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Mössbauer study of $Hf_{0.5}Ta_{0.5}Fe_2$

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Laves phase materials

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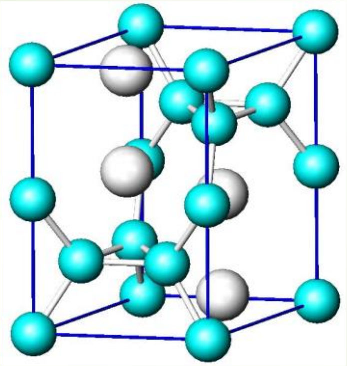
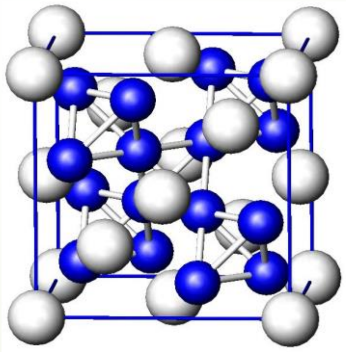
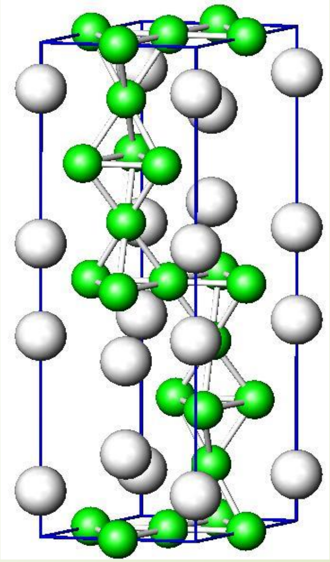
- intermetallic phases
- one of the largest groups of intermetallic compounds (over 1400)
- AB_2 stoichiometry composition
- crystallizing in three possible structure types:
  - hexagonal “$MgZn_2$”(**C14**); space group *$P6_3/mmc$*
  - hexagonal “$MgNi_2$”(**C36**); space group *$P6_3/mmc$*
  - cubic “$MgCu_2$” (**C15**); space group *Fd3m*



C14



C15



C36

- polytypic phase transformations !!!!!

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Laves phase materials. Interesting? Why?

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- abnormal physical and chemical properties
  - high-temperature applications
  - oxidation resistance
  - perfect el. conductivity; e.g. superconductive $(Hf, Zn)V_2$
  - **various magnetic properties**; e.g. $(Tb, Dy)Fe_2$
  - hydrogen storage; e.g. $Zr(Cr, Fe)_2$
  - high brittleness (few exceptions with satisfactory ductility)
- thermodynamic information is very limited (sc. papers are often contradictory)

  -> investigation of possible laves phase alloys are mostly *ab initio* calculations
- there is no applicable theory that predicts the existence or non-existence of certain laves phase.

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$HfFe_2$ and $TaFe_2$

FINE TUNING OF MAGNETIC PROPERTIES

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- binary AFe_2 laves phases
  - itinerant-electron nature of the magnetism due to Fe
  - 6h and 2a Fe sites (3 : 1)

- **$HfFe_2$**
  - ferromagnetic up to 600 K
  - C14, C15 or C36 structure

- **$TaFe_2$**
  - Pauli paramagnet
  - C14, C15 or C36 structure

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Belosevic-Cavor J, Koteski V, Novakovic N, Concas G, Congiu F and Spano G 2006 Eur. Phys. J. B 50 425
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Ternary Laves phase alloys $Hf_{1-x}Ta_xFe_2$

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- Ta substitution for Hf in $HfFe_2$
  → **desirable magnetic properties**

- C14 structure stabilizes and shows a first order transition from FM to AF state
  (spin fluctuation theory)

- at room temperature
  - ferromagnetic for $0 \leq x < 0.3$,
  - **antiferromagnetic for $0.3 \leq x \leq 0.7$** and
  - paramagnetic at around $x = 1.0$

- for $x > 0.225$ is FM only at T = 0 K

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Investigation of $Hf_{0.5}Ta_{0.5}Fe_2$

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- Materials and methods:
  - **XRD** → structure determination
  - **MPMS** → macroscopic magnetic properties
  - **<u>Mössbauer spectroscopy</u>**

