Epitaxial Fe/Si/Fe(001)
Structure and Magnetism of a Unique System

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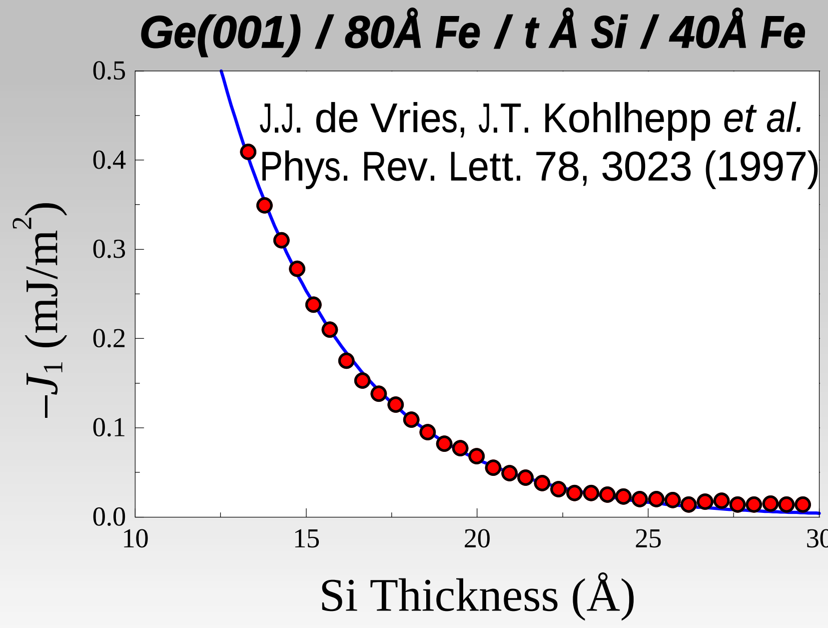
Motivation (1)

- exploring new materials, combining ferromagnetic metals (Fe, Co, ...) and traditional semiconducting materials (Si, Ge, ...)
- new type of interlayer exchange coupling
- investigation of iron-silicide formation in well-defined systems

Motivation (2)

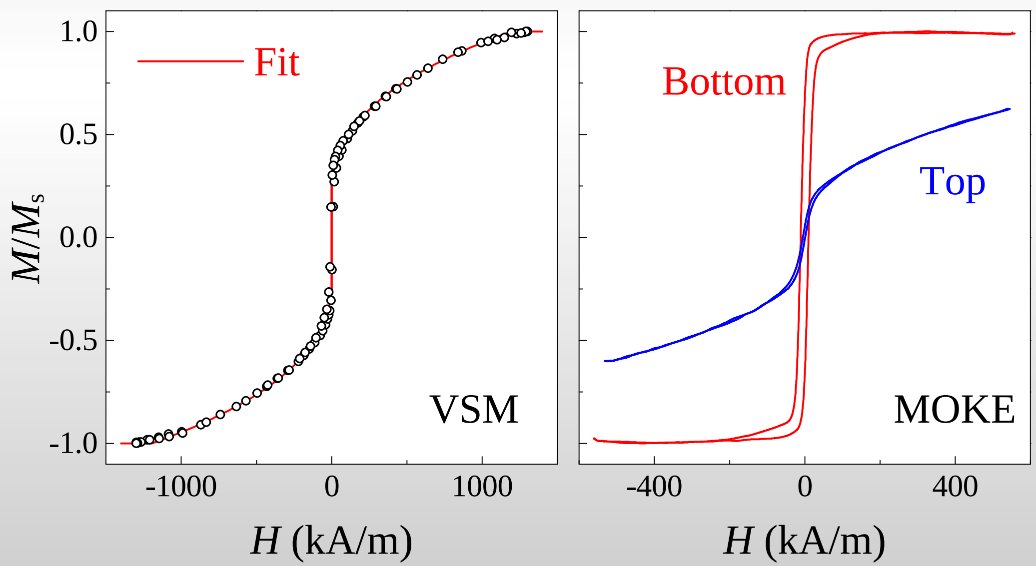
- ***bilinear (antiferromagnetic) coupling***
  in epitaxial Fe/Si/Fe(001) sandwiches and textured Si/Fe(110) multilayers observed

- formation of *c*-FeSi in the spacer
  - special band structure and density of states features
  - Fermi - surface of *c*-FeSi



