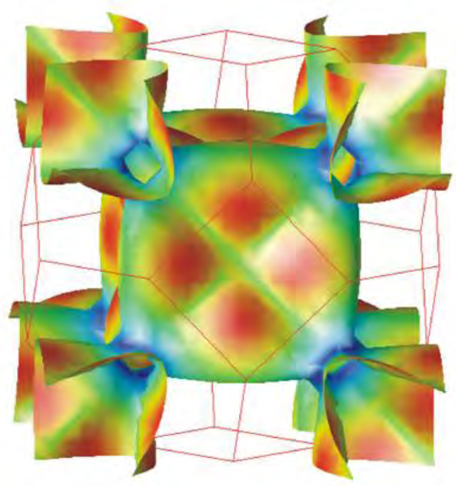
MOMENT

Materials for Optical, Magnetic, and Energy Technologies

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Semiconducting and half metallic Heusler compounds for multifunctional applications



Claudia Felser

Heusler Compounds as Multifunctional Materials

ISABELLENHÜTTE

1905	Magnetic material:	Cu_2MnAl
1983	Halfmetallic ferromagnet:	NiMnSb
	Magneto-optical:	PtMnSb
	Magneto-mechanic:	Ni_2MnGa
	Superconductor:	Pd_2YSn
	Semiconductors:	CoTiSb
	Heavy fermion:	Fe_2VAl
	Li-conductor:	LiMnSb
	Magneto-electronic:	Co_2FeSi
2001	Thermo-electric:	TiNiSn
	Magneto-caloric:	CoMnSb:Nb

- Concept
- Semiconducting Half Heusler
  - Thermoelectric materials
  - Diluted Semiconductors
- Half metallic Heusler compounds
  - High Curie temperatures
  - Ferrimagnets
- High energy photoemission for Devices
- Summary

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Rational Design

Half metallicity

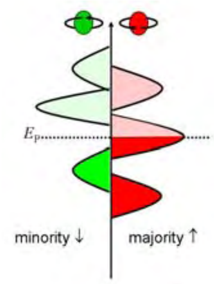
High density of states at E_F

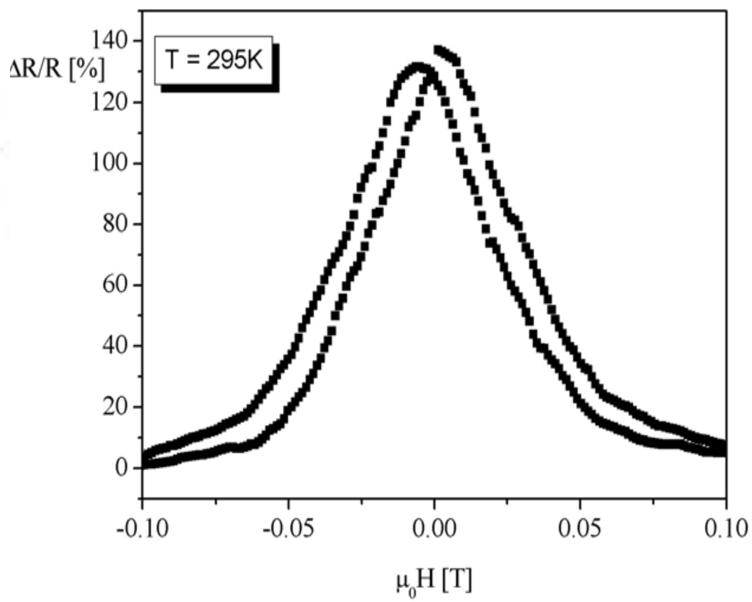
↓

Large MR at room temperature

Intermag 2002: $Co_2Cr_{0.4}Fe_{0.6}Al$

CCFA





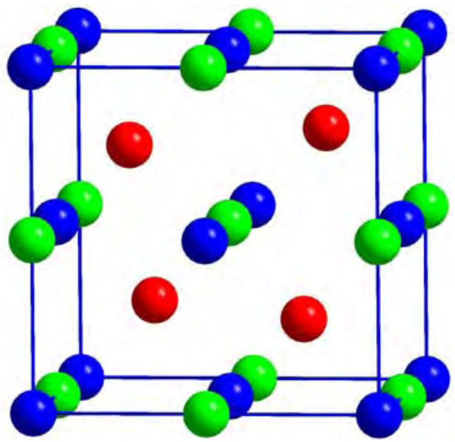
- First TMR device (Inomata et al.) 19% at RT
- TMR-device with MgO (Marukame et al. APL 90 (2007) 012508)
  109% TMR at RT ⇒ 88 % spin polarisation at 4K
- Point contact 80% MR (Coey et al.)

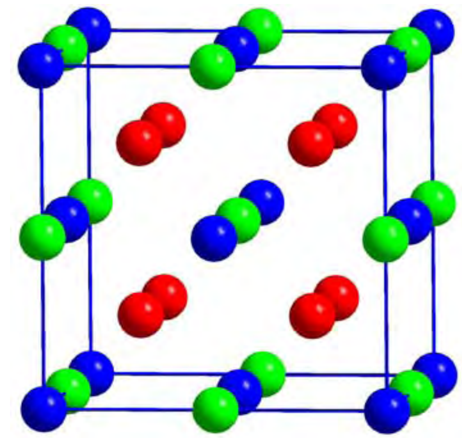
Patent (Felser, Block, DE 101 08 760, H01 L43/08)

Block, Felser, et al. J. Solid State Chem. **176**, 646 (2003)

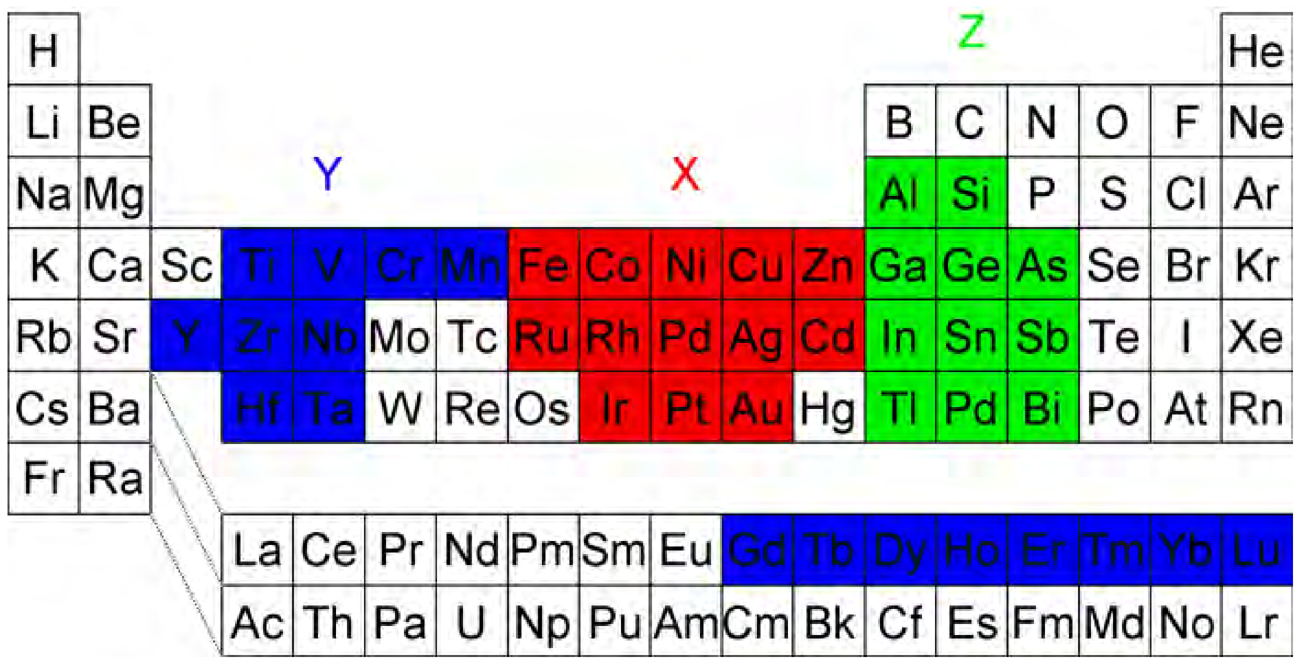
Semiconducting Heuslers – Stuffed ZnS

XYZ





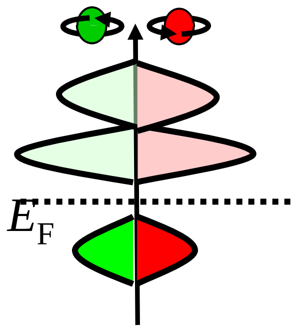
X_2YZ



Slater-Pauling Rule

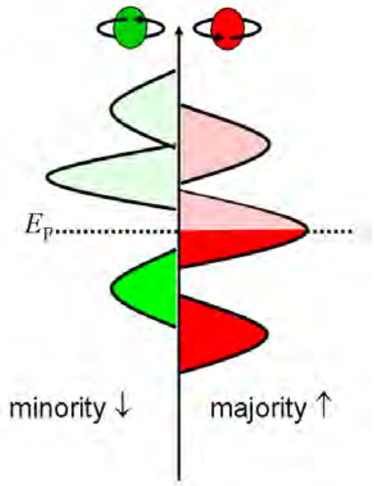
Magic valence electron number X_2YZ 24

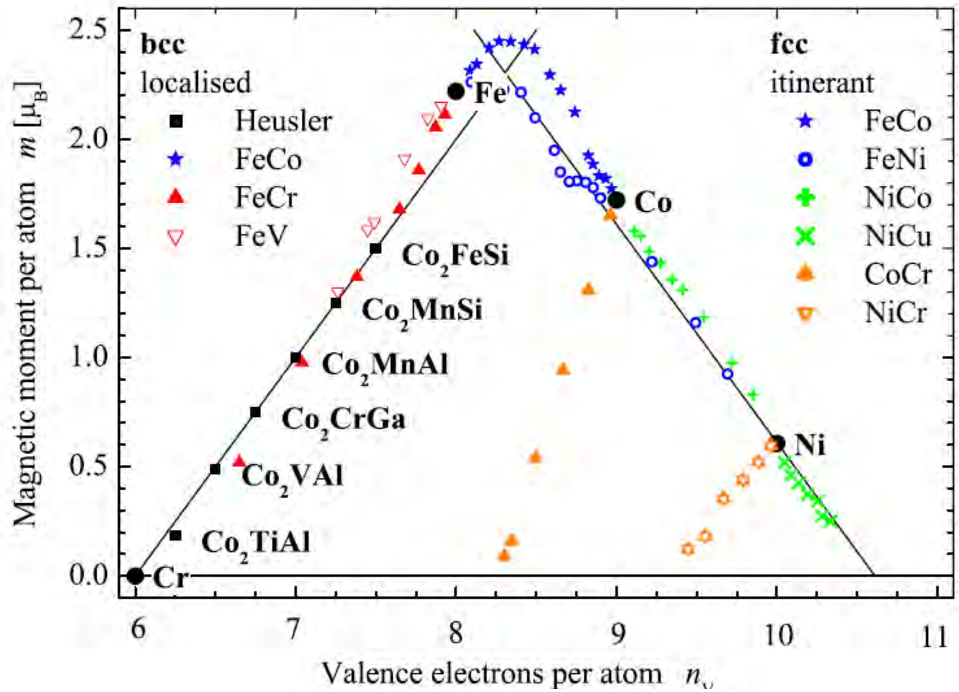
Valence electrons =^24 + sat. magnetization