    - nuclear method in material science

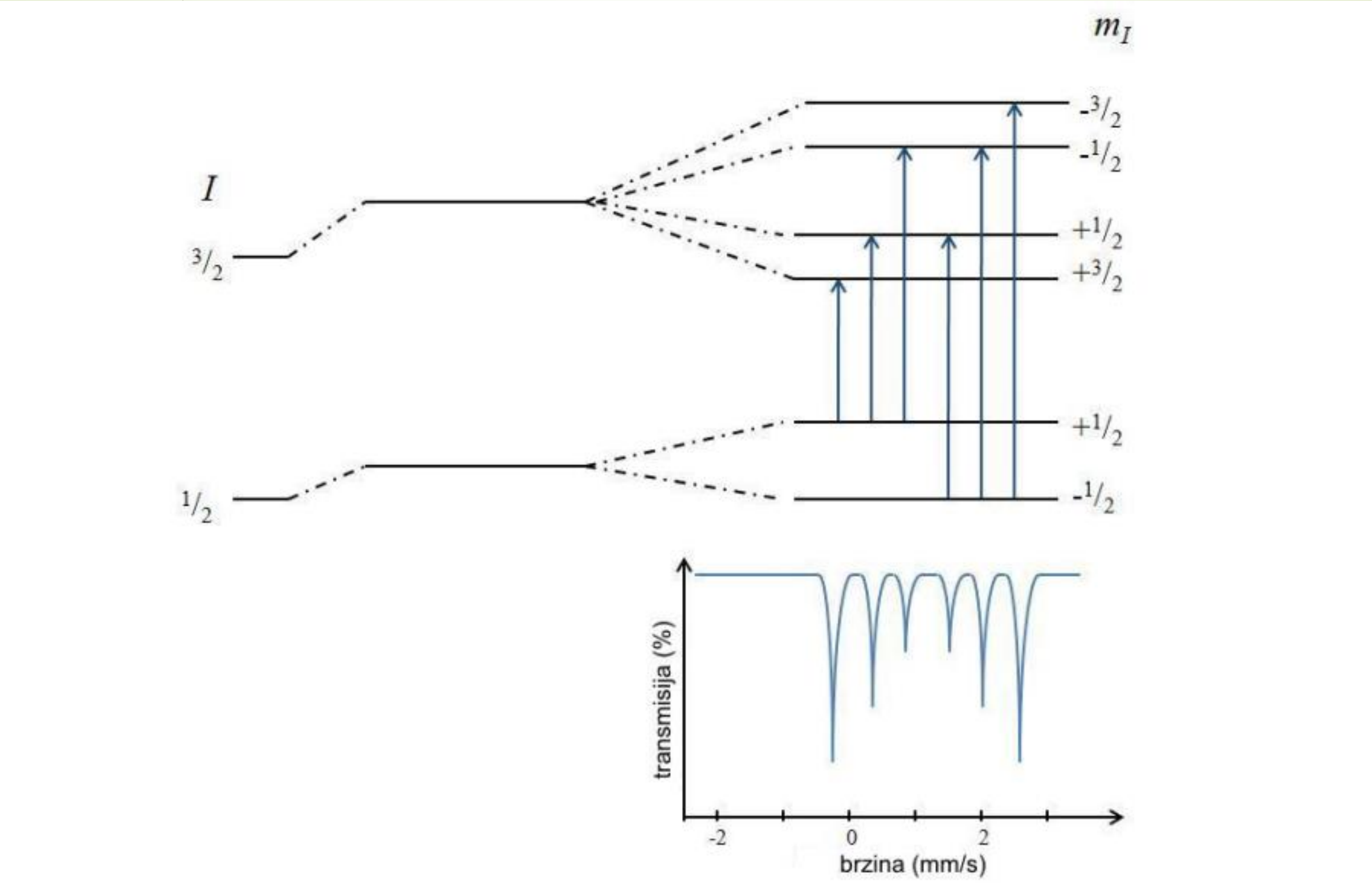
    - ^{57}Fe (Eγ = 14,4 keV) source accelerated through a range of velocities

    - 1mm/s = 48.075 neV

    - resonant absorption on sample

    → hyperfine interactions information (local magnetic field on Fe site)

Mössbauer spectroscopy: local magnetic interaction



Results:
XRD - $Hf_{0.5}Ta_{0.5}Fe_2$

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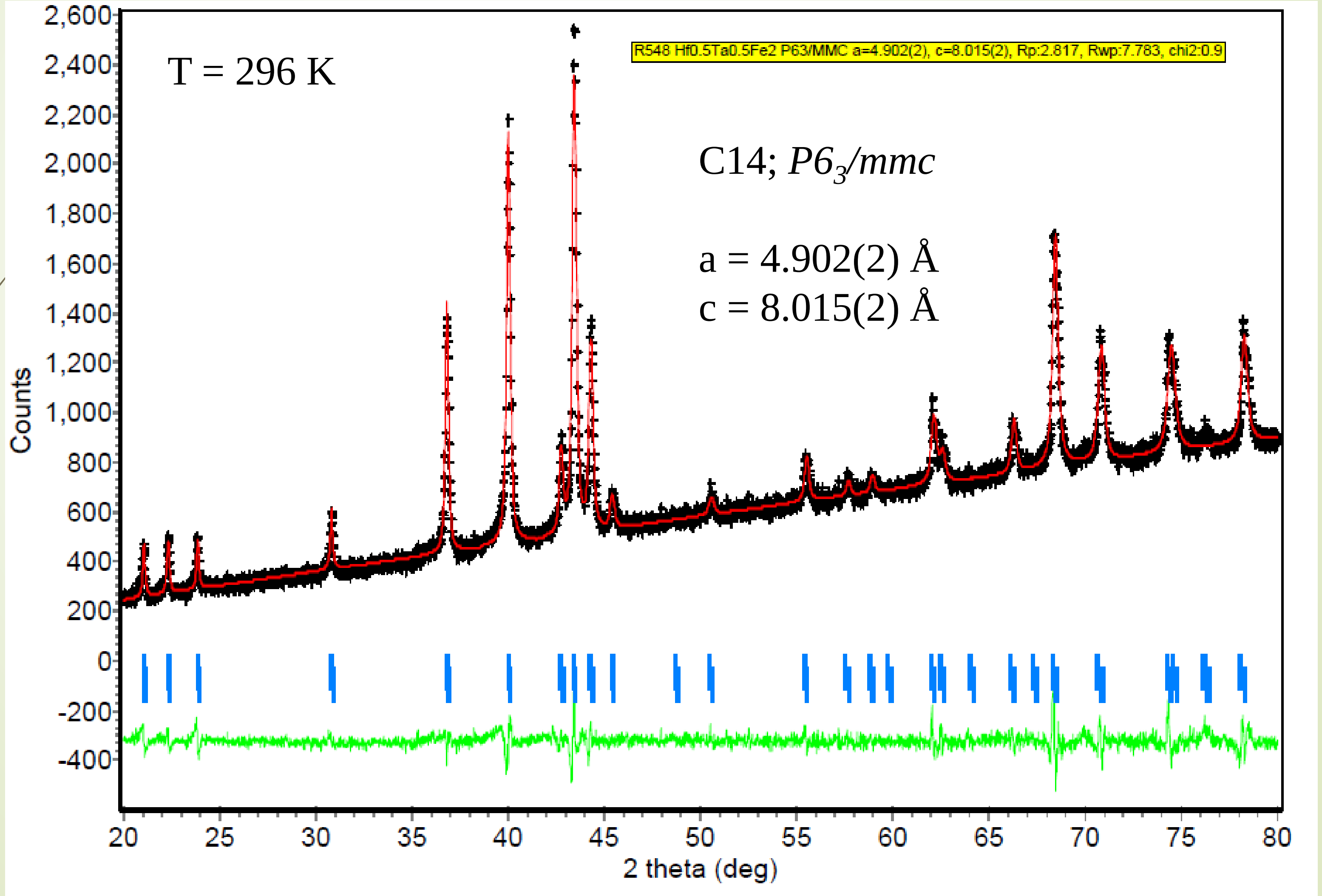