- additionally, observation of a strong ***biquadratic (orthogonal) coupling***
  however, origin was still unknown

- Fe/Si multilayers are not suitable for studying biquadratic coupling



J.T. Kohlhepp *et al.*
Phys. Rev. B 55, R696 (1997)

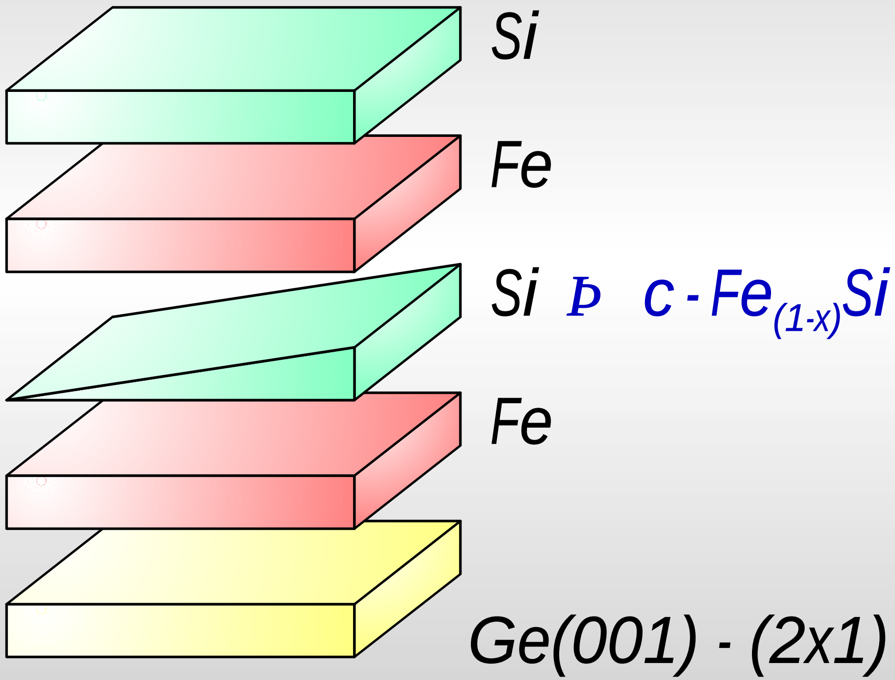
Þ ***well-defined MBE grown trilayers***

Þ ***temperature dependence of coupling strengths***

Experimental

preparation

MBE - grown sandwiches



characterization

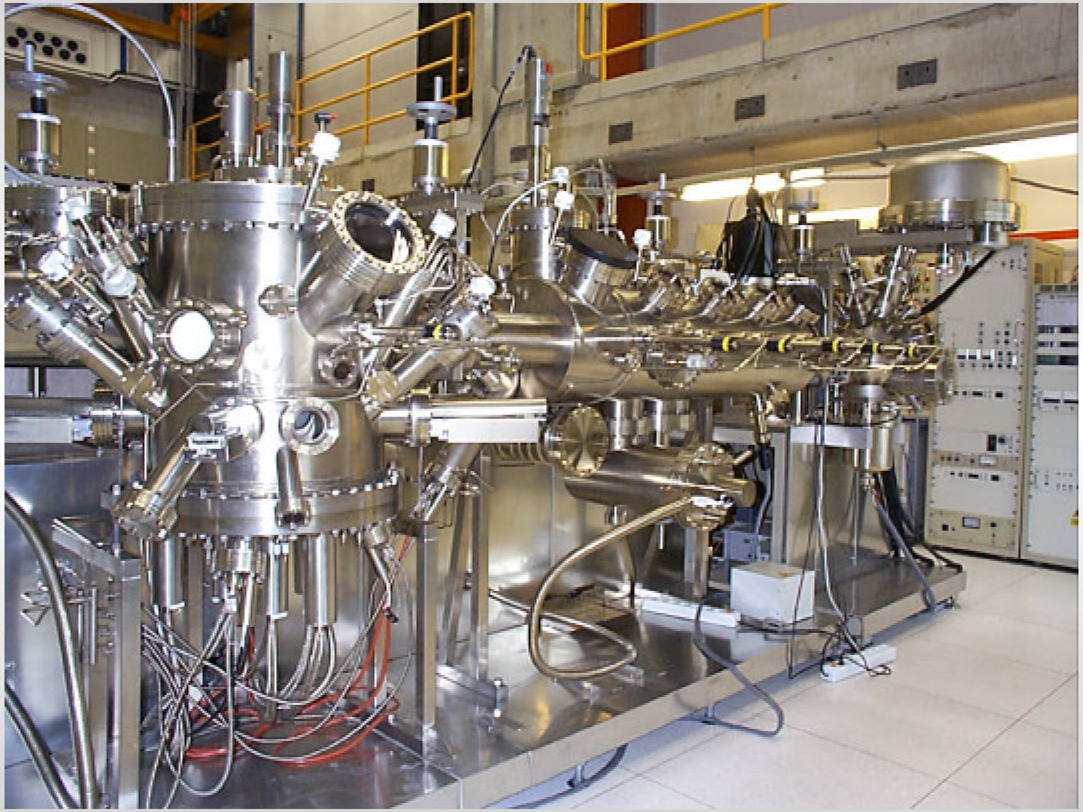
in-situ:

- AES
- XPS
- LEED
- STM

ex-situ:

- temperature dependent MOKE
- SQUID
- Mössbauer spectroscopy (CEMS)
- XRD
- Polarized Neutron Reflectometry (ISIS, Rutherford Appleton Labs)

VG Semicon V80M MBE system



features:

- base pressure < 2×10^{-11} mbar
- separate growth, preparation and analysis chambers
- deposition chamber:
  - 3 e-guns, 4 Knudsen cells
  - quartz crystal monitors
  - RHEED
  - variable temperature 240-1100 K
- preparation chamber:
  - sputter cleaning (300-1100 K)
  - LEED
  - fast entry load lock

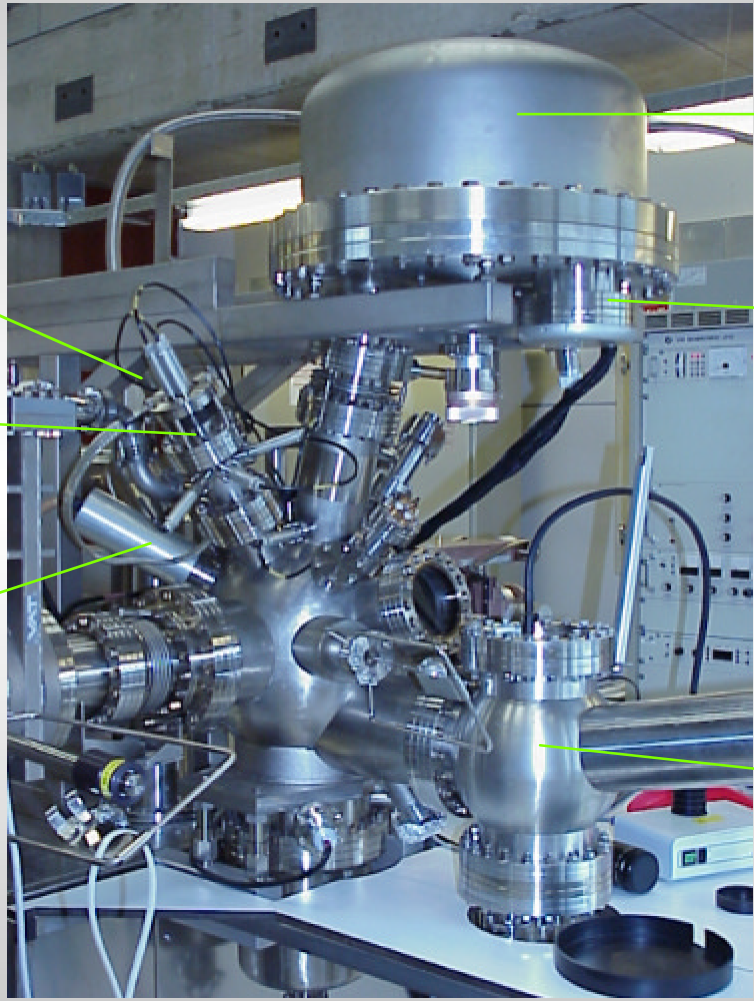
VG Semicon V80M MBE system

- surface analysis chamber (ESCA - lab) -

Al / Mg twin anode
X-ray source

10 keV electron gun

photomultiplier (SEM)



electron energy
analyzer

triple channeltron
detector

Omicron
STM1

/n

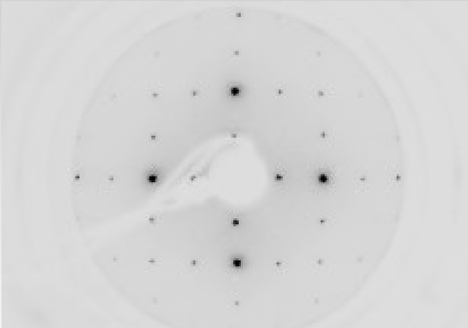
cNM

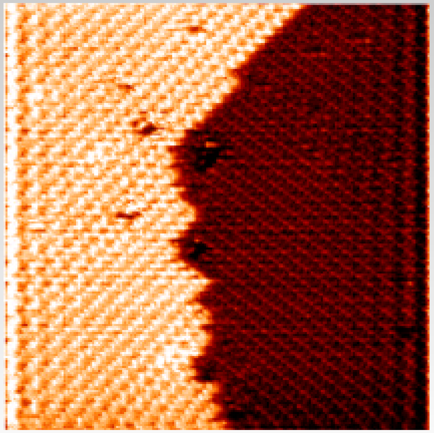
Properties of Fe on Ge(001)

LEED

STM

Ge(001)
2x1

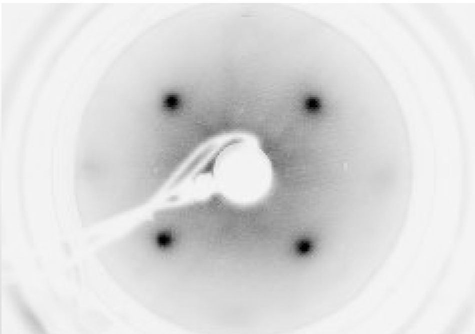


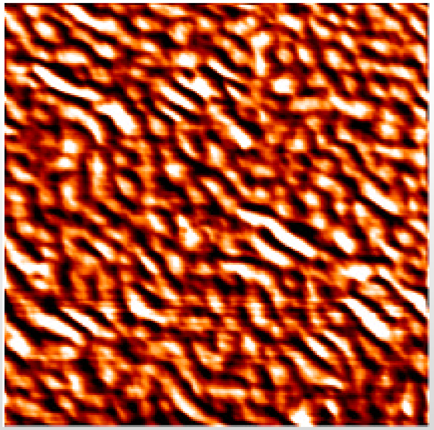


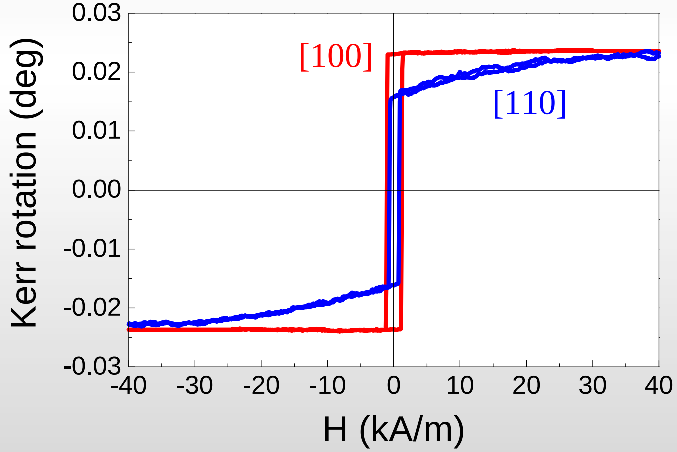
25 x 25 nm², atomically flat

MOKE

+ 60Å Fe







bcc(001) growth

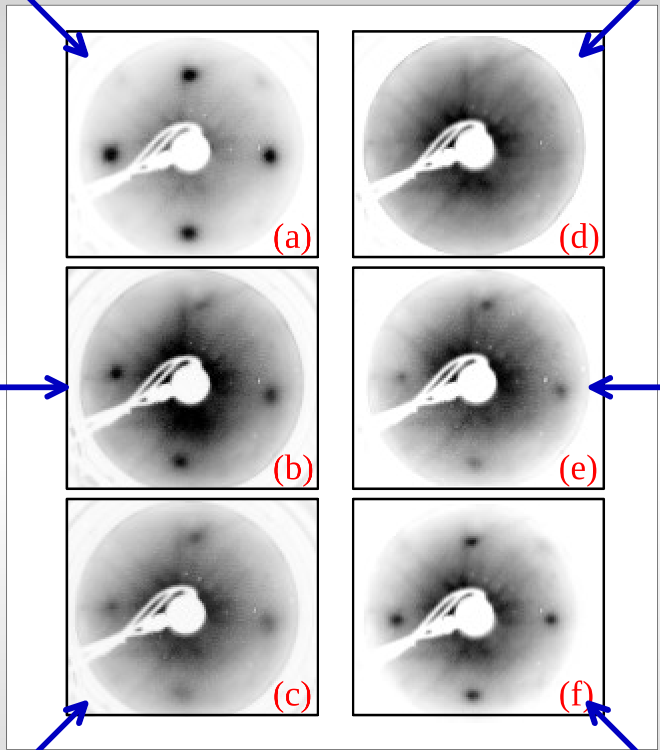
100 x 100 nm²
0.24 nm rms roughness

small coercivity
fourfold cubic anisotropy

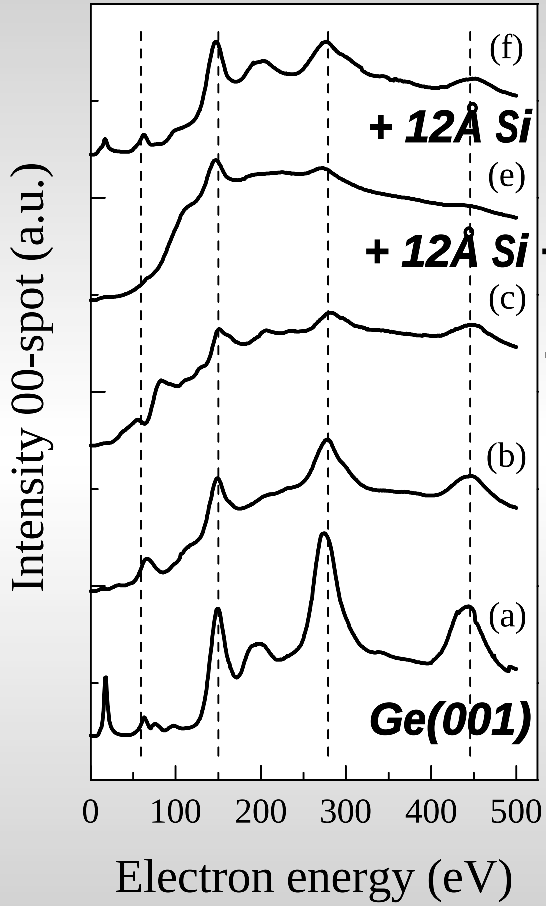
Structure of Ge(001)/Fe/Si/Fe

LEED studies:

Pattern:

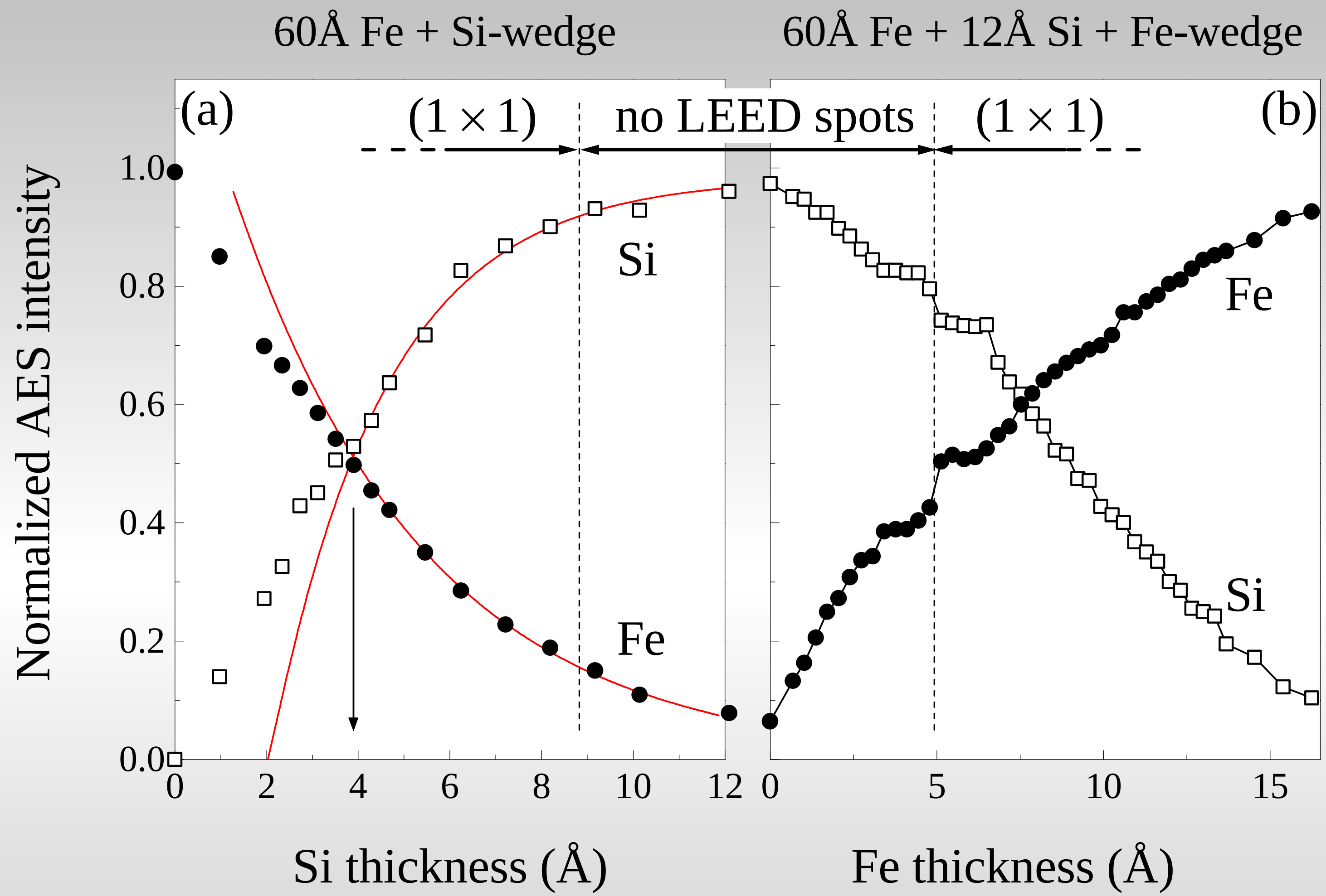


I-V spectra:



Þ *bcc-like (001)-structure maintained in stack*

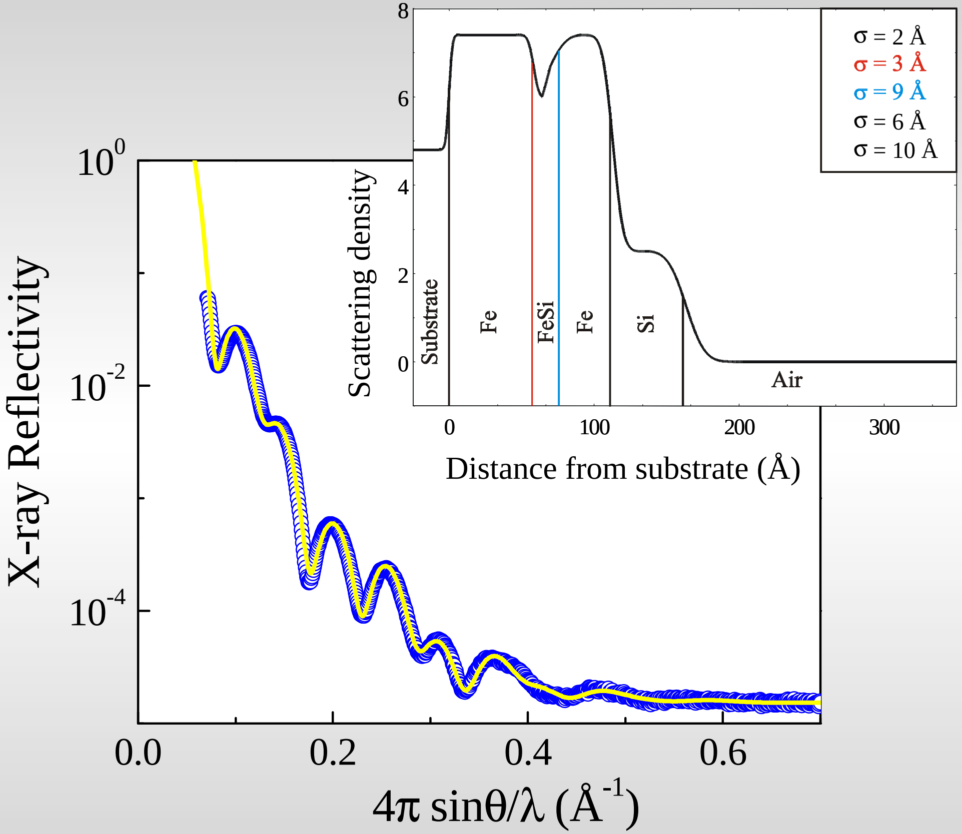
AES studies:



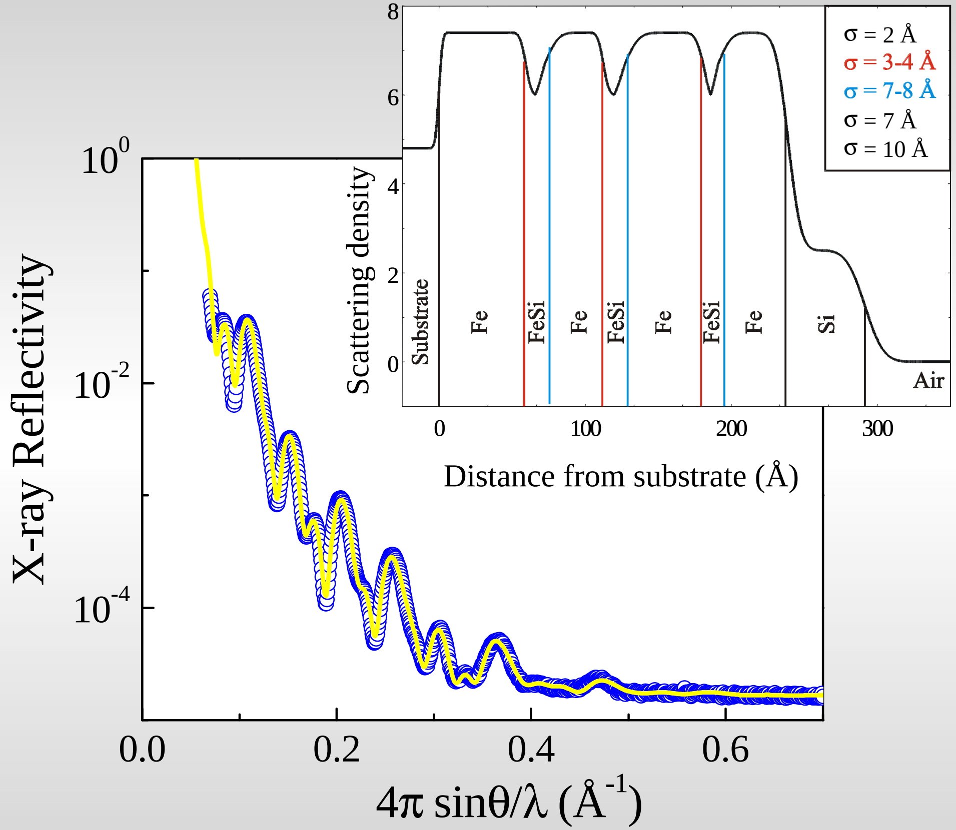
Þ **Fe diffuses from the bottom and top into the Si spacer accompanied by a reappearance of LEED spots**

GIXR studies:

Ge(001) / 60 Å Fe / 14 Å Si / 45 Å Fe / 40Å Si

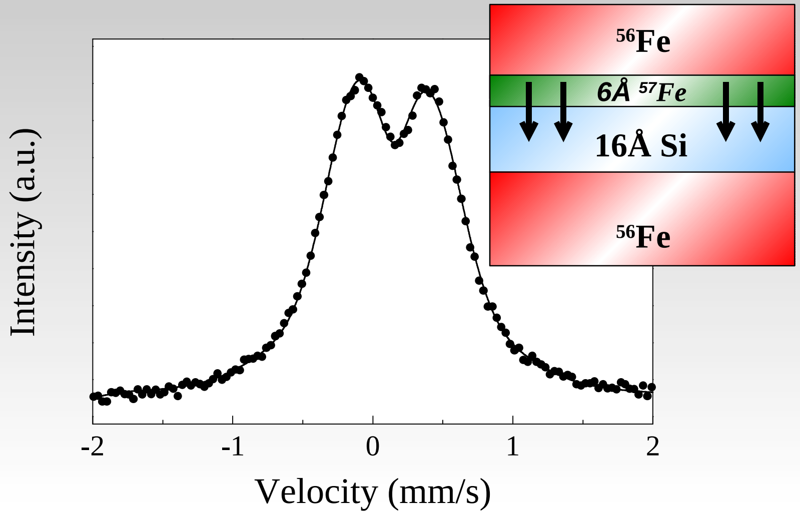


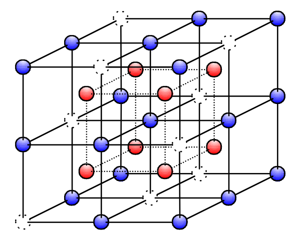
Ge(001) / (60 Å Fe / 14 Å Si / 45 Å Fe /14 Å Si)$_2$ / 26Å Si



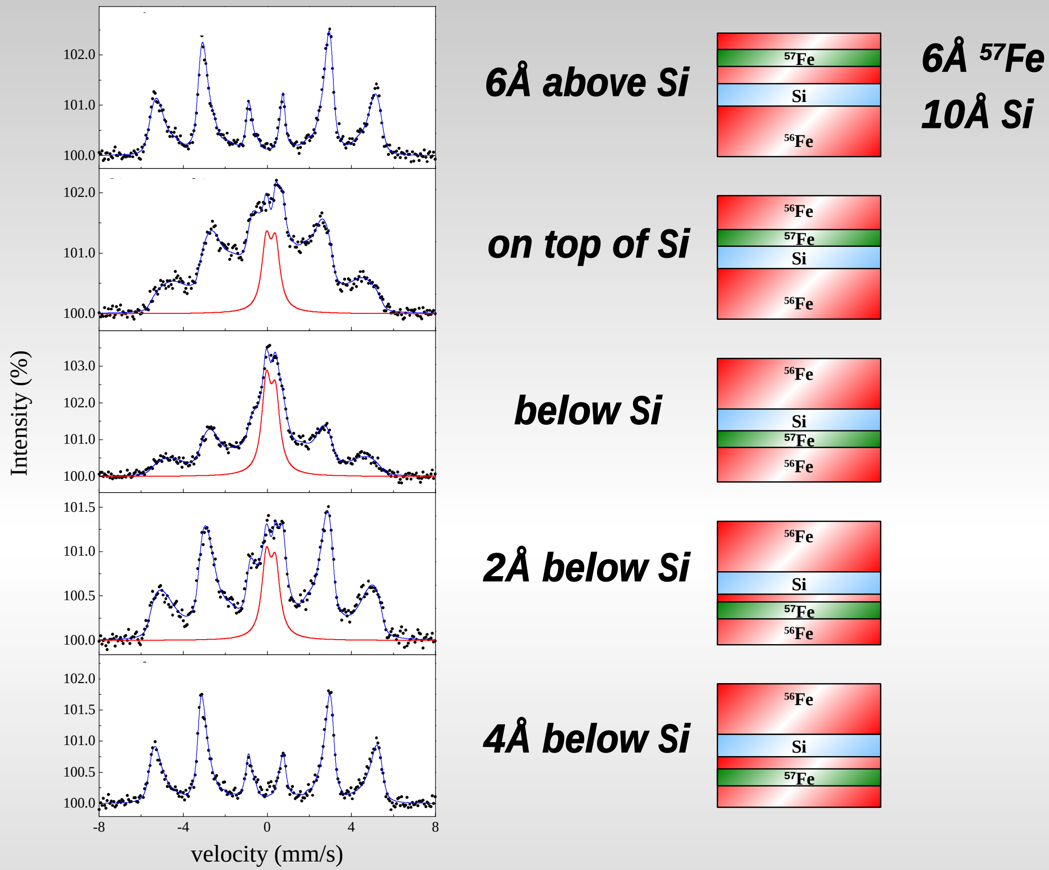
Þ Si spacer completely gone; transformed to FeSi

CEMS studies:





