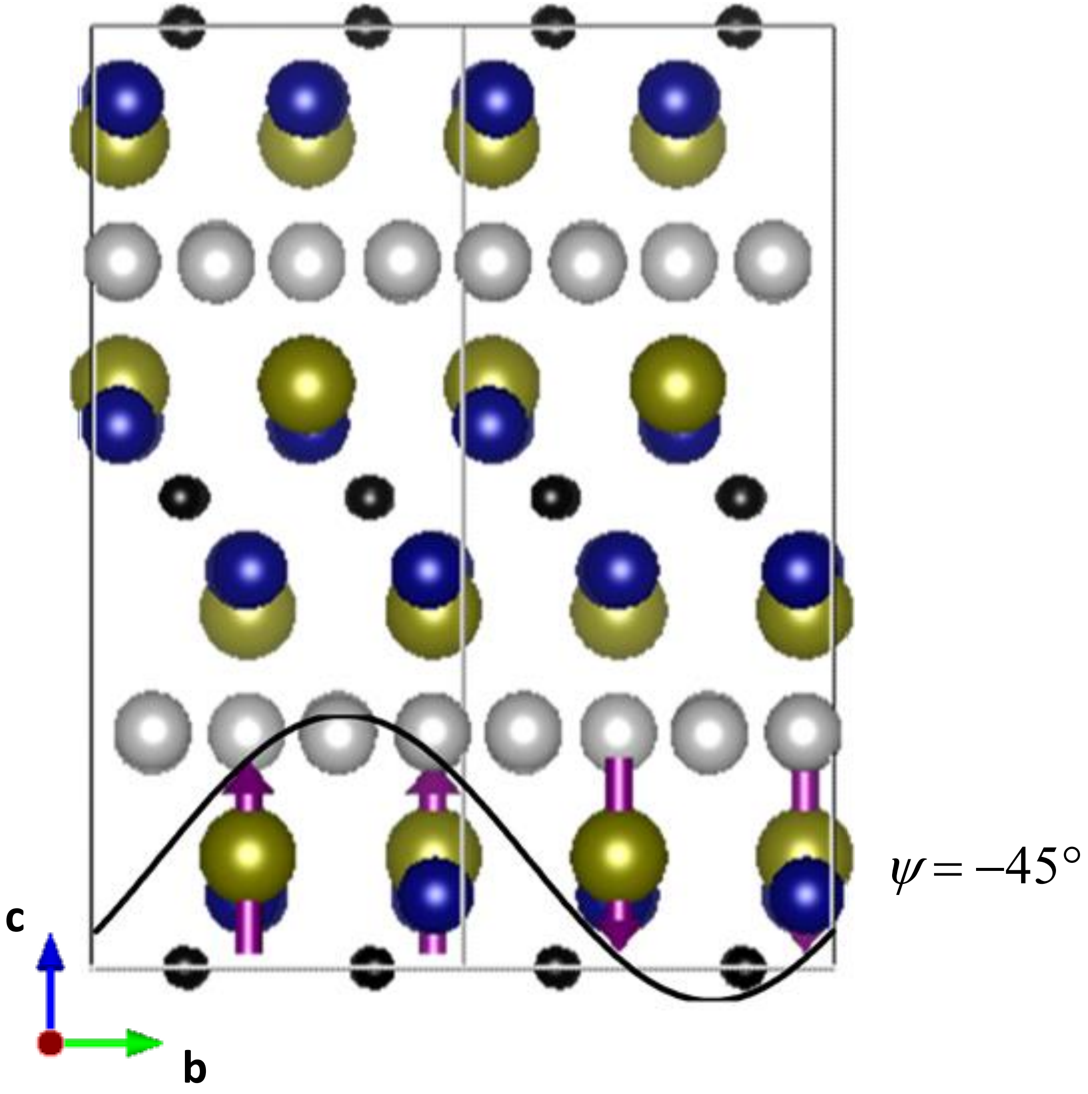
Parametrizing the magnetic structure of Gd

- For **k** = (0, 0.5, 0), the magnetic structure requires 3 parameters
- *m* – SDW amplitude



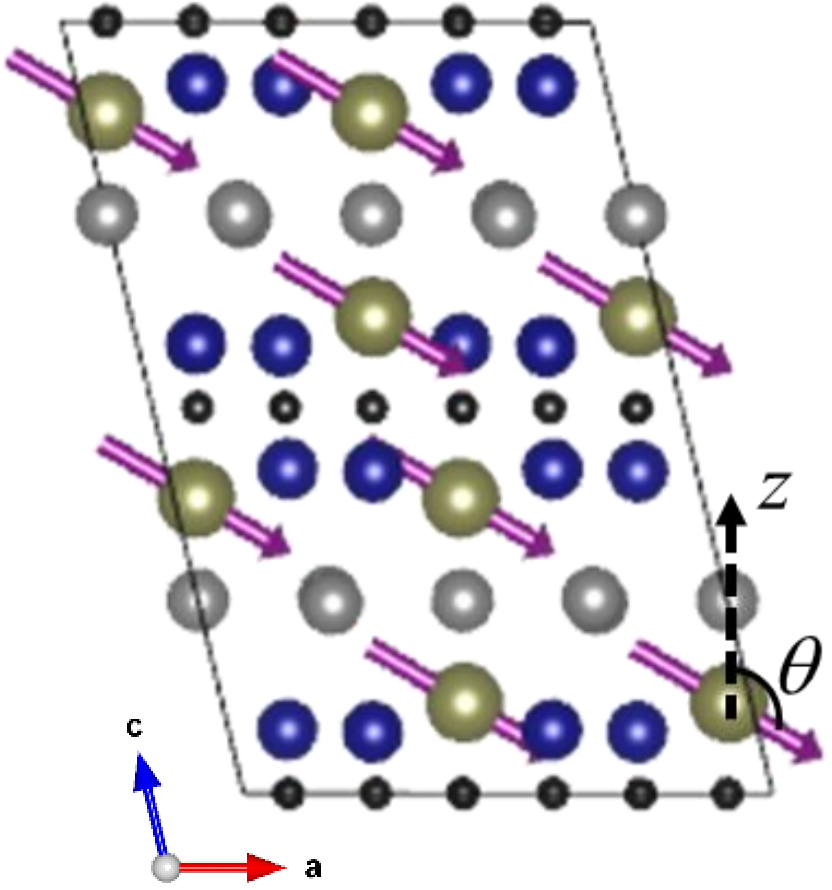
Parametrizing the magnetic structure of Gd

- For k = (0, 0.5, 0), the magnetic structure requires 3 parameters
- m – SDW amplitude
- ψ – magnetic phase