Results:
MPMS -$Hf_{0.5}Ta_{0.5}Fe_2$

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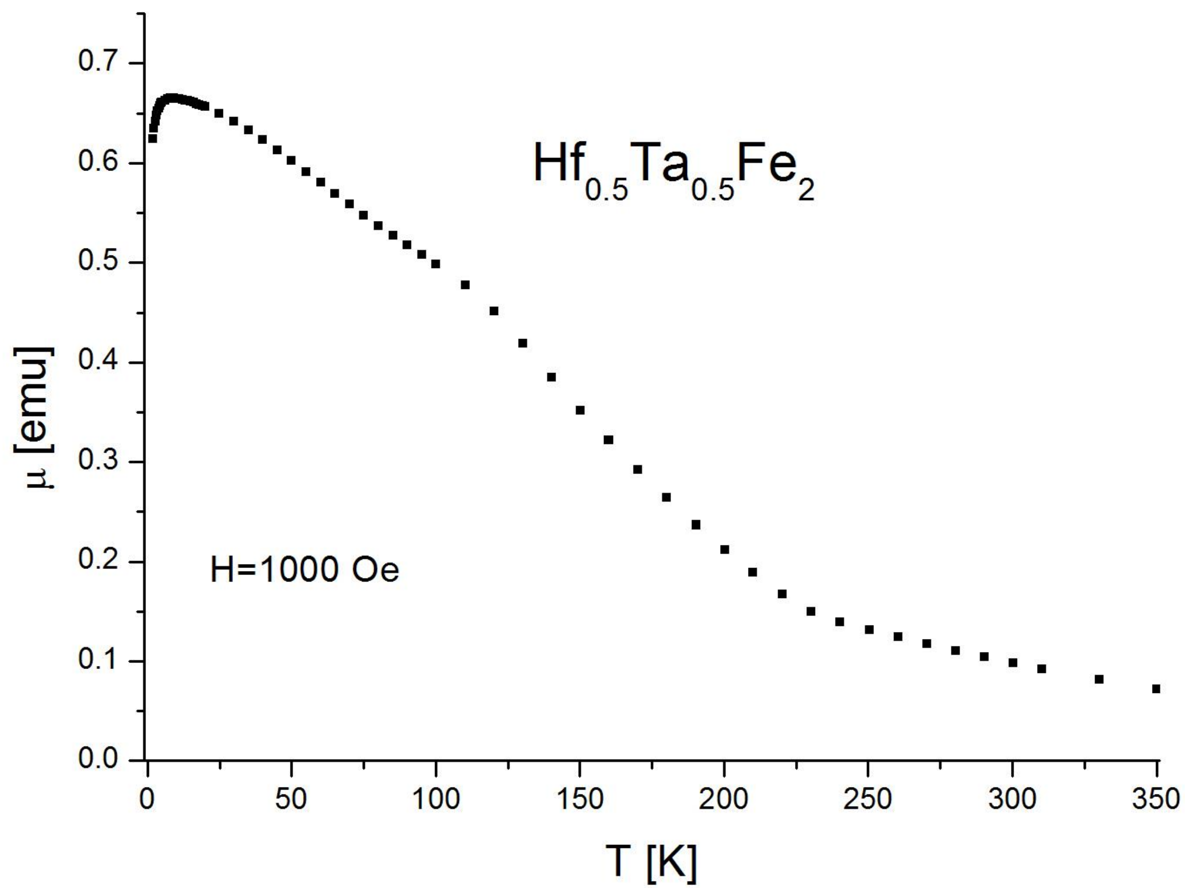