Co_2FeAl

2*9 + 8 + 3 = 29 Ms = $5\mu_B$





Kübler 1983

Galanakis et al., PRB **66**, 012406 (2002)

B. Balke et al., Sci. Technol. Adv. Mater. **9** (2008) 014102.

- Concept

- Semiconducting Half Heusler
  - Thermoelectric materials
  - Diluted Semiconductors

- Halfmetallic Heusler compounds
  - High Curie temperatures
  - Ferrimagnets

- High energy photoemission for Devices

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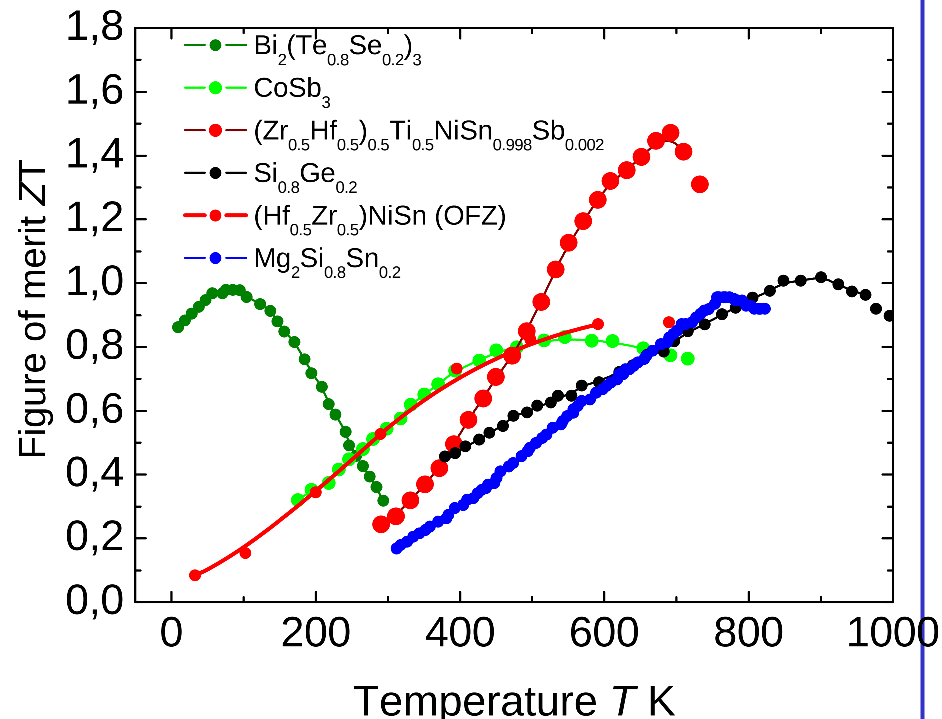
Half Heusler: 18 valence-electrons

Thermoelectrica

Typ	Material	Price in $/kg (metals)
V-VI	Bi_2Te_3	140
IV-VI	PbTe	99
Zn_4Sb_3	Zn_4Sb_3	4
Silicides	p-MnSi1.73	24
	n-$Mg_2Si_{0.4}Sn_{0.6}$	18
	$Si_{0.80}Ge_{0.20}$	660
	$Si_{0.94}Ge_{0.06}$	270
Skutterutides	$CoSb_3$	11
Half-Heusler	TiNiSn	55
n/p-Clathrate	$Ba_8Ga_{16}Ge_{30}$	1000 without Ba
Oxides	p-$NaCo_2O_4$,	17 without Na, O
Zintl Phasen	p-$Yb_{14}MnSb_{11}$	92
Th_3P_4	$La_{3-X}Te_4$	160

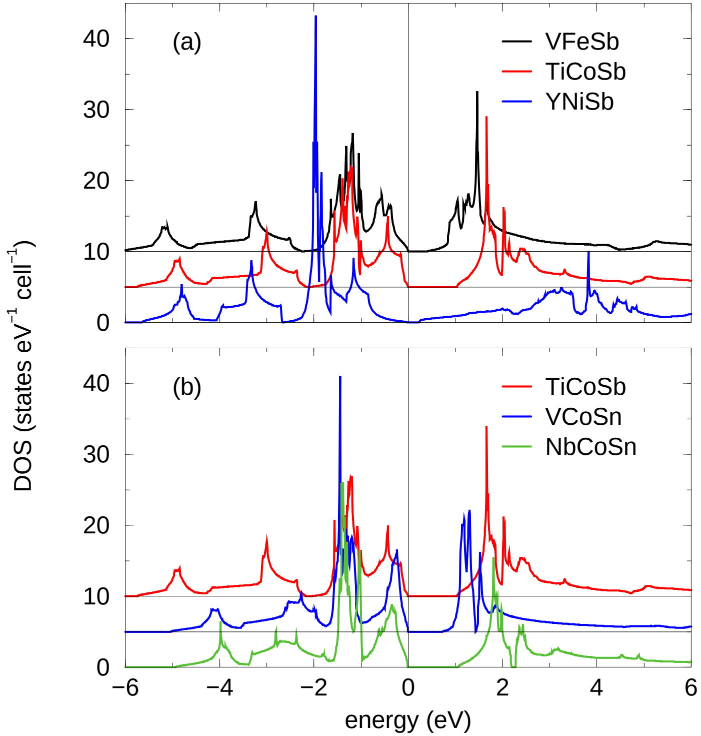


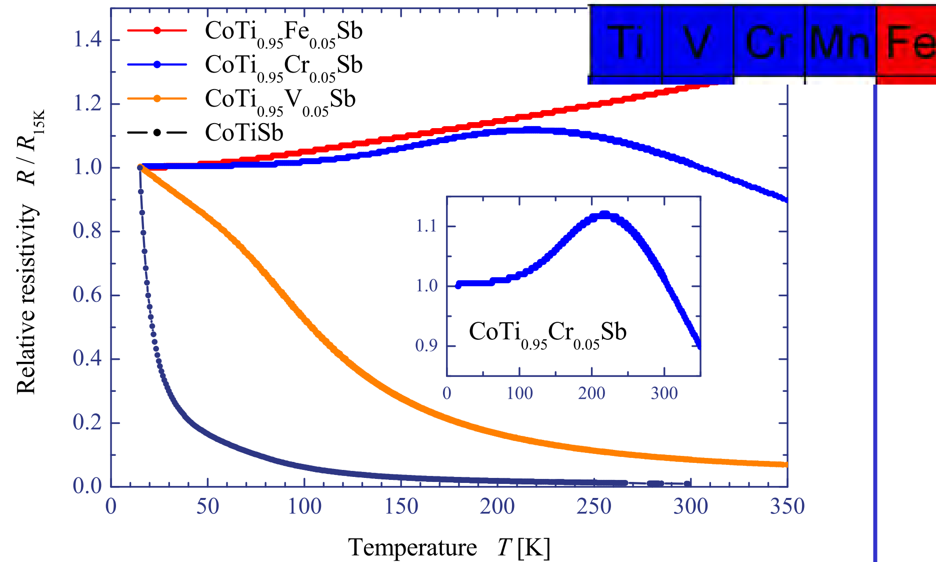
Information H. Böttcher

Fraunhofer Institut Physikalische Messtechnik IPM

R. Asahi et al. J. Phys.: Cond. Mat. **20** (2008) 64227
K. Miyamoto et al. Appl. Phys. Express **1** (2008) 081901
E. Toberer, Nature Mat. **7** (2008) 105
VK Zaitsev et al. PRB **74** (2006) 045207

Half Heusler for Thermoelectrics





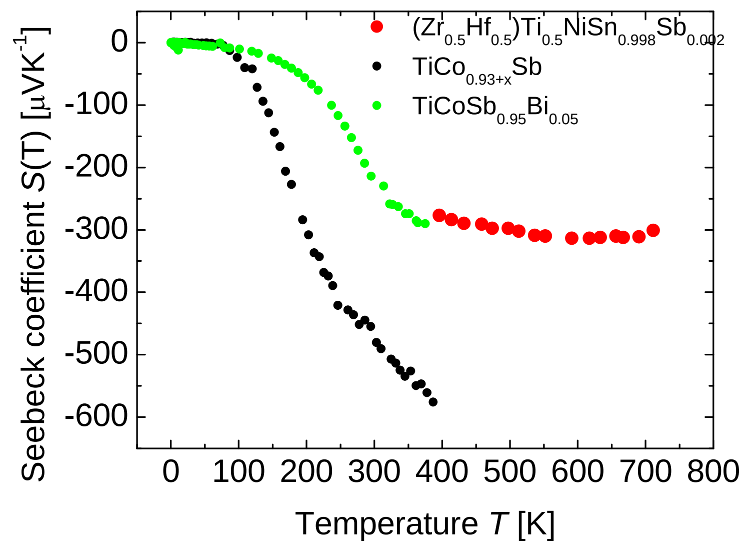
$$ZT = \frac{\alpha^2 \sigma}{\lambda} T$$

α: Seebeck coeffizient

σ: Electrical conductivity

λ: Thermo conductivity

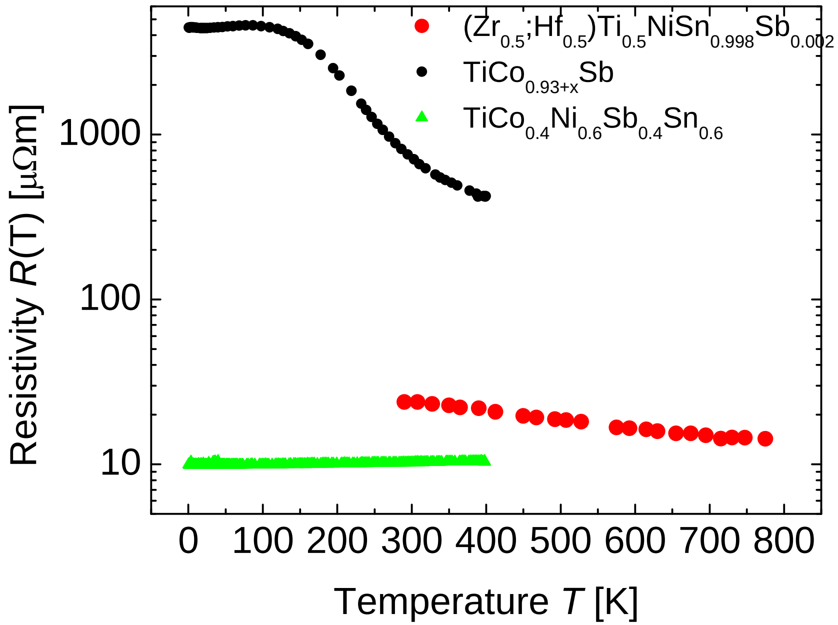
T: Temperatur (K)

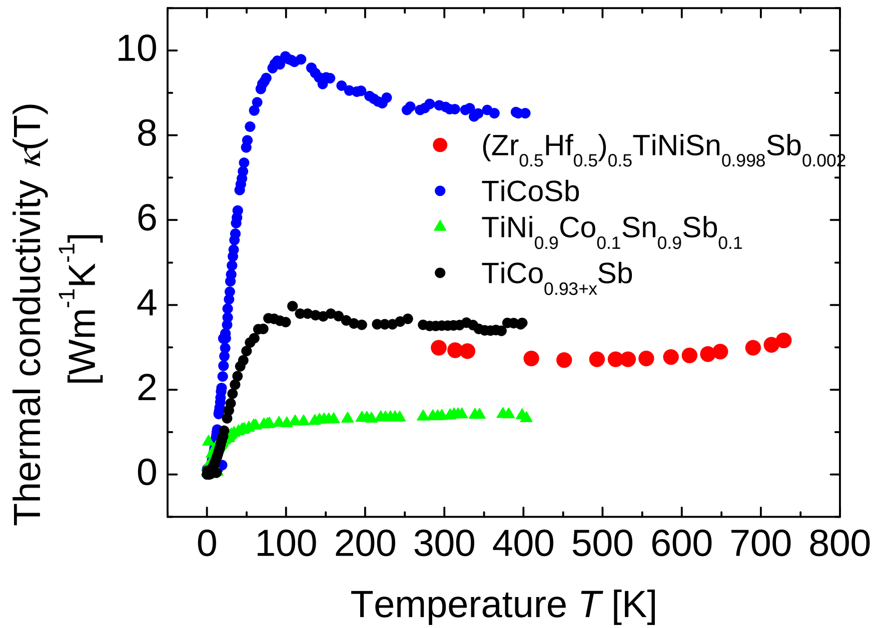


Kandpal et al. J. Phys. **D 39** (2006) 776

Balke et al. PRB **77**, 045209 (2008)

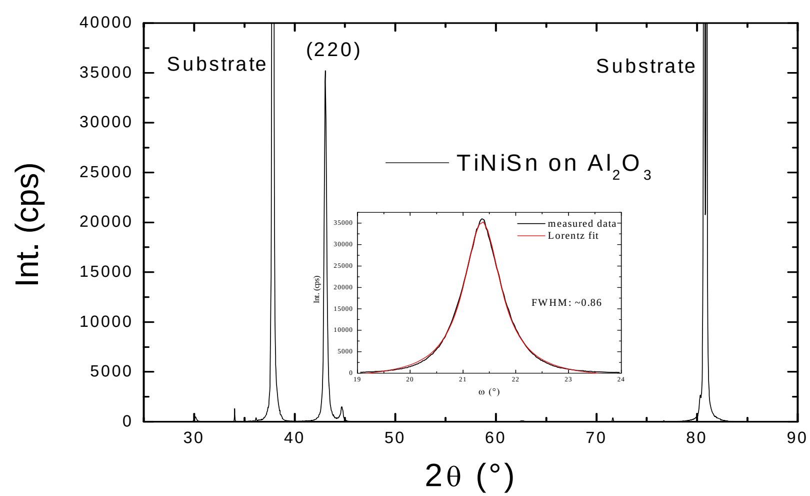
Thermoelectrica





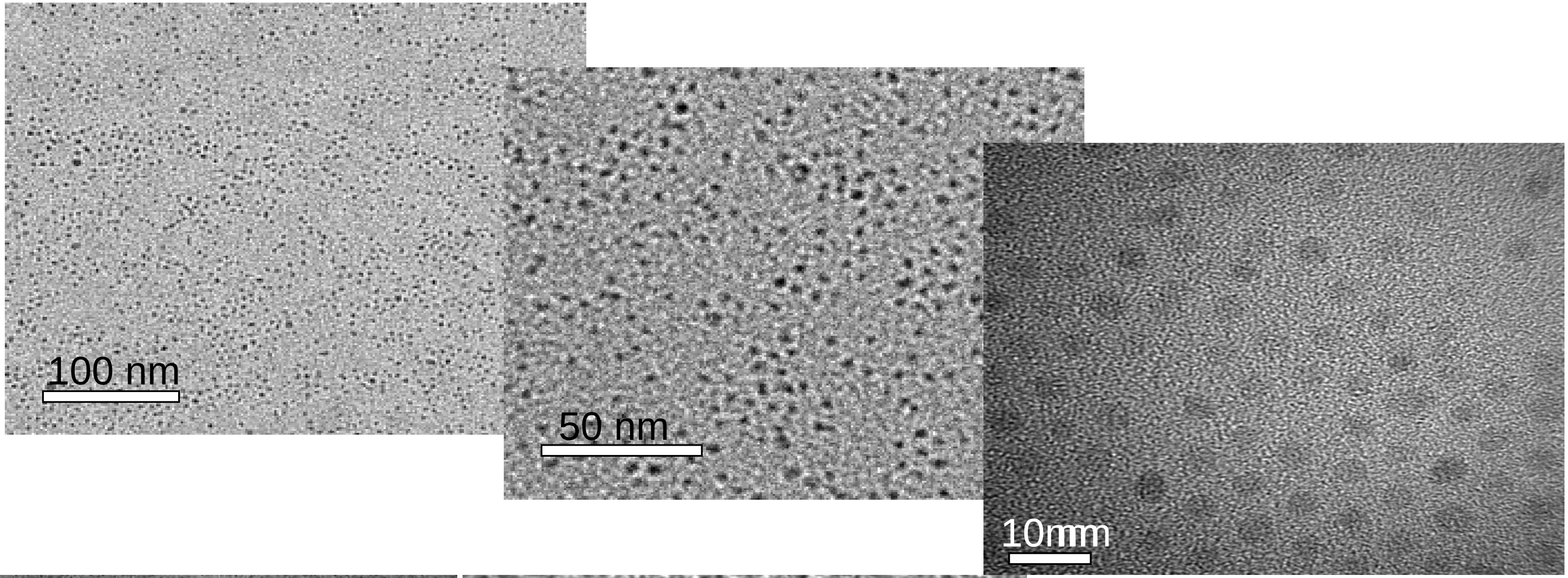
Improvement of the thermal conductivity

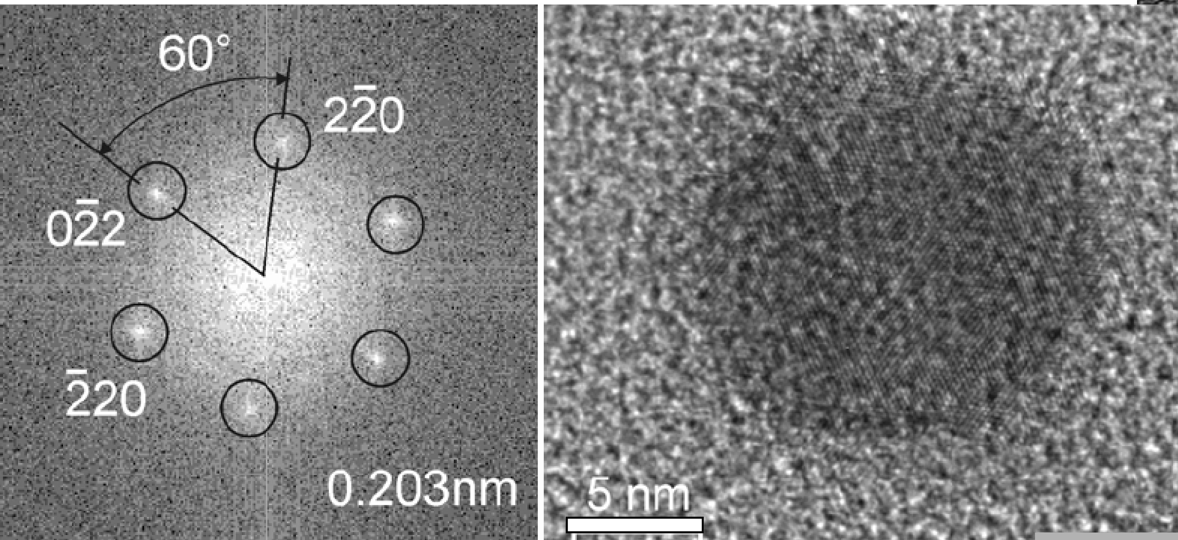
- Melt Spinning
- Ball milling – Spark Plasma
- Multilayer
- Nanoparticles
- Rattlers such as Lithium-Ions



Barth et al., in preparation (2009)

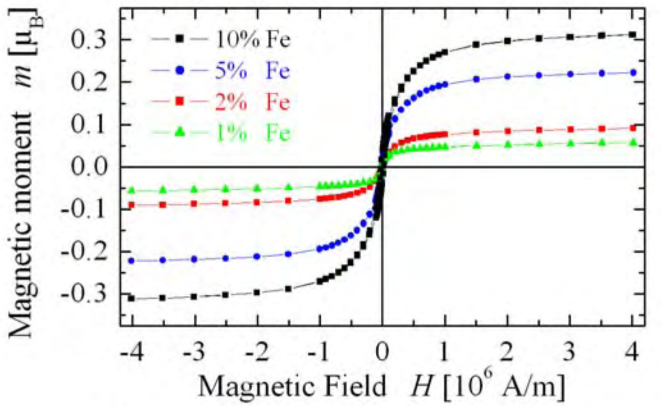
First Heusler Nanoparticles: Co_2FeGa

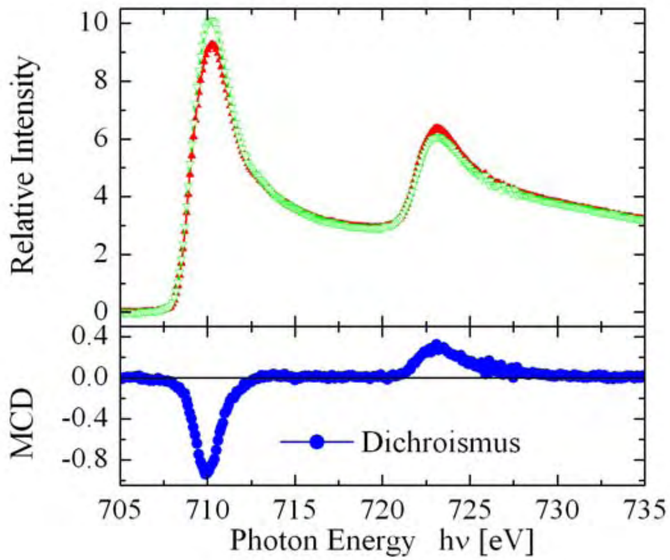




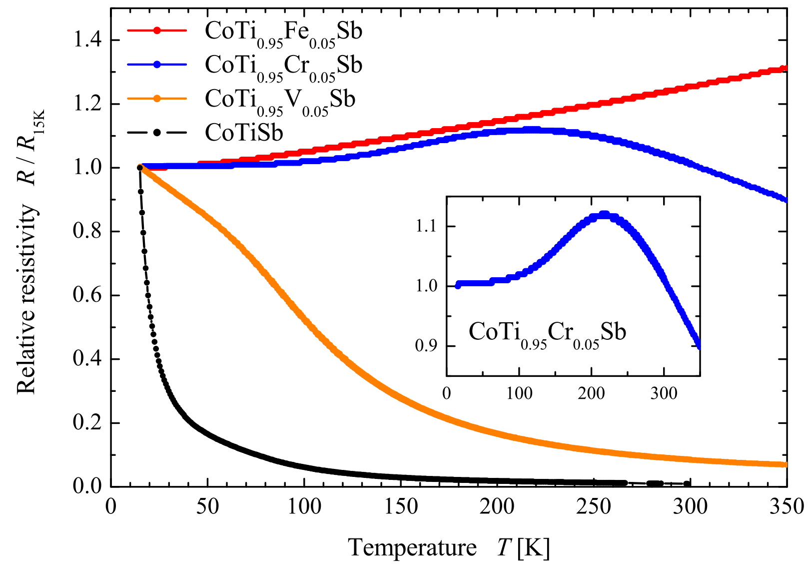
Basnit et al. J. Phys. D, (2009) accepted

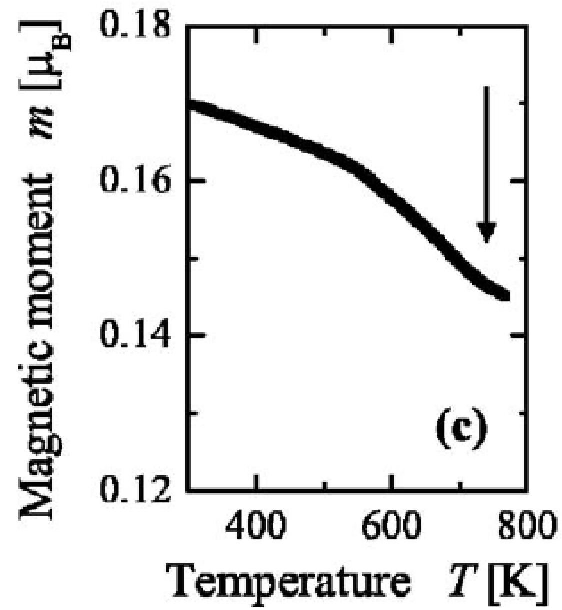
For Spin Injection





XMCD-Investigation on Fe

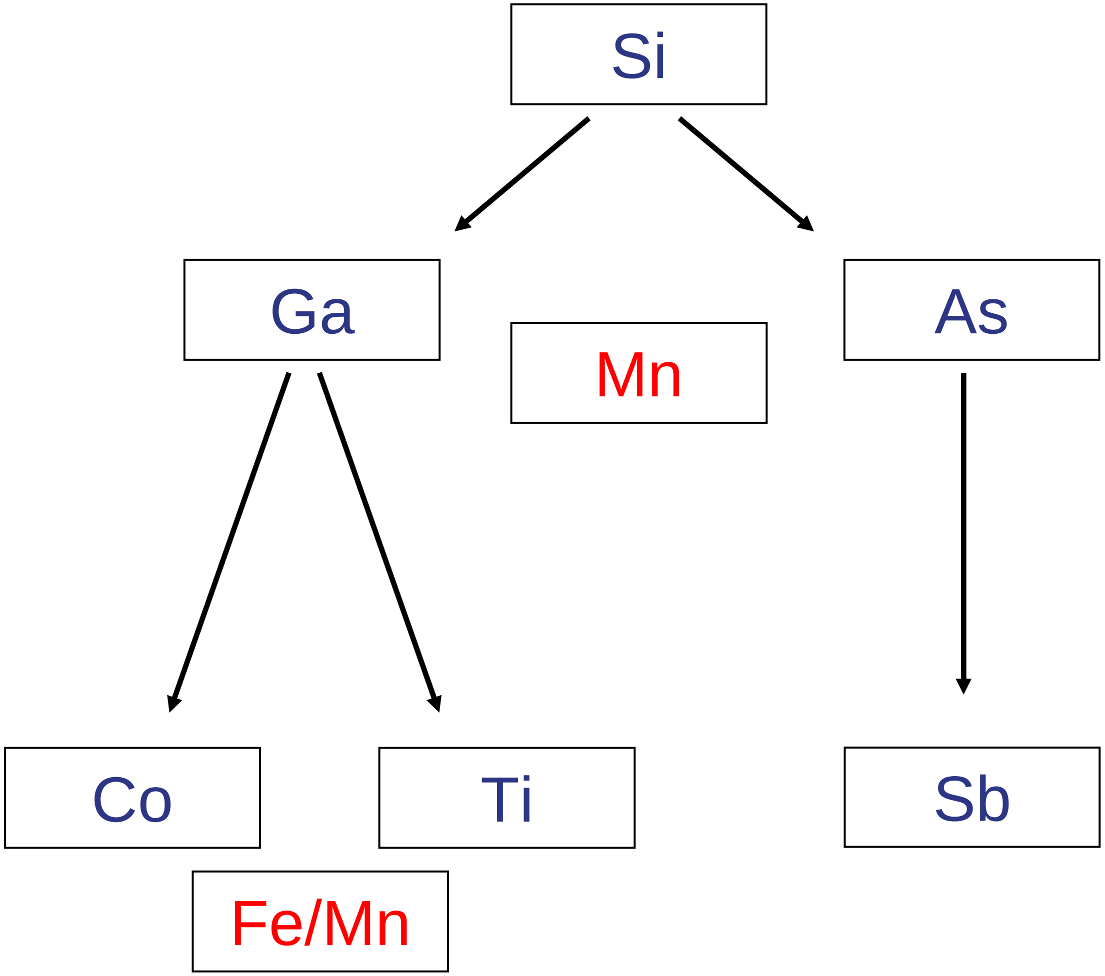




Kroth et al. APL **89** 202509 (2006)

Balke et al. PRB **77**, 045209 (2008)

Design of Diluted Semiconductors



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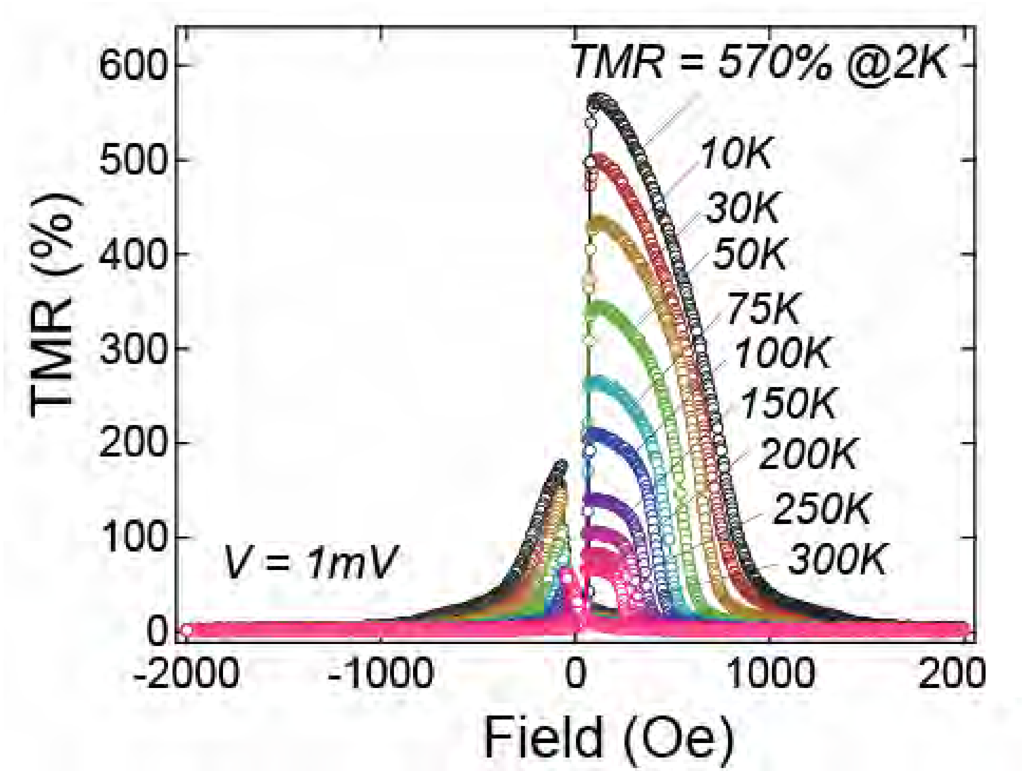
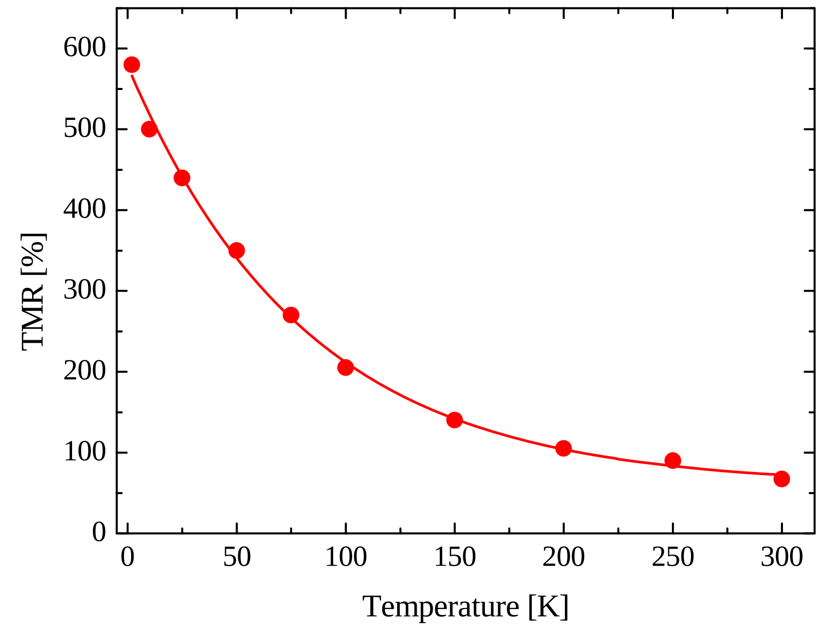
Tunneljunction





TMR ratio = 67%@RT, 580%@2K

Large temperature dependence of TMR ratio should be solved.

Sakuraba et al. APL **89** (2006) 052508

Sakuraba et al. APL **88** (2006) 192508

Half metallic ferromagnets

- for Tunnelmagnetoresistance TMR
- for CPP GMR

What do we need?

High Curie Temperature

Ordered $L2_1$ structure

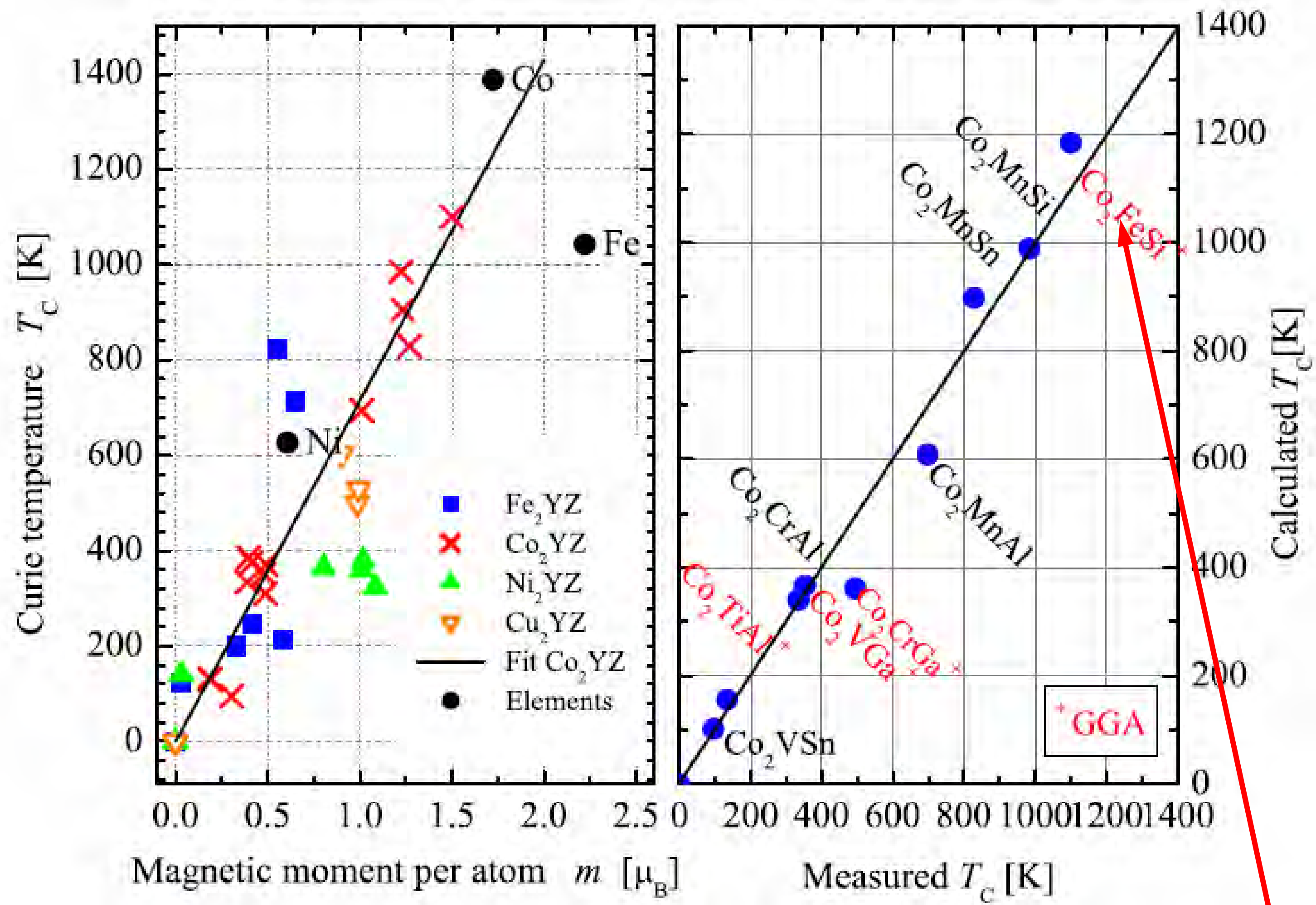
Good interfaces

Adjusted E_F: middle of the gap

no magnons

Designed electronic structure

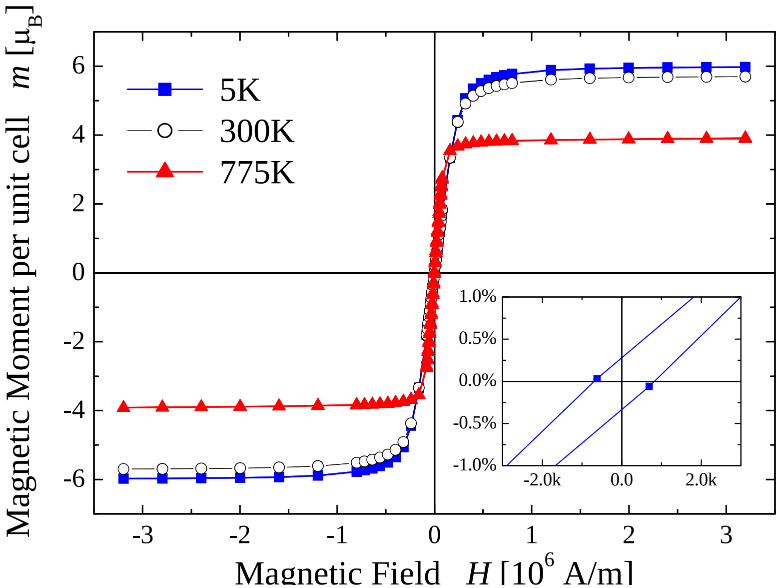
High Curie Temperatures

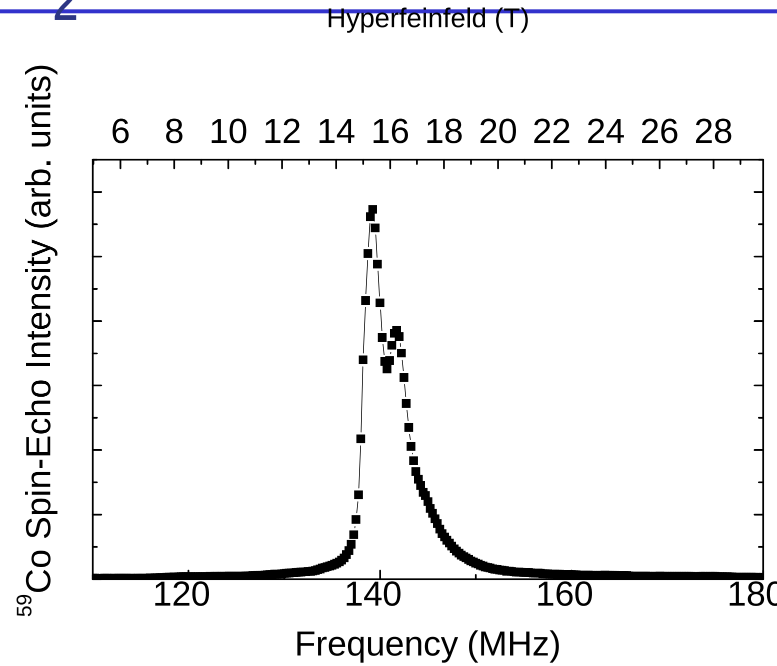


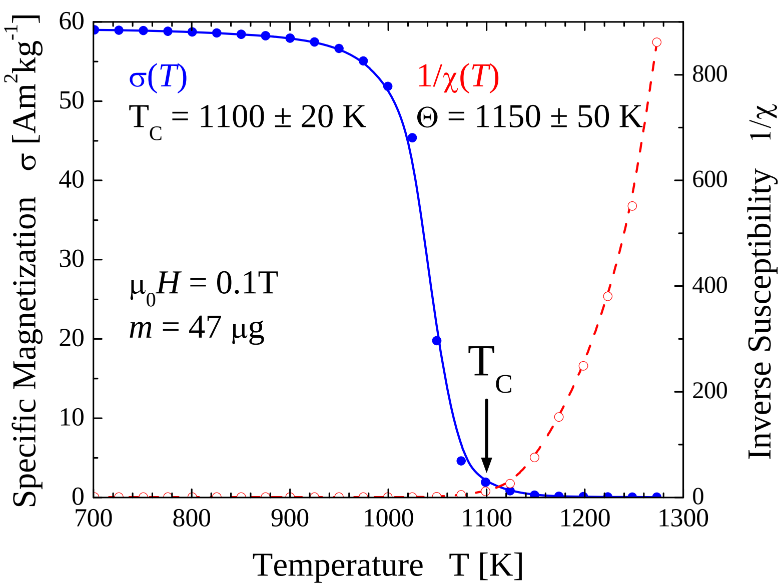
Expected Curie temperature for Co_2FeSi **: > 1000K**

Fecher, J. Appl. Phys. **99** (2006) 08J106
Kübler et al., Phys. Rev. **B 76** (2007) 024414

Co_2FeSi







Magnetic moment in saturation: $5.97\mu_B \pm 0.1\mu_B$ at 5K

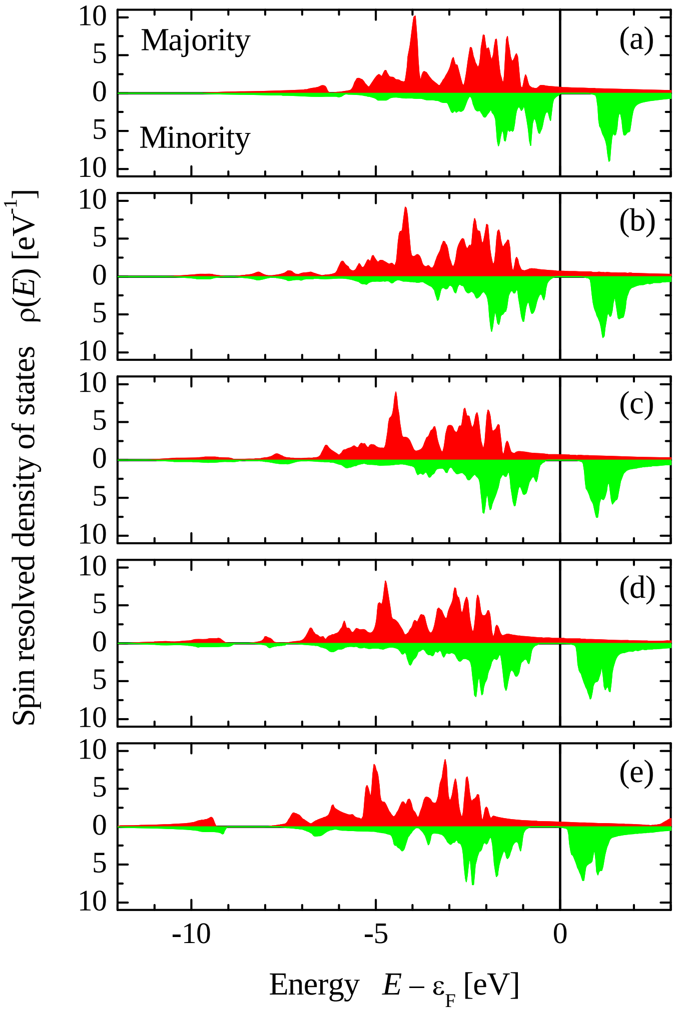
Extrapolation to 0K :Slater-Pauling rule: 6 μ_B

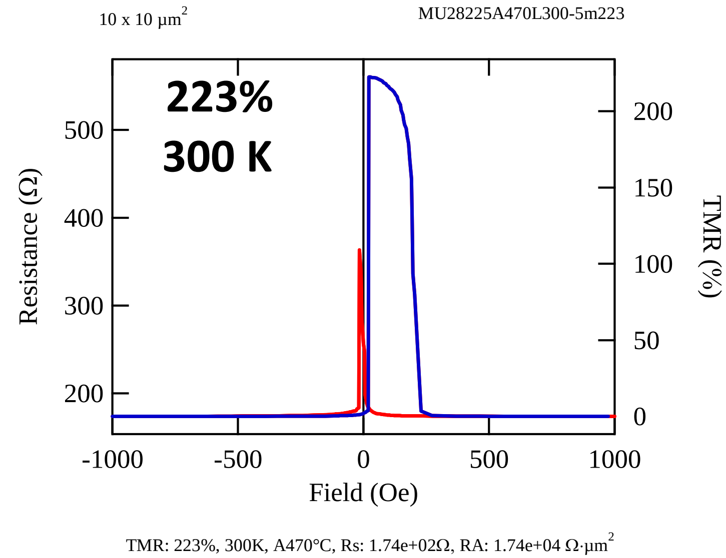
Curie Temperature 1120 K

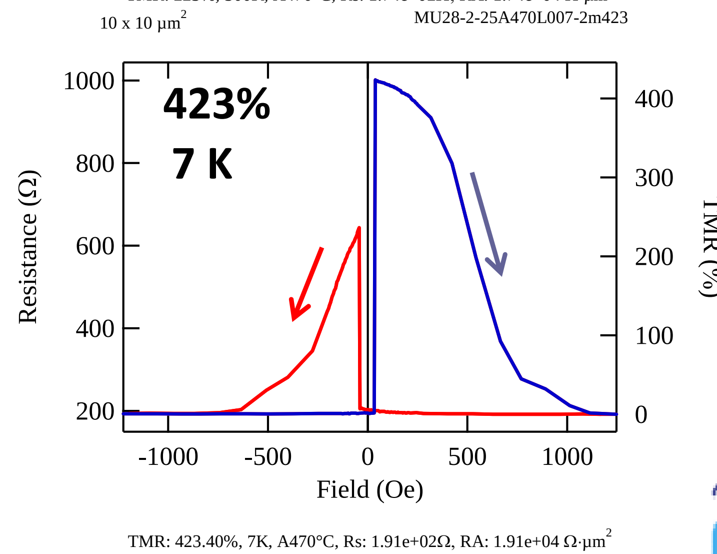
Wurmehl, et al ., APL **88** (2006) 032502.
Wurmehl, et al ., Phys. Rev. B **72** (2005) 184434

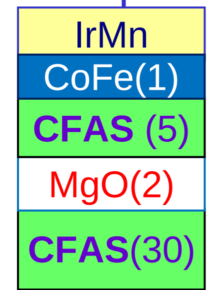
Heusler in Spintronic Devices: TMR

$Co_2FeSi_{1-x}Al_x$







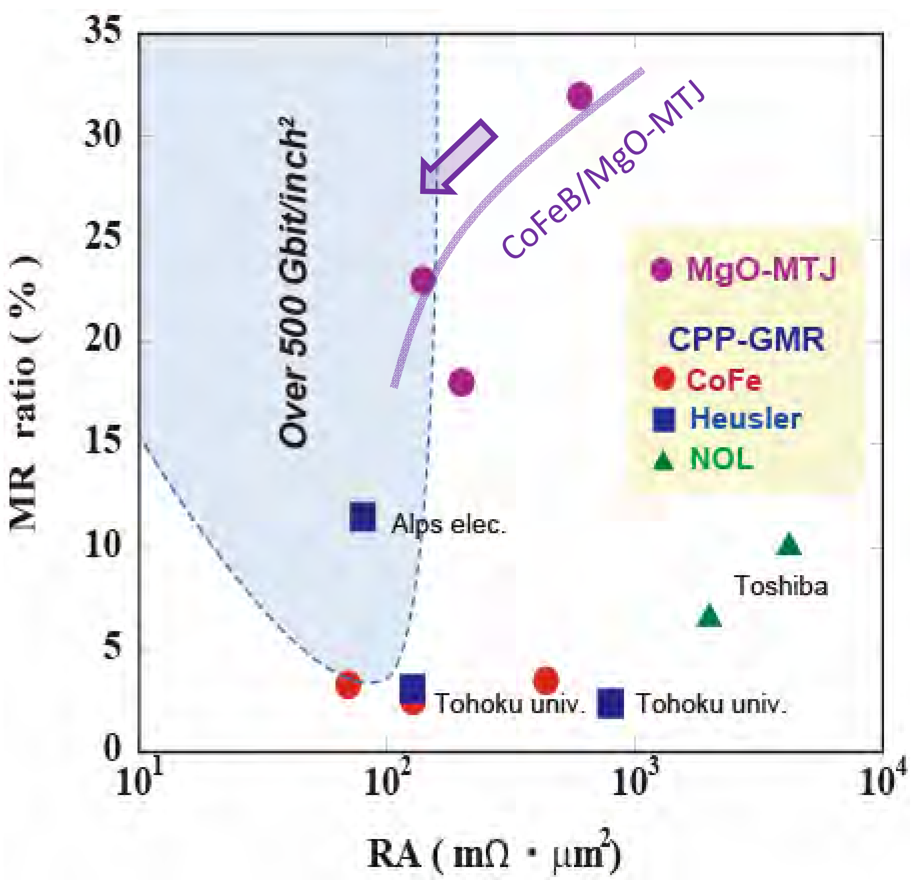


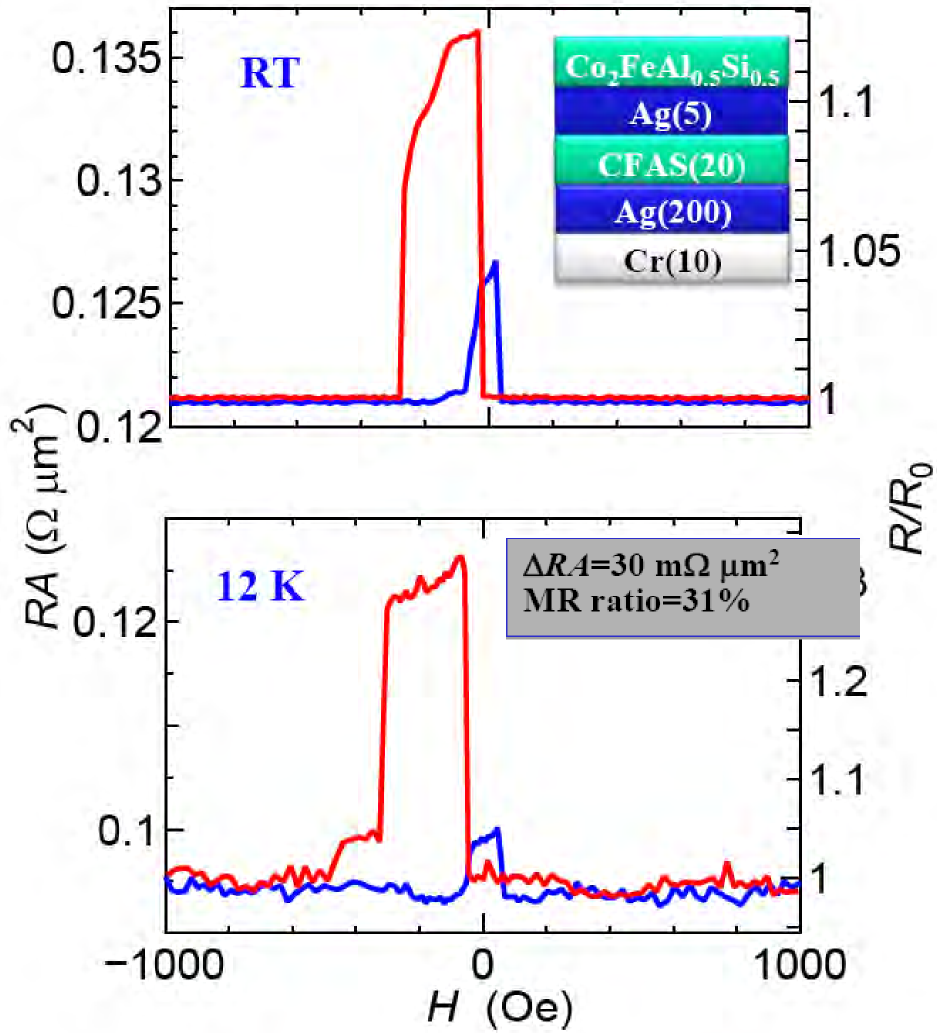
Fecher, Felser J. Phys. D **40** 1582 (2007)

N. Tezuka et al.,Jpn. J. Appl. Phys. **46**, L454 (2007)

Heusler in Spintronic Devices: CPP-GMR

Courtesy of Koki Takanashi, Sendai





Challenge: fitting spacer

Interlayer exchange coupling!

Inomata et al. to be published

Ferrimagnets

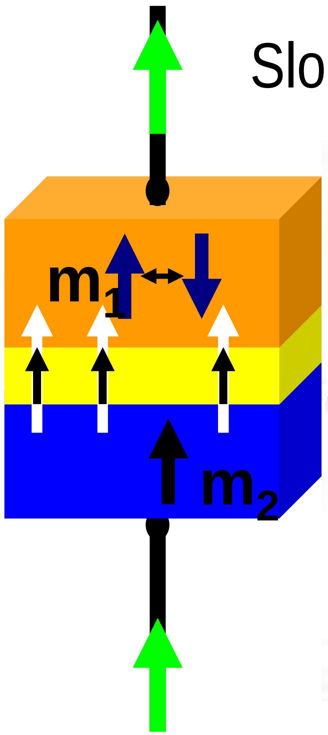
Application: Spintorque

Compensated ferrimagnet?

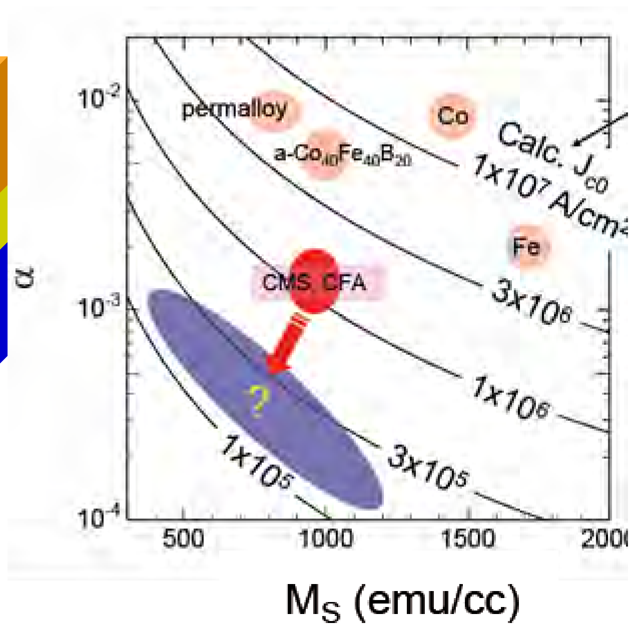
no net magnetization
two magnetic sublattices
with compensating moments

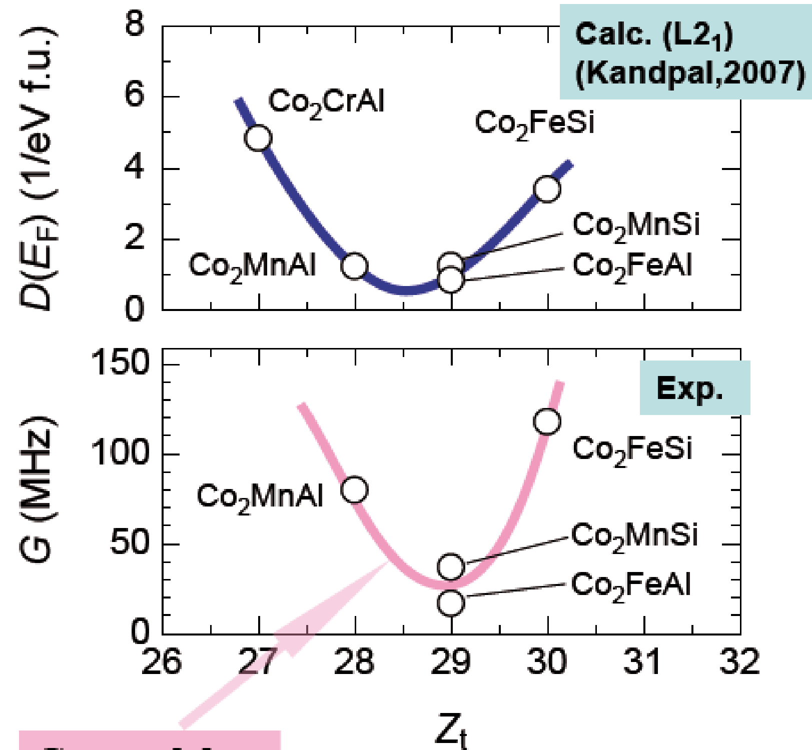
Warren E. Pickett Phys. Rev. B 57 (1998) 10613.

Spin transfer switching



Sloczewski 1996





$$G = \gamma \alpha M_s \propto D_\uparrow + D_\downarrow$$

$J \approx 1 – 100\ \mathrm{MA/cm}^2$

$$J \approx \frac{e}{\hbar g} \alpha M_s H_U d$$

Heinrich et al. (JAP2004)

Yilgin et al. (IEEE2005)

Yilgin et al. (JJAP2007)

Oogane et al. (JAP2007)

reduction of α & M_S

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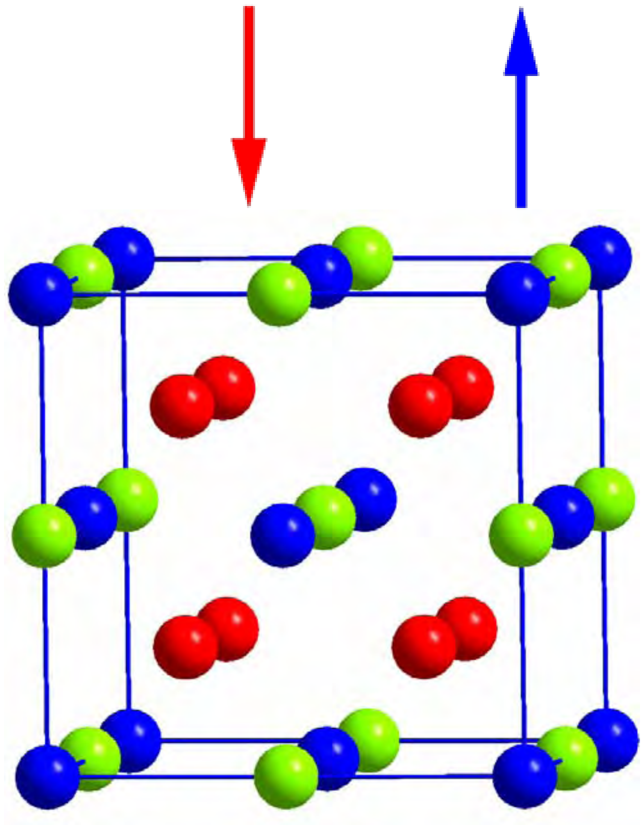
Courtesy after Shigemi Mizukami

Halfmetallic Ferrimagnet



Kübler's Rule
Slater Pauling Rule

Mn_2MnGa

Two magnetic sublattice
•24 Valence electrons – 0 μ_B
•Mn^{3+} at octahedral site – 4 μ_B
•Mn compensates

⇒Compensated ferrimagnet

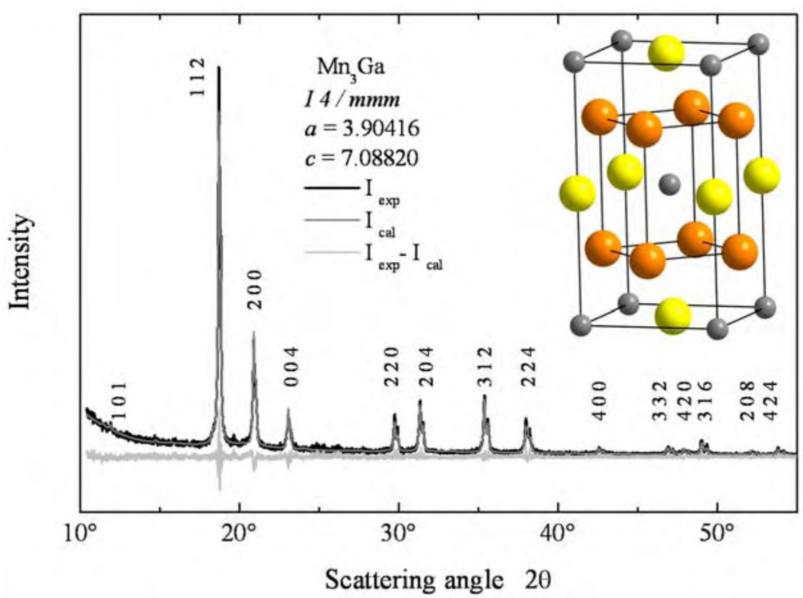
Wurmehl, et al. J. Phys. Cond. Mat**. 18** (2006) 6171
Balke et al. APL **90** (2007) 152504

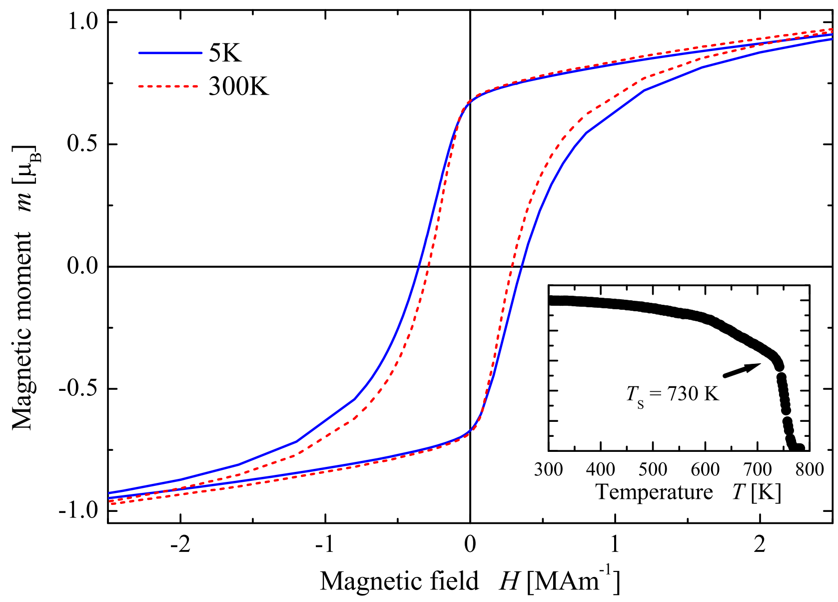
Compensated Ferrimagnet: Heusler

Mn_2MnGa

Low Moment – High Curie Temperature: low current for spinswitch

Tetragonal distorted Heusler: Mn^{3+} Jahn Teller Ion



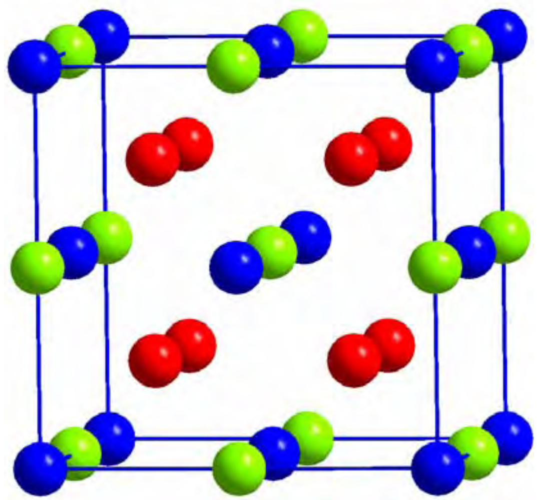


Compensated ferrimagnet: $1\mu_B$
Theoretical Spinpolarisation: 88%
Curie temperature: 730 K

Balke et al. APL **90** (2007) 152504
Winterlik et al. Phys. Rev. B **77** (2008) 054406

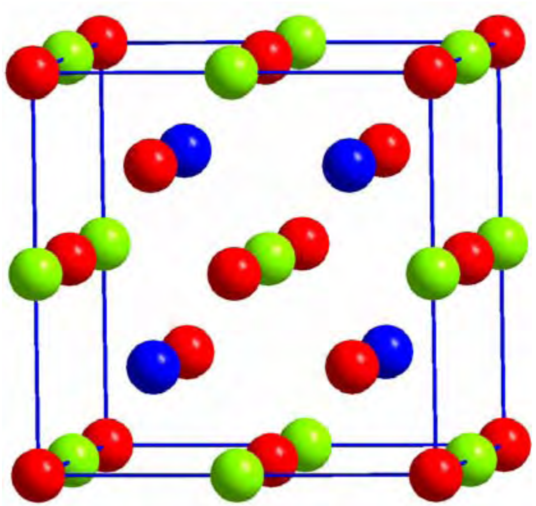
Heusler and relates Structures

X_2MnZ



XMnMnZ

XCrCrZ



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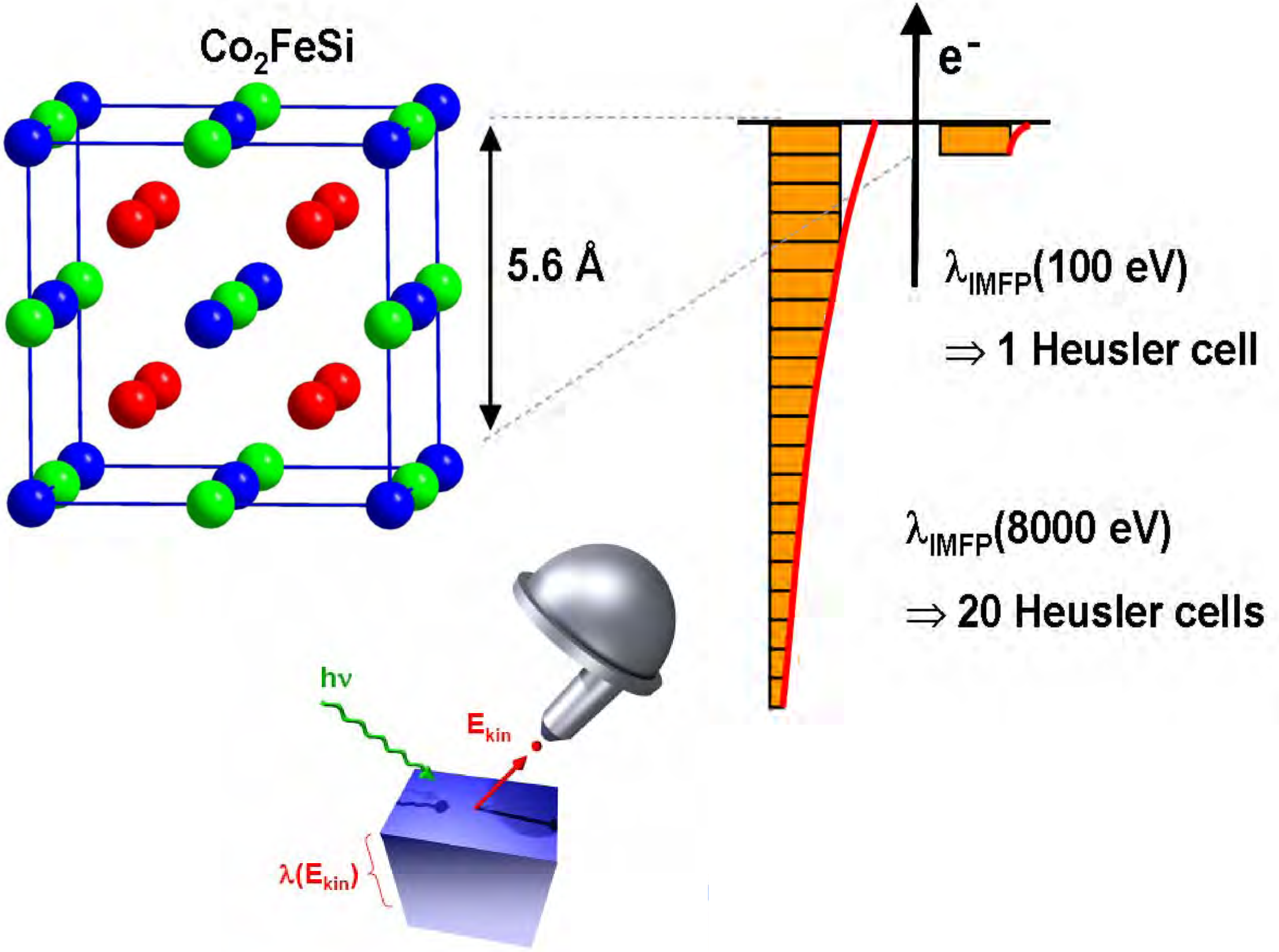
High Energy Photoemission



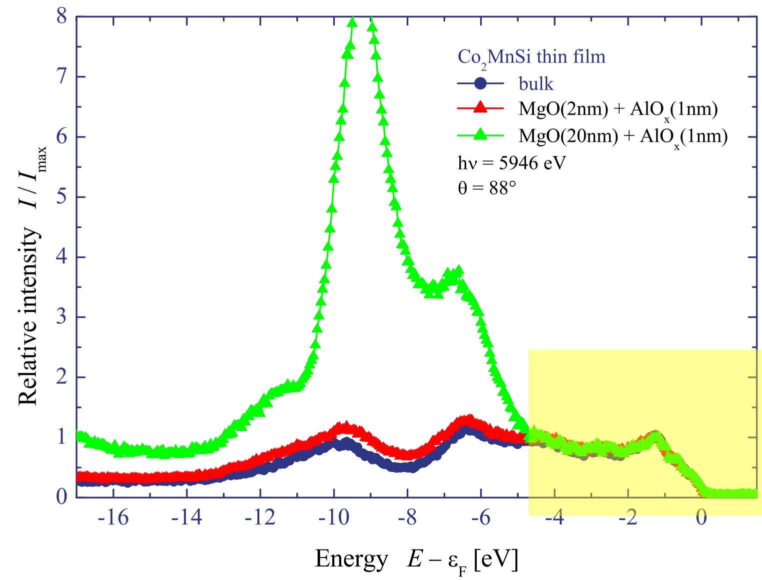
High Energy Photoemission: buried films

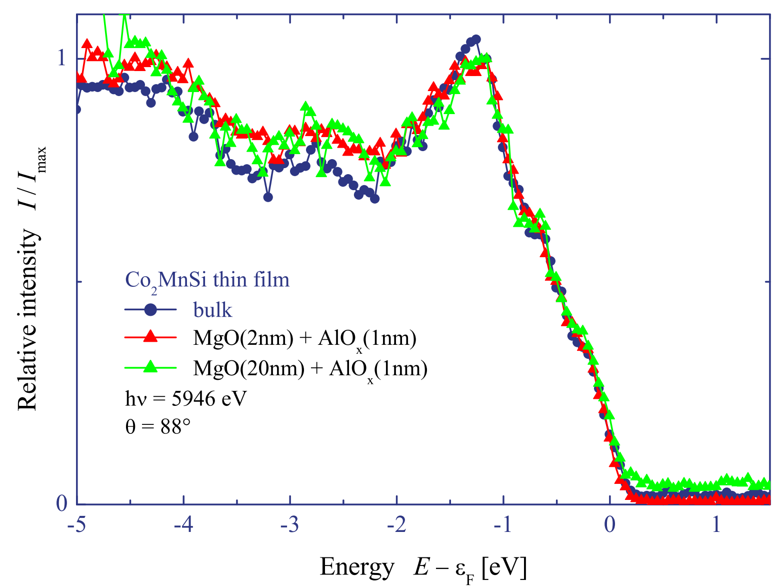
hν = 7.94 keV

Films Yamamoto Sapporo

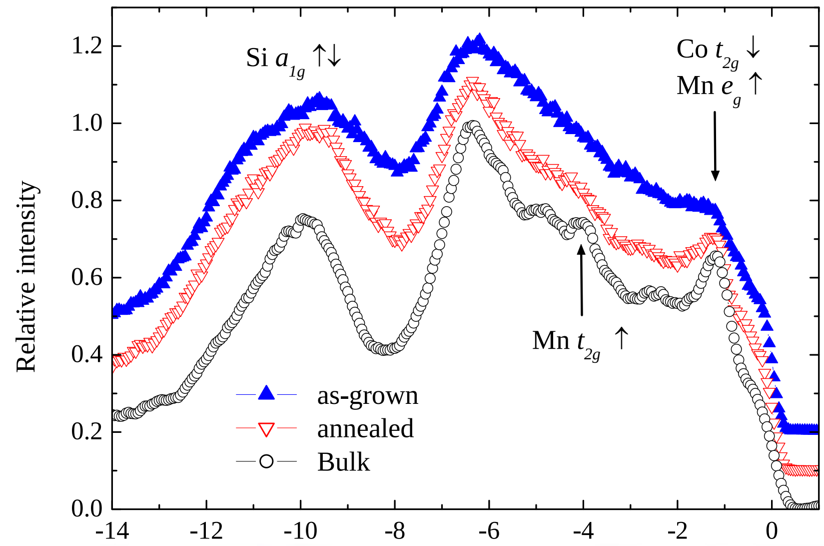
Measurements SPring8

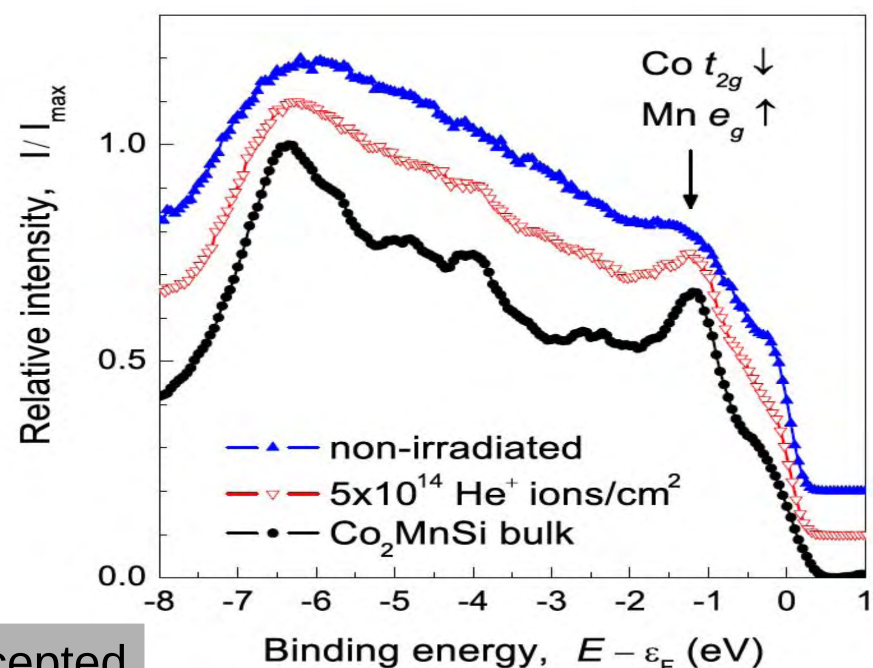
Fecher et al. APL **92** 195313 (2008)





Film quality studied by High Energy PES





$h\nu$ = 7.94 keV

Annealing and Irradiation improves the film quality

Ouardi et al. J. Phys. D (2009) accepted

TOHOKU UNIVERSITY

Summary

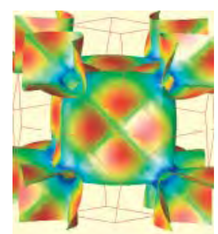
- Half Heusler compounds (Stuffed ZnS) are candidates for thermoelectric applications and for diluted semiconductors
- Nanostructured Heuslers are need for low thermoconductivity
- Heusler compounds are half metals with high Curie temperatures Co_2YZ
- Compensated ferrimagnetic Heuslers Mn_2YZ with 24 Valenceelectrons
- Halfmetallic ferrimagnets for spintorque application Mn_2CoZ
- High energy photoemission is an excellent tool to study devices
- SPINHAXPES is needed

Co-workers

JST-DFG Project:

- NIMS, Tohoku: K. Inomata
- Saporro: M. Yamamoto
- SPring8: K. Kobayashi

Deutsche Forschungsgemeinschaft DFG



MultiMag

HeuSpin

Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit

Dresden: S. Wurmehl

Augsburg: A. Reller

FG 559: G. Jakob, B. Hillebrands, J. Kübler, Y. Ando (Tohoku)

DFG-FG559, FE633, SP1166, BMBF: HEUSPIN, MULTIMAG

MATERIALS SCIENCE IN MAINZ