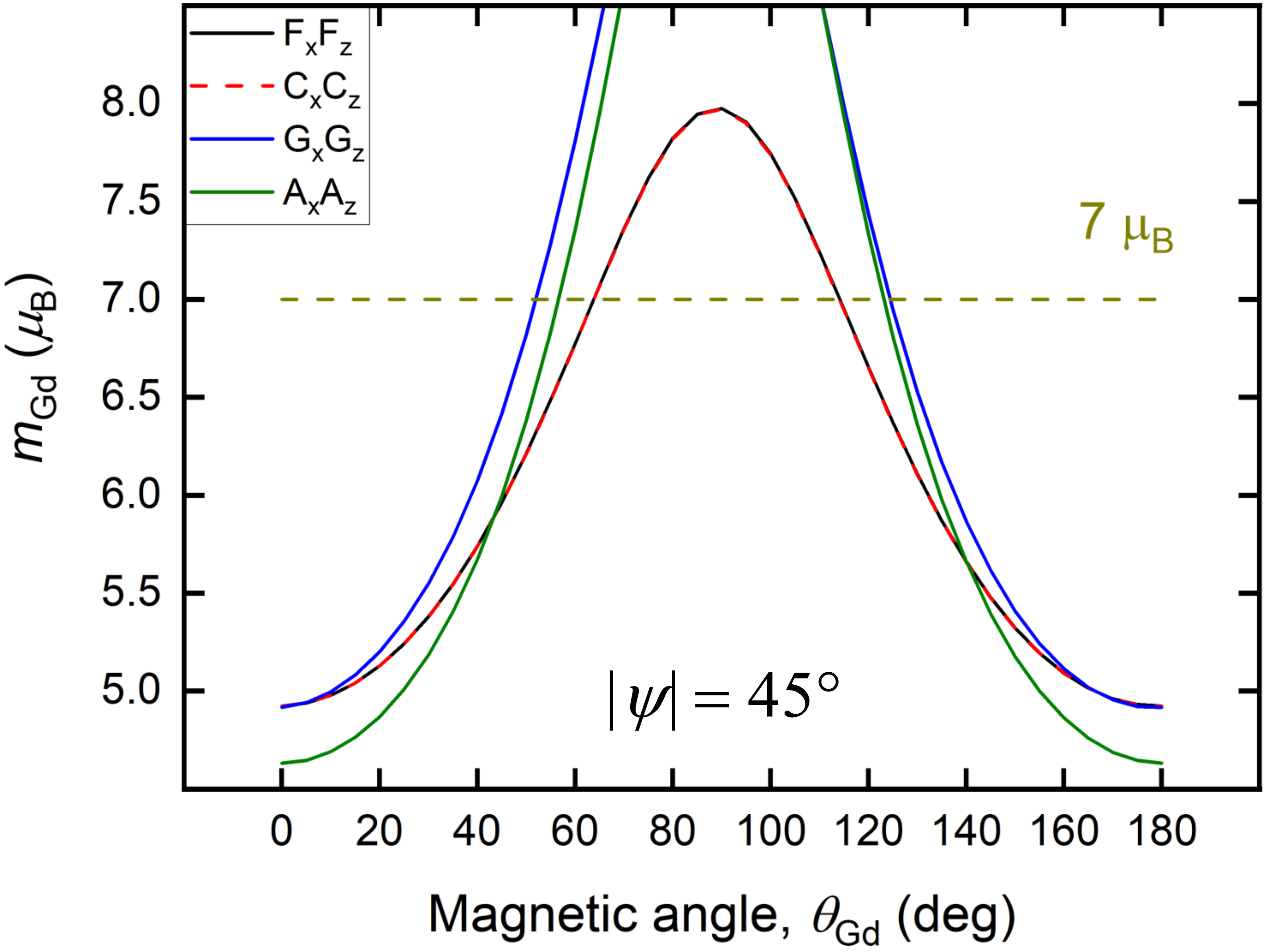
Parametrizing the magnetic structure of Gd

- For k = (0, 0.5, 0), the magnetic structure requires 3 parameters
- m – SDW amplitude
- ψ – magnetic phase
- θ – moment direction



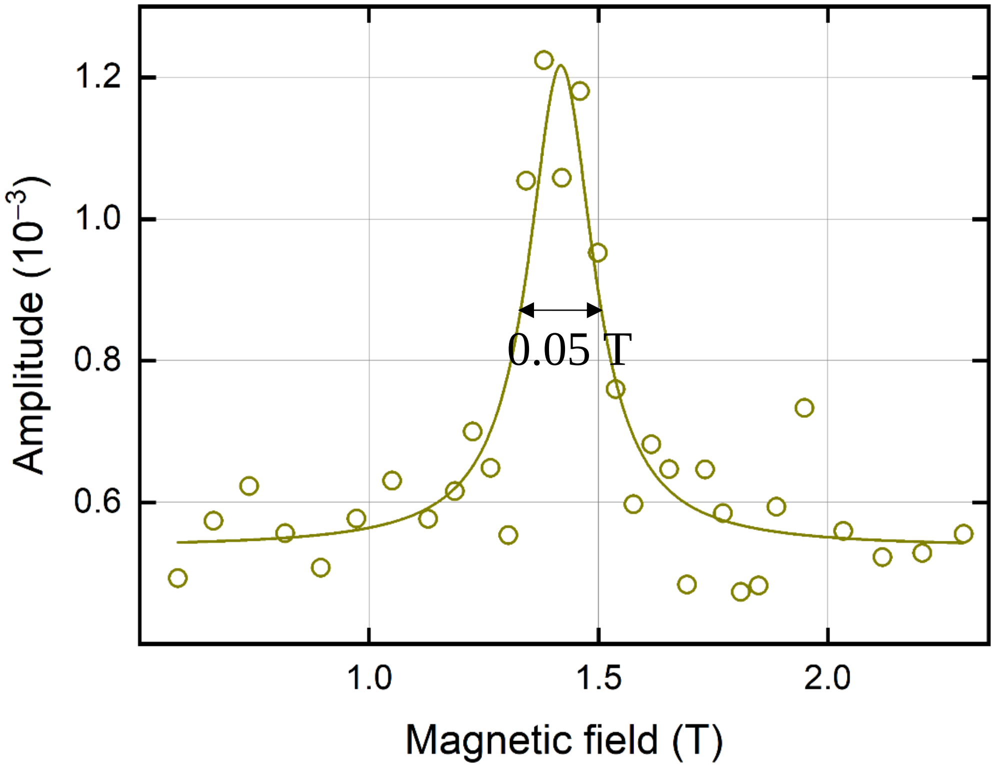
Magnetic structure determination of Gd *i*-MAX

- A scan over θ and ψ is performed with m calculated for each pair
- m is constrained to be less than 7 μ_B – the free ion moment of Gd^{3+}

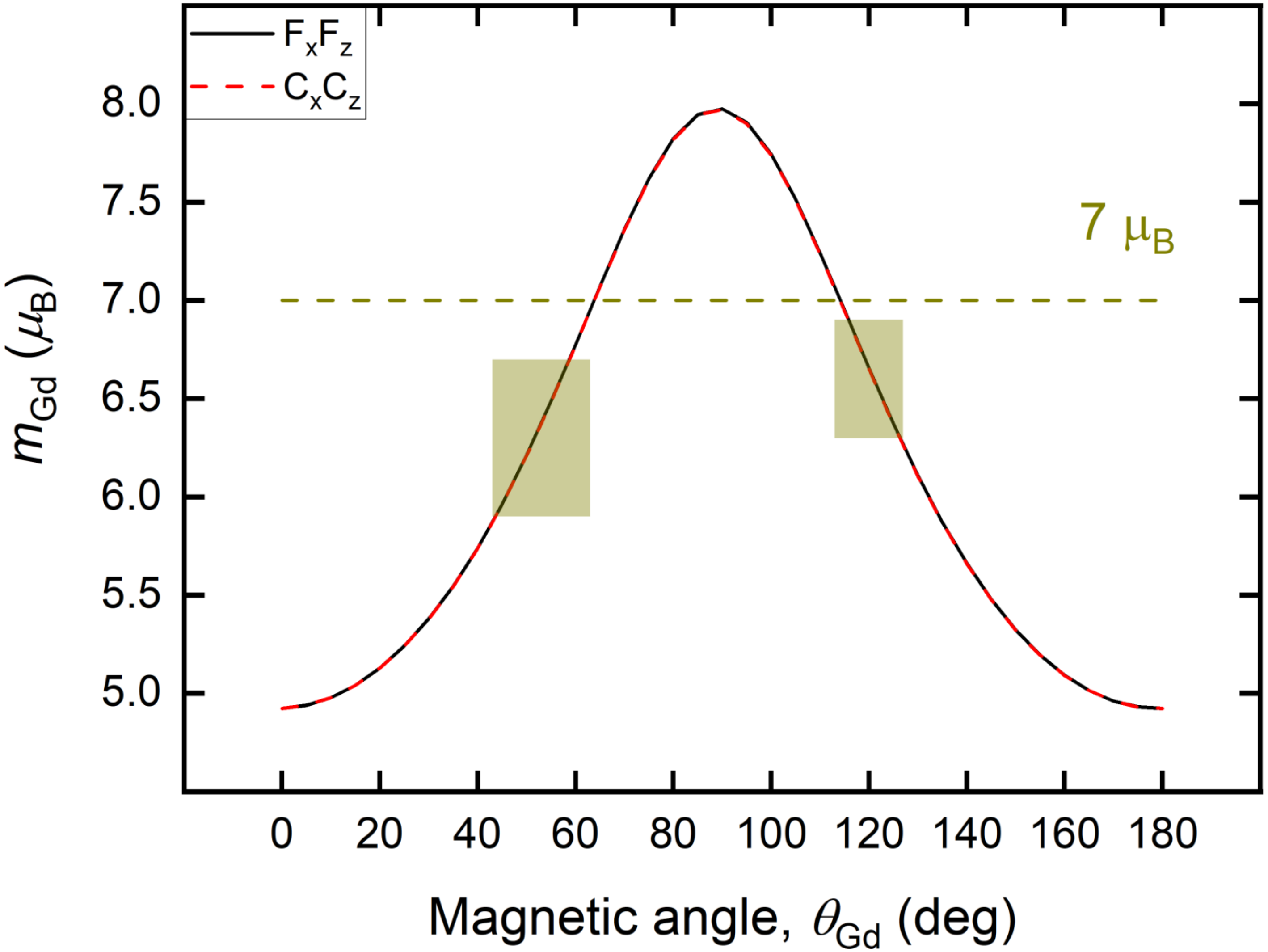


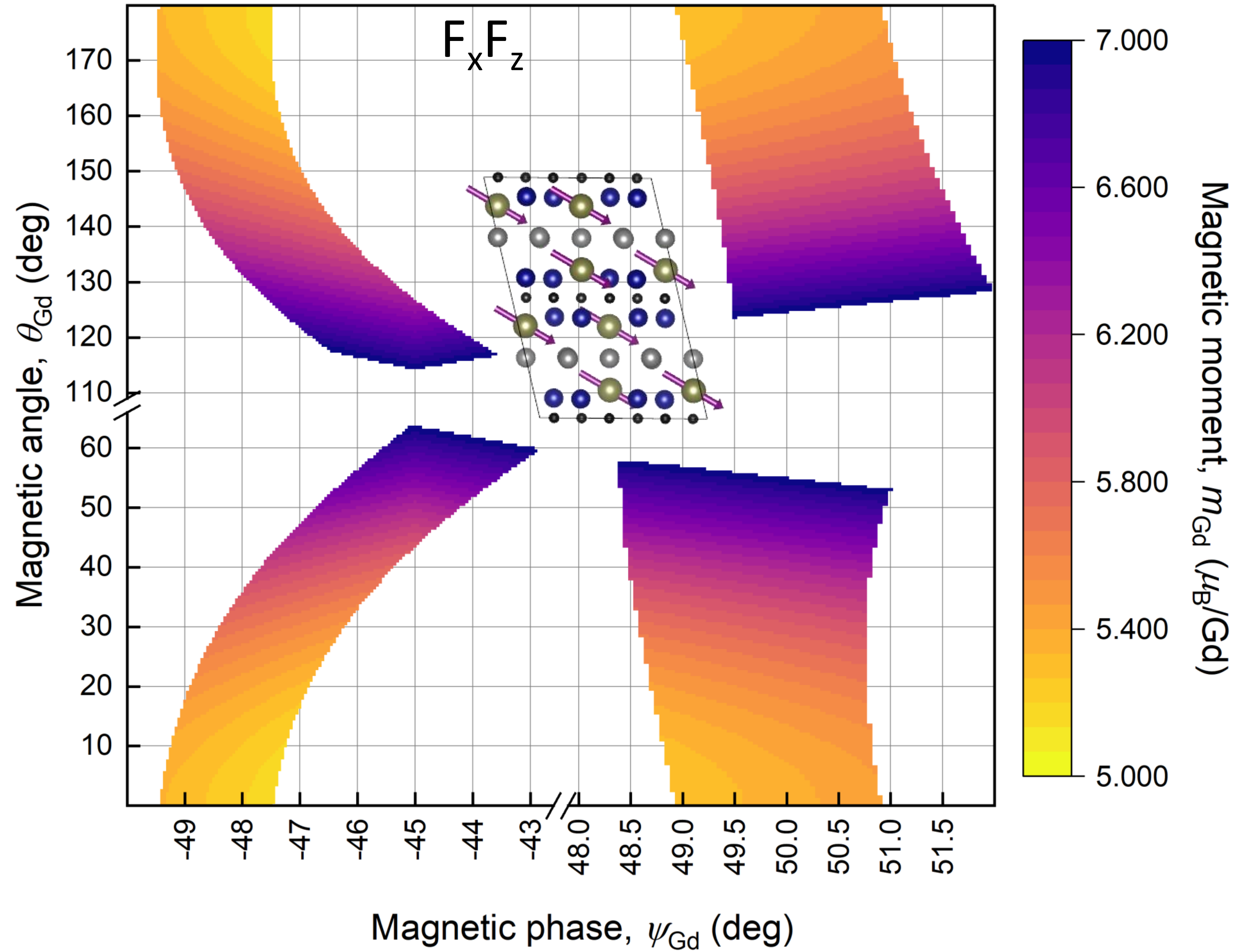
Magnetic structure determination of Gd *i*-MAX