Results: Mössbauer spectroscopy

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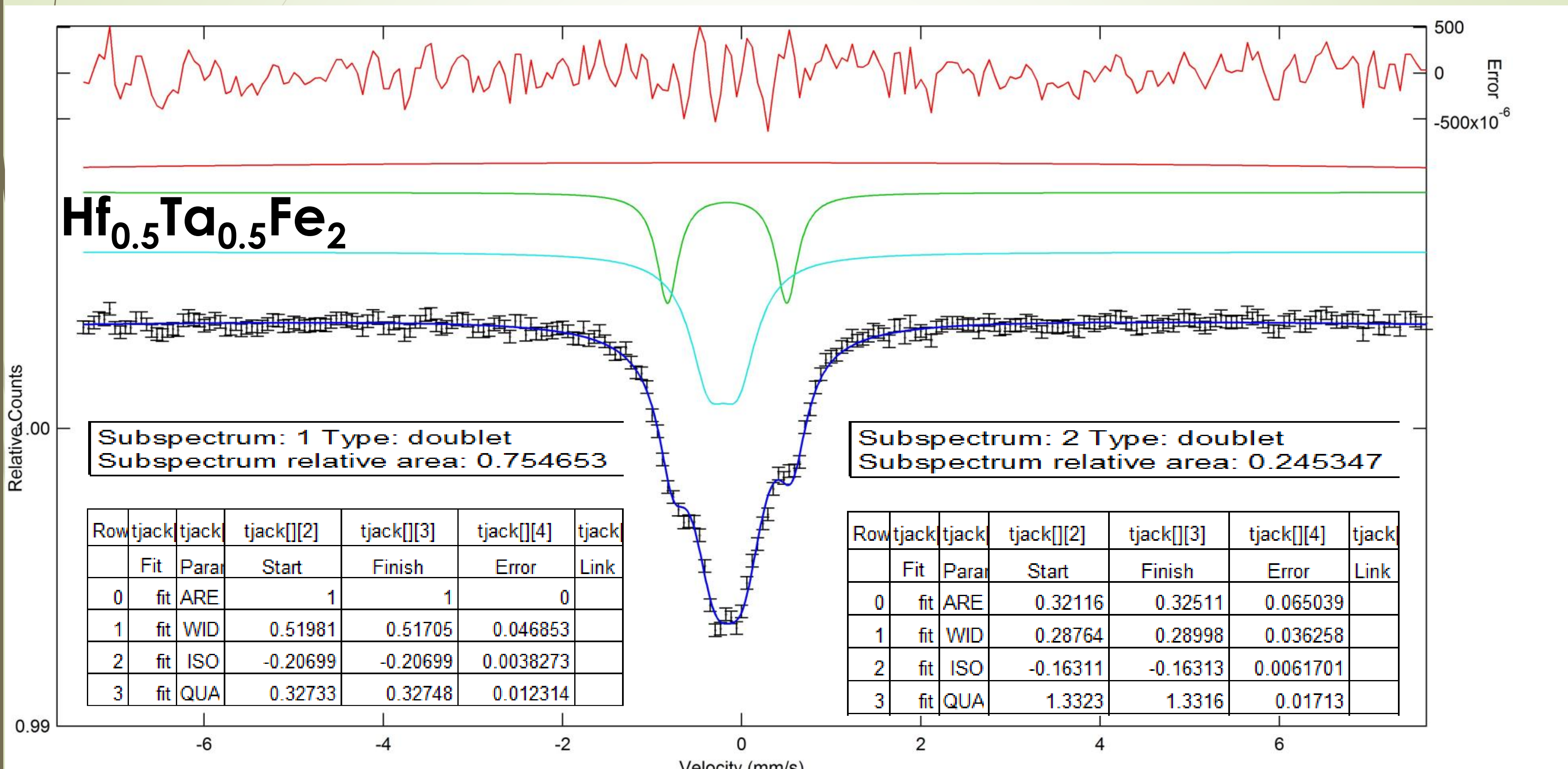

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1	fit	WID	0.51981	0.51705	0.046853	
2	fit	ISO	-0.20699	-0.20699	0.0038273	
3	fit	QUA	0.32733	0.32748	0.012314	

Row	tjack	tjack	tjack[][2]	tjack[][3]	tjack[][4]	tjack
	Fit	Para	Start	Finish	Error	Link
0	fit	ARE	0.32116	0.32511	0.065039	
1	fit	WID	0.28764	0.28998	0.036258	
2	fit	ISO	-0.16311	-0.16313	0.0061701	
3	fit	QUA	1.3323	1.3316	0.01713	

- **AREA(Doublet 1) : AREA(Doublet 2) = 3 : 1**

Summary

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- macroscopic magnetic measurements imply sample paramagnetism at room temperature

- two quadrupole doublets on Mössbauer spectrum imply the absence of local magnetic interactions on the 6h and 2a Fe site

  → $\mathbf{Hf_{0.5}Ta_{0.5}Fe_2}$ is paramagnetic at room temperature

- room temperature paramagnetism occurs at less than 70% Ta substitution of Hf

- magnetic phase transitions → strong spin fluctuations which are local in these compounds

Plans

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- similar investigations on prepared samples:

  $HfFe_2$

  $Hf_{0.95}Ta_{0.05}Fe_2$

  $Hf_{0.75}Ta_{0.25}Fe_2$

  $Hf_{0.95}Ta_{0.05}Fe_2$

  $Hf_{0.25}Ta_{0.75}Fe_2$

  $Hf_{0.05}Ta_{0.95}Fe_2$

  $TaFe_2$

- + possible **TDPAC** measurements

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Thank You !!!