- The field homogeneity is

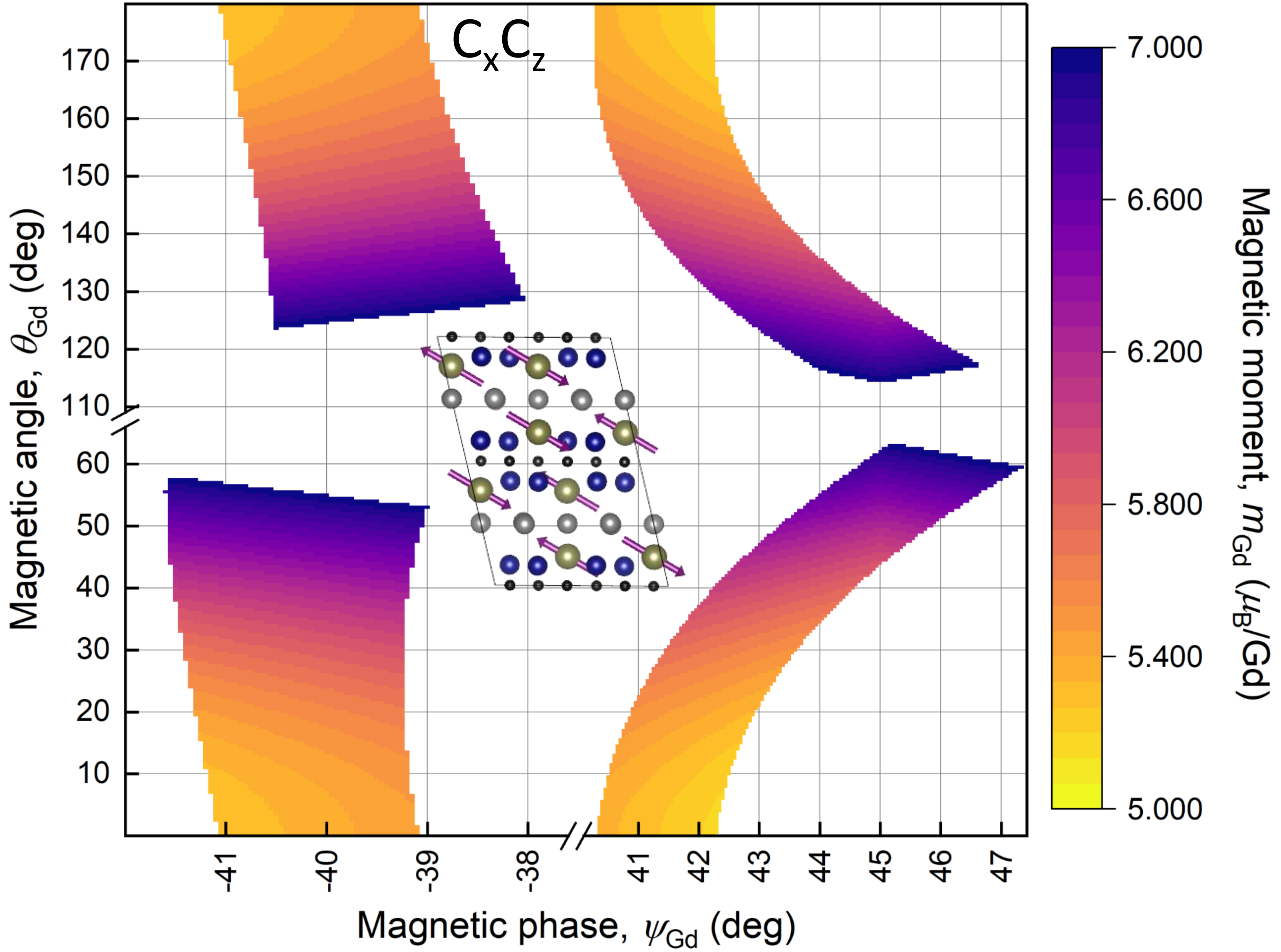


- This, in turn gives constraints on m_{Gd}





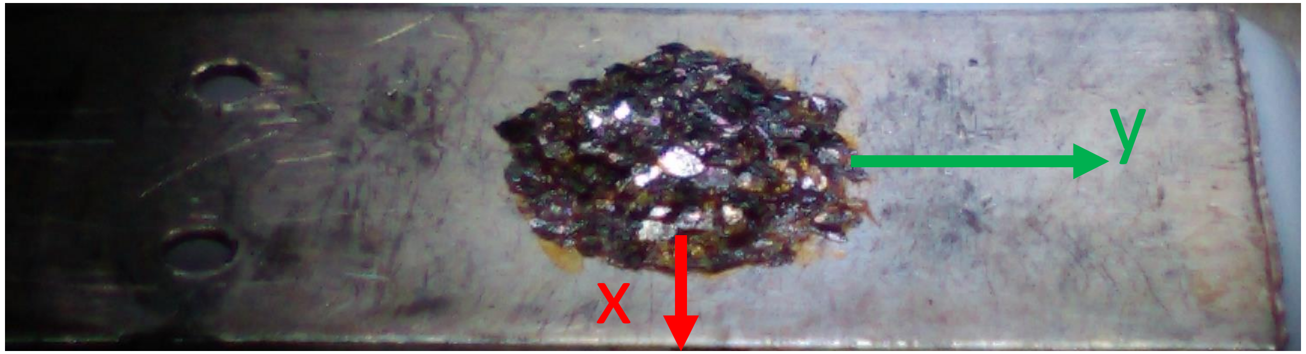
F_xF_z
Magnetic angle, θ_{Gd} (deg)
170
160
150
140
130
120
110
60
50
40
30
20
10
-49
-48
-47
-46
-45
-44
-43
48.0
48.5
49.0
49.5
50.0
50.5
51.0
51.5
Magnetic phase, ψ_{Gd} (deg)
7.000
6.600
6.200
5.800
5.400
5.000
Magnetic moment, m_{Gd} (μ_B/Gd)

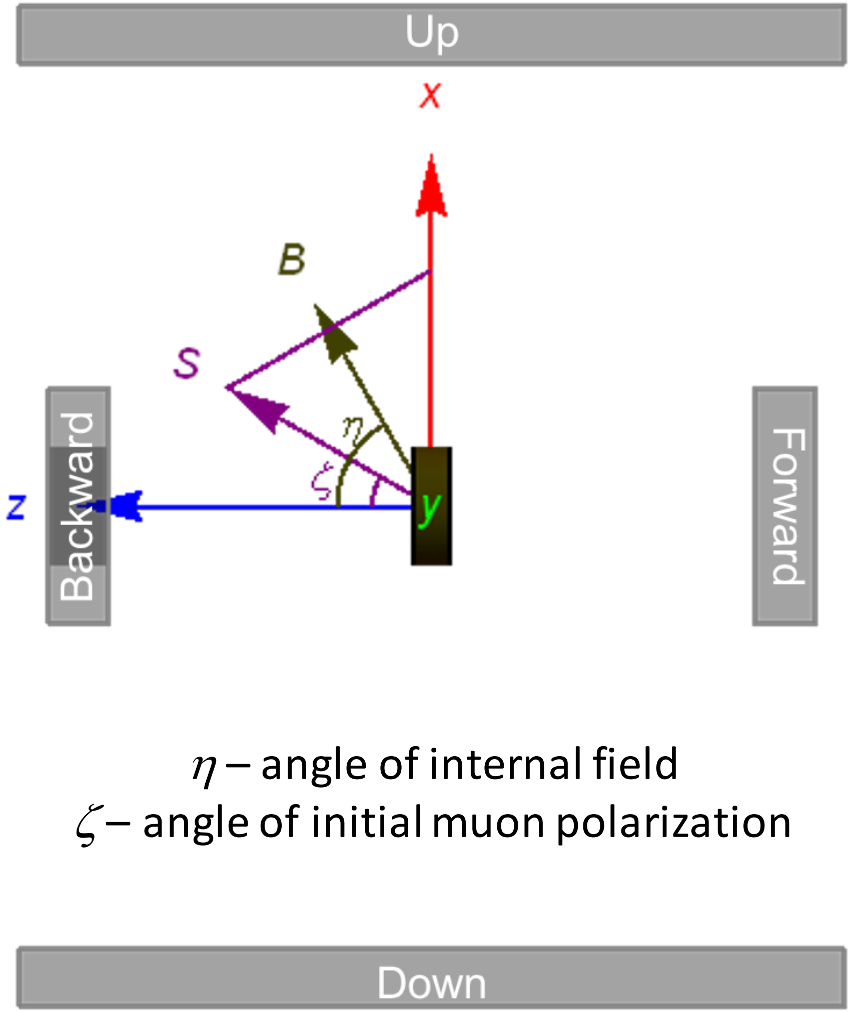


C_xC_z
Magnetic angle, θ_{Gd} (deg)
170
160
150
140
130
120
110
60
50
40
30
20
10
-41
-40
-39
-38
41
42
43
44
45
46
47
Magnetic phase, ψ_{Gd} (deg)
7.000
6.600
6.200
5.800
5.400
5.000
Magnetic moment, m_{Gd} (μ_B/Gd)

Single crystal measurements of Gd *i*-MAX

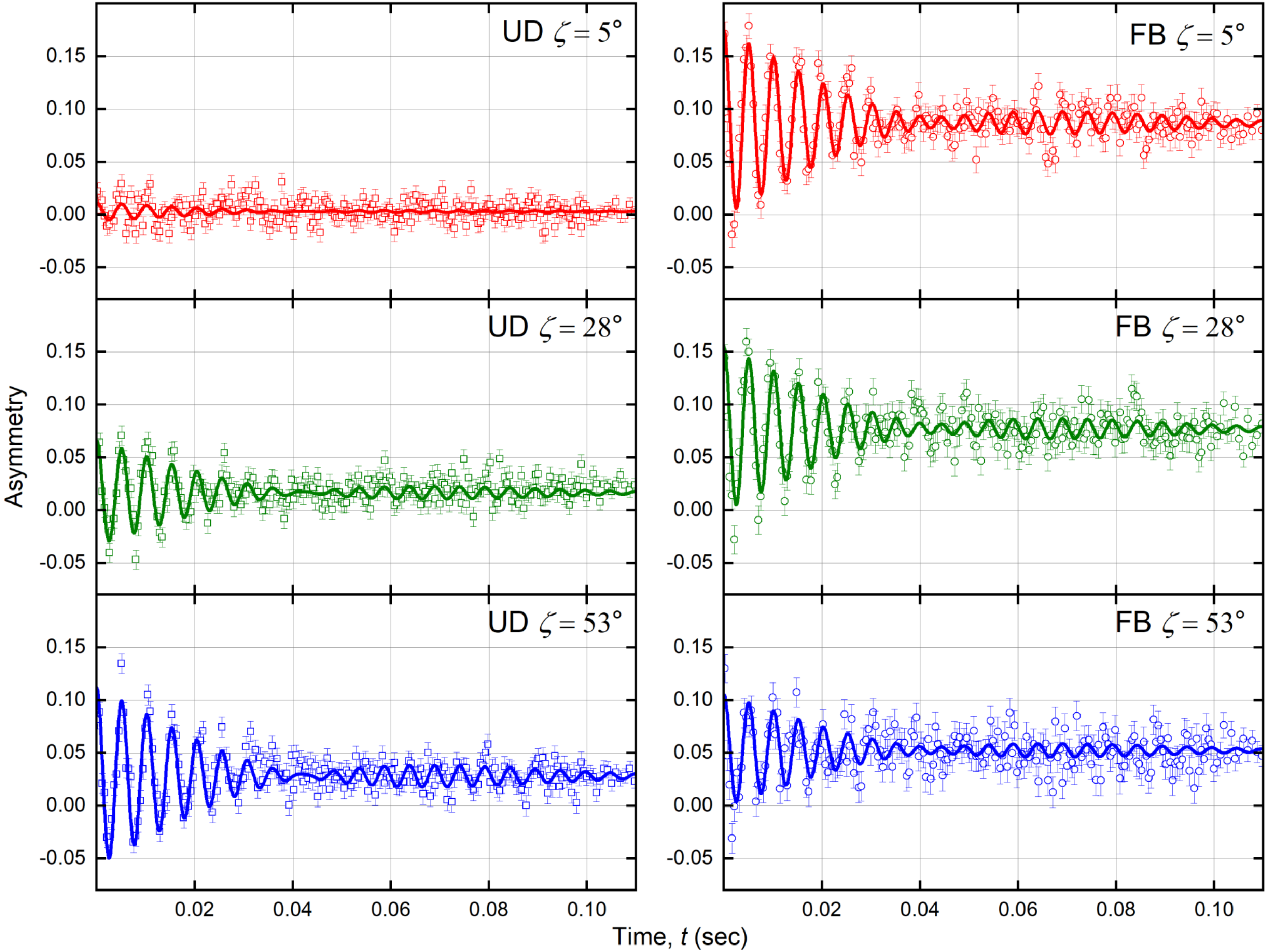
- As single crystals of Gd *i*-MAX became available, it became possible to add more constraints
- The crystals were oriented along the c^* axis but not oriented in the *a*-*b* plane
- Measurements at different polarization angles ζ allow to determine the direction of B





η – angle of internal field

ζ – angle of initial muon polarization



UD ζ = 5°
FB ζ = 5°
UD ζ = 28°
FB ζ = 28°
UD ζ = 53°
FB ζ = 53°
Asymmetry
Time, t (sec)
0.15
0.10
0.05
0.00
-0.05
0.02
0.04
0.06
0.08
0.10

Gd *i*-MAX single crystal analysis

- The asymmetry can be simultaneously fitted using the model

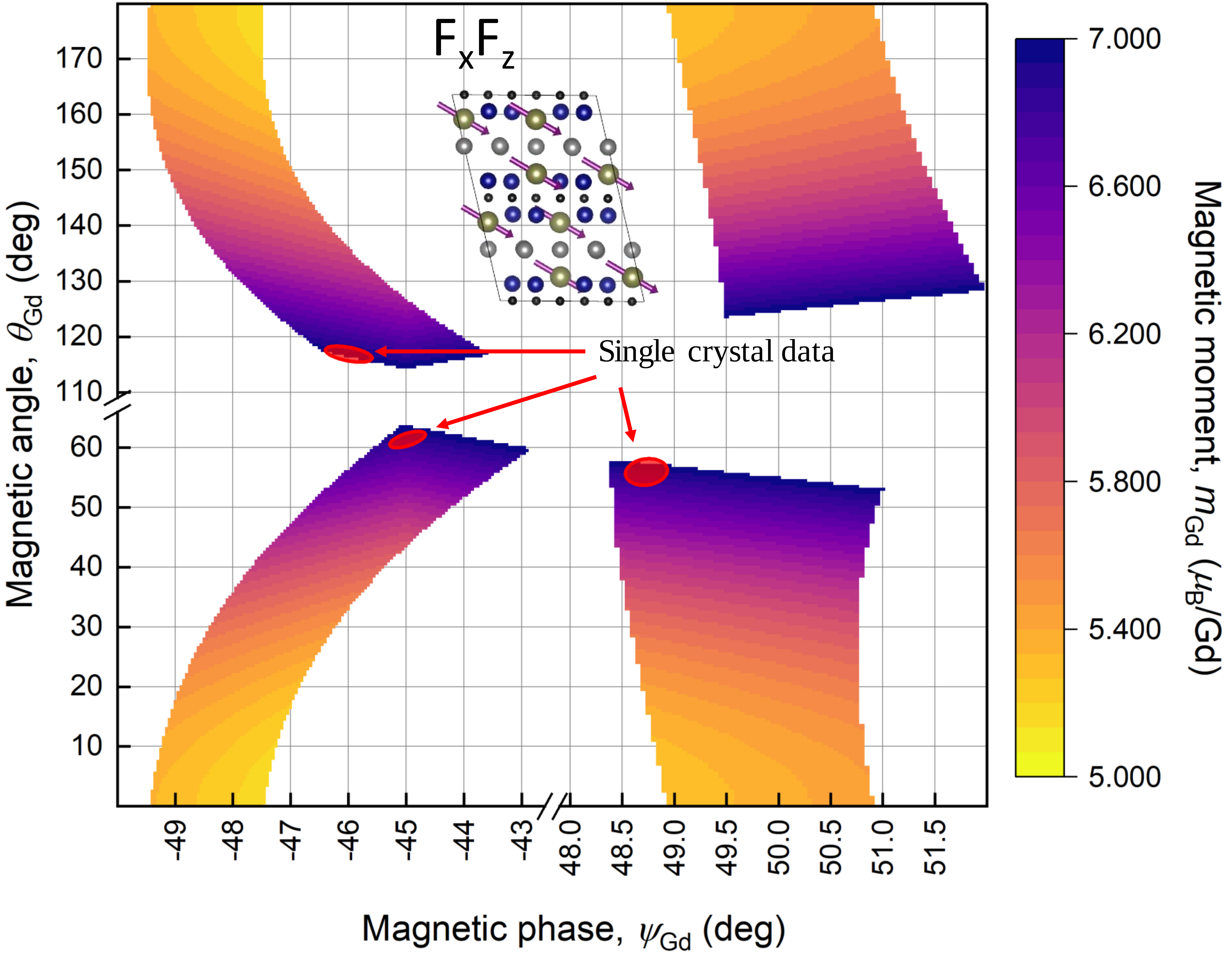
$$S_{\mathrm{UD}}(t) = \tfrac{1}{4} A_{\mathrm{UD}} \boxed{\sin\zeta}\left[e^{-\lambda_F t}\cos(\gamma B t)\boxed{(3+\cos 2\eta)} + 2e^{-\lambda_S t}\boxed{\sin^2\eta}\right]$$

$$S_{\mathrm{FB}}(t) = A_{\mathrm{FB}} \boxed{\cos\zeta}\left[e^{-\lambda_F t}\cos(\gamma B t)\boxed{\sin^2\eta} + e^{-\lambda_S t}\boxed{\cos^2\eta}\right]$$

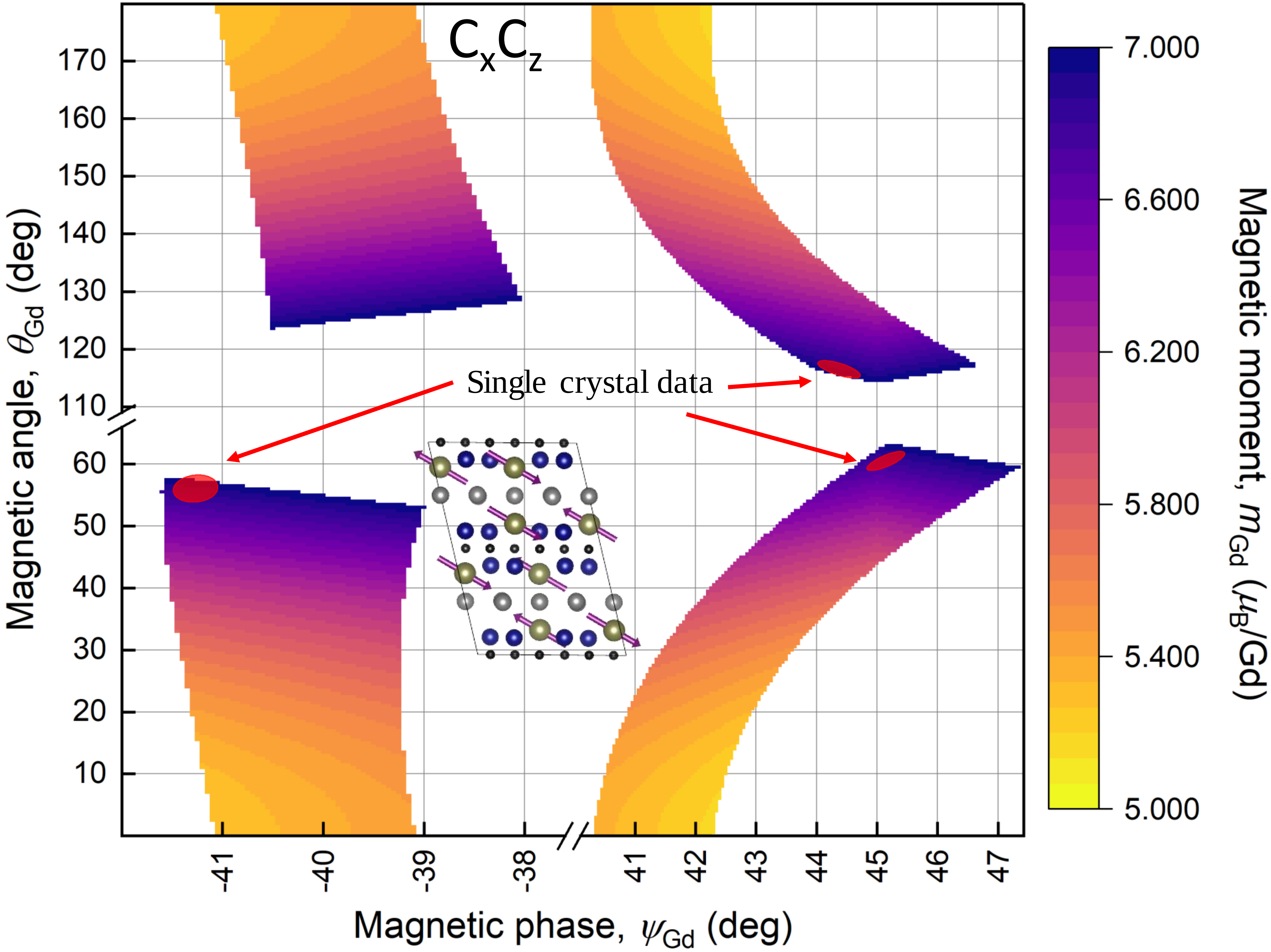
Initial muon polarization

Projection along the field direction

- By calculating B and η from (m_{Gd}, θ_{Gd}, ψ_{Gd}) then fitting S_{UD} and S_{FB} to the observed asymmetry for all angles ζ, the magnetic structure can be determined



F_xF_z
Single crystal data
Magnetic angle, θ_{Gd} (deg)
Magnetic phase, ψ_{Gd} (deg)
Magnetic moment, m_{Gd} (μ_B/Gd)
7.000
6.600
6.200
5.800
5.400
5.000


C_xC_z
Single crystal data
Magnetic angle, θ_{Gd} (deg)
170
160
150
140
130
120
110
60
50
40
30
20
10
-41
-40
-39
-38
41
42
43
44
45
46
47
Magnetic phase, ψ_{Gd} (deg)
7.000
6.600
6.200
5.800
5.400
5.000
Magnetic moment, m_{Gd} (μ_B/Gd)

Temperature evolution and modelling

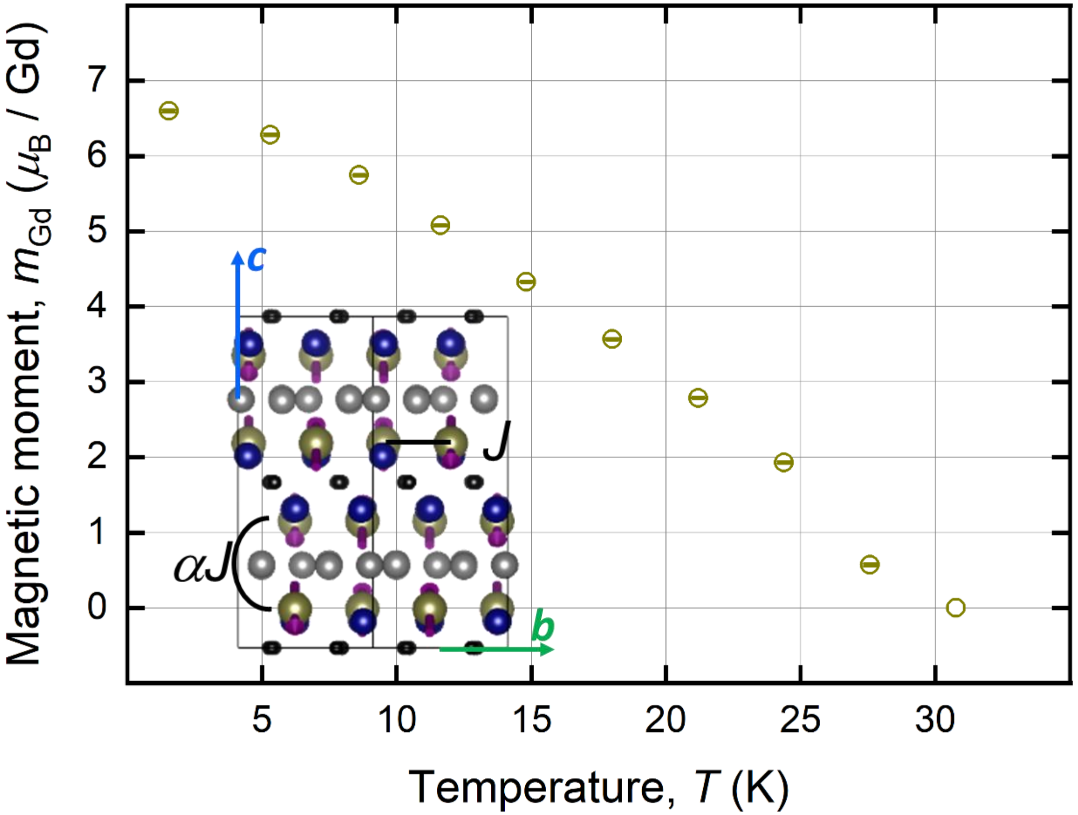
- The magnetic moment of the Gd *i*-MAX shows a gradual second order-like transition

- Motivated by the non-zero slope near $T = 0$, the data was fitted using a model [1] of an anisotropic layered antiferromagnet

SBMFT

$$H = J\left(\sum_{i,\delta_\parallel} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta_\parallel} + \alpha \sum_{i,\delta_\perp} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta_\perp}\right)$$

- The thermodynamic properties of this Hamiltonian are calculated using Schwinger boson mean field theory (SBMFT)

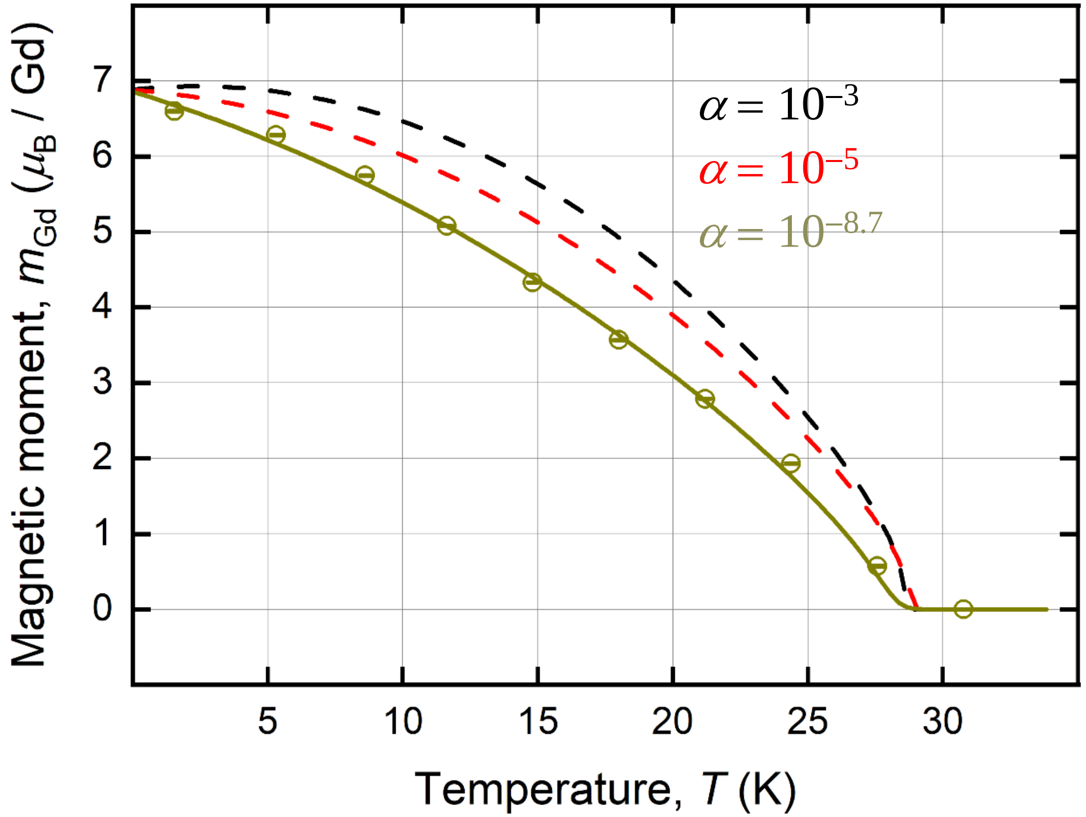


J – Exchange interaction, $\delta_\parallel$ - In plane nearest neighbors, $\delta_\perp$ - Out of plane nearest neighbors
α – Anisotropy, $\mathbf{S}$ – Spin opeartor

[1] Keimer et al. Phys. Rev. B **45**, 13 (1992)

Temperature evolution and modelling

- The observed data is well described using the SBMFT calculation which gives almost the full free ion moment of Gd^{3+} (7 m_B) and a high Néel temperature of 29 K.



- The smallness of α confirms the strong anisotropy and nearly 2D nature of the Gd *i*-MAX

Conclusions

- The magnetic structure of the Gd *i*-MAX was solved using a combination of NPD on isostructural compounds with μSR, AD-μSR, symmetry analysis and muon site determination

- The Gd *i*-MAX is a nearly 2D magnet with a high magnetic moment of 7 μ_B, T_N of 29 K and a magnetic structure which shows long time stability (at least order of μs) and is ideal as parent compound for 2D sheets

Thank you

Special thanks to our collaborators:

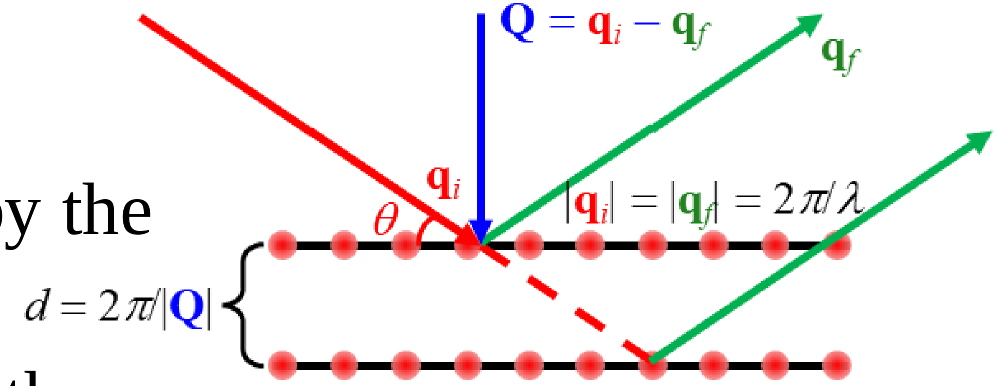
E. N. Caspi and A. Pesach – Physics department, NRCN
H. Shaked – Physics department, Ben Gurion University Negev
Quanzheng Tao, Johanna Rosen – Linköping University, Sweden
C. Ritter – Institut Laue Langevin, France
H. Evans – National Institute for Standards and Technology, USA
D. Sheptyakov, Z. Salman – Paul Scherrer Institut, Switzerland
P. Bonfá – University of Parma, Italy
T. Ouisse, M. Barbier – University of Grenoble, France

Appendix

A. Neutron scattering theory

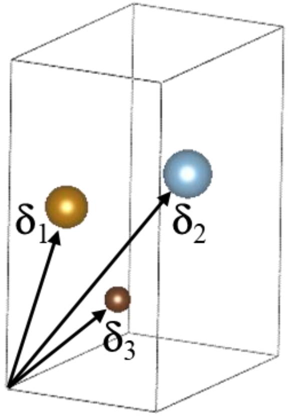
Neutron scattering - theory

- Neutron scattering by crystals occurs when the Bragg condition is met
  $\lambda = 2d \sin\theta$



- The position of Bragg peaks is determined by the crystal lattice type
- The intensity of the peaks is proportional to the square of the structure factor

$$F(\mathbf{Q}) = \sum_j b_j e^{i\mathbf{Q}\cdot\boldsymbol{\delta}_j}$$



$\mathbf{q}_i$ – Initial neutron momentum
$\mathbf{q}_i$ – Final neutron momentum
$\mathbf{Q}$ – Momentum transfer
λ – Neutron wavelength
θ – Bragg angle
d – Crystal plane spacing

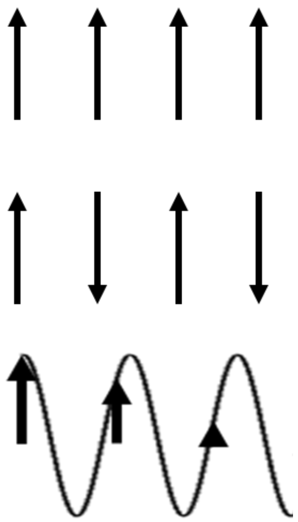
Magnetic neutron scattering

- Since the neutron has spin ½, it can interact with the magnetic field present in magnetic materials.

- It is useful to describe a general magnetic structure in a crystal using propagation vectors $\mathbf{k}_j$: $\mathbf{m}_i = \sum_j \mathbf{m}(\mathbf{k}_j) e^{-i\mathbf{k}_j \cdot \mathbf{r}_i}$

- In this case, magnetic reflections will appear at scattering vectors $\mathbf{Q} \pm \mathbf{k}_j$ with a magnetic structure factor

$$\mathbf{F}_m(\mathbf{Q} \pm \mathbf{k}_n) = \sum_j f_j(\mathbf{Q} \pm \mathbf{k}_n) \mathbf{m}_j(\mathbf{k}_n) e^{i(\mathbf{Q} \pm \mathbf{k}_n) \cdot \boldsymbol{\delta}_j}$$



k = 0

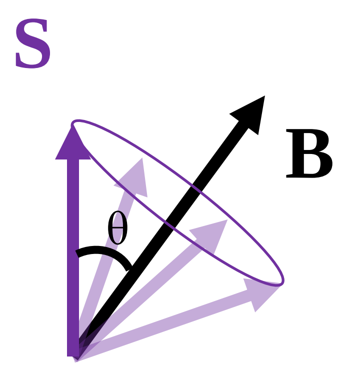
k = 0.5

k ∉ [illegible]

f – Magnetic form factor **m** – Magnetic moment **Q** – Momentum transfer of crystallographic reflection

B. Muon spin rotation theory

μSR theoretical background



- Muon spin in a magnetic field performs Larmor precession

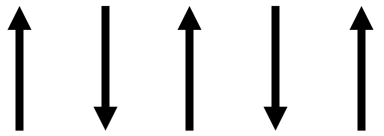
$$\mathbf{S}(t)=\cos\theta\,\hat{\mathbf{B}}_{\mathrm{P}}+\sin\theta\left[\cos(\gamma Bt)\,\hat{\mathbf{B}}_{\perp,1}+\sin(\gamma Bt)\,\hat{\mathbf{B}}_{\perp,2}\right]$$

- Implanting muons in the sample gives an average over all magnetic fields

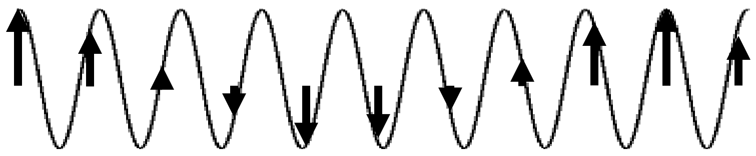
$$P(t)=\int(\mathbf{S}(t)\cdot\hat{\mathbf{z}})\,\rho(\mathbf{B})\,d^3\mathbf{B}=\frac{1}{3}+\frac{2}{3}\int\cos(\gamma Bt)\,\rho(B)\,B^2\,dB$$

Powder

- Different types of magnetic order can give different types of μSR signal



$$\Rightarrow\begin{cases}\rho(B)=\delta(B-B_0)\\ P(t)=\cos(\gamma B_0 t)\end{cases}$$



$$\Rightarrow\begin{cases}\rho(B)=\dfrac{4}{\pi\sqrt{B_0^2-B^2}}\\ P(t)=\mathrm{J}_0(\gamma B_0 t)\end{cases}$$

C. Schwinger boson mean field theory

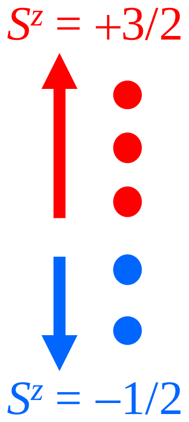
Schwinger boson mean field theory (SBMFT)

- SBMFT [1] is a self-consistent spin wave theory which uses the Schwinger boson representation of spin operators

- In the Schwinger boson representation, a spin state $|S_z\rangle$ is represented using two boson operators $b_\uparrow$ and $b_\downarrow$

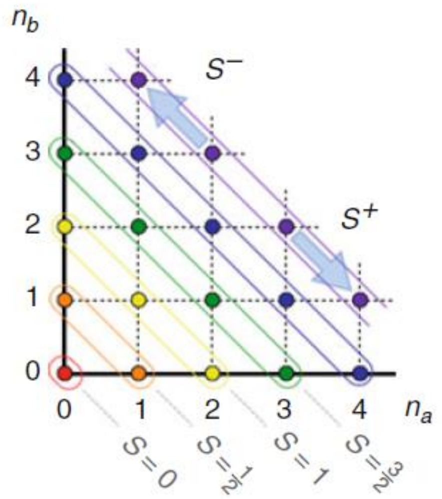
$$S^+ = b_\uparrow^\dagger b_\downarrow$$

$$S^z = \tfrac{1}{2}\left(b_\uparrow^\dagger b_\uparrow - b_\downarrow^\dagger b_\downarrow\right)$$



- A constraint is added to ensure physical spin values

$$b_\uparrow^\dagger b_\uparrow + b_\downarrow^\dagger b_\downarrow = 2S$$



Taken from [2]

[1] A. Auerbach, "*Interacting electrons and quantum magnetism*", Springer Science & Business Media 2012

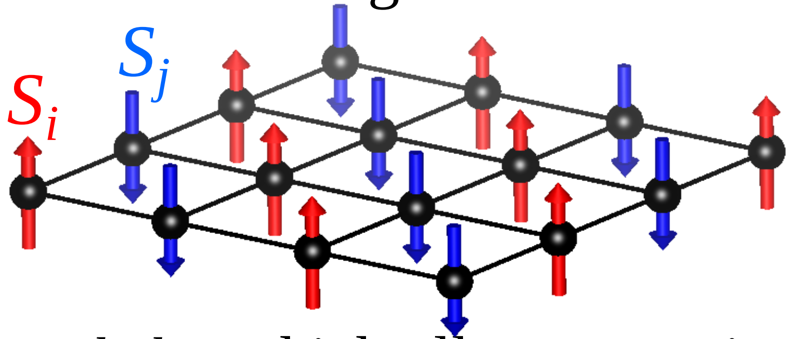
[2] C. Lacroix, "*Introduction to frustrated magnetism*", Springer Science & Business Media, 2011

Schwinger boson mean field theory (SBMFT)

- We want to transform the Heisenberg antiferromagnet on a bipartite lattice $H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j$ into the Schwinger boson representation

- Define a Schwinger boson $b_{\uparrow i}$ or $b_{\downarrow i}$ on each site and perform a rotation by π around the y axis on the j sublattice to expand around the classical Néel ground state

$$\begin{cases} S_j^x \to -S_j^x \\ S_j^y \to S_j^y \\ S_j^z \to -S_j^z \end{cases} \Rightarrow \begin{cases} b_{\uparrow j} \to -b_{\downarrow j} \\ b_{\downarrow j} \to b_{\uparrow j} \end{cases}$$



- It is convenient to define a bond operator $A_{ij} = b_{\uparrow i}b_{\uparrow j} + b_{\downarrow i}b_{\downarrow j}$ which allows to write

$$H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j = -\frac{J}{2}\sum_{\langle ij\rangle}\left(A_{ij}^\dagger A_{ij} - 2S^2\right)$$

Schwinger boson mean field theory (SBMFT)

- H is now a four-body operator. Introduce the mean field approximation $A_{ij} \to Q \propto \langle A_{ij} \rangle$ to obtain the mean field Hamiltonian

$$H_{\mathrm{MF}} = \frac{NQ^2}{4J} + Q\sum_{\langle ij \rangle}\left(\mathrm{A}_{ij} + \mathrm{A}_{ij}^{\dagger}\right) + \lambda\sum_{i=1}^{N}\left(b_{\uparrow i}^{\dagger}b_{\uparrow i} + b_{\downarrow i}^{\dagger}b_{\downarrow i} - 2S\right)$$

Scalar — Quadratic part — Schwinger boson constraint

N – number of lattice sites
Q – mean field parameter
λ – Lagrange multiplier

- The mean field Hamiltonian can be diagonalized using a Bogoliubov transformation $\beta_{\mathbf{k}\sigma} = \cosh\theta_{\mathbf{k}} b_{\mathbf{k}\sigma} - \sinh\theta_{\mathbf{k}} b_{-\mathbf{k}\sigma}^{\dagger},\ \sigma = \uparrow,\downarrow$ and we obtain

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}\sigma}\left(\omega_{\mathbf{k}}\beta_{\mathbf{k}\sigma}^{\dagger}\beta_{\mathbf{k}\sigma} + \frac{1}{2}\right) + \frac{NQ^2}{4J} - N\lambda\left(2S+1\right)$$

$\omega_{\mathbf{k}} = \sqrt{\lambda^2 - \left(zQ\gamma_{\mathbf{k}}\right)^2}$ - dispersion relation

$z = 4$ – number of nearest neighbors

$\gamma_{\mathbf{k}} = \sum_{\boldsymbol{\delta} \in \mathrm{n.n}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}$ - band structure

Schwinger boson mean field theory (SBMFT)

- The layered antiferromagnet Hamiltonian $H = J\left(\sum_{i,\delta_{P}} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta_{P}} + \alpha \sum_{i,\delta_{\perp}} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta_{\perp}}\right)$

  can be written as an effective 2D antiferromagnet in an external field

$$H = J\left(\sum_{i,\delta_{P}} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta_{P}} - 2\alpha h \sum_i S_i^z\right)$$

Self-consistency: $h = 2\alpha \left\langle S^z \right\rangle = 2\alpha M$

- An external field modifies the spin wave spectrum of the SBMFT Hamiltonian as follows

$$\omega_{\mathbf{k}\sigma} = \sqrt{\left(\lambda + \sigma h\right)^2 - \left(zQ\gamma_{\mathbf{k}}\right)^2}$$

Schwinger boson mean field theory (SBMFT)

- To obtain the temperature evolution, we calculate the free energy from the SBMFT Hamiltonian:

$$F = \frac{1}{T}\sum_{\mathbf{k}\sigma} \ln\left[2\sinh\left(\frac{\omega_{\mathbf{k}\sigma}}{2T}\right)\right] - N\lambda\left(2S+1\right) + \frac{NQ^2}{4J}$$

- The mean field parameters are obtained by minimizing F:

$$\frac{\partial F}{\partial Q} = 0 \Rightarrow \frac{1}{2N}\sum_{\mathbf{k}\sigma} \frac{\gamma_{\mathbf{k}} z^2 Q^2}{\omega_{\mathbf{k}\sigma}}\left(n_{\mathbf{k}\sigma} + \frac{1}{2}\right) = \frac{zQ}{J}$$

$$\frac{\partial F}{\partial \lambda} = 0 \Rightarrow \frac{1}{2N}\sum_{\mathbf{k}\sigma} \frac{\lambda + \sigma h}{\omega_{\mathbf{k}\sigma}}\left(n_{\mathbf{k}\sigma} + \frac{1}{2}\right) = S + \frac{1}{2}$$

$$n_{\mathbf{k}\sigma} = \left(e^{\omega_{\mathbf{k}\sigma}/T} - 1\right)^{-1}$$ - Boltzmann weight

- Finally, the magnetization is solved for self-consistently using

$$M = -\lim_{N\to\infty}\left\langle \frac{\partial F}{\partial h}\right\rangle = \frac{h}{2\alpha}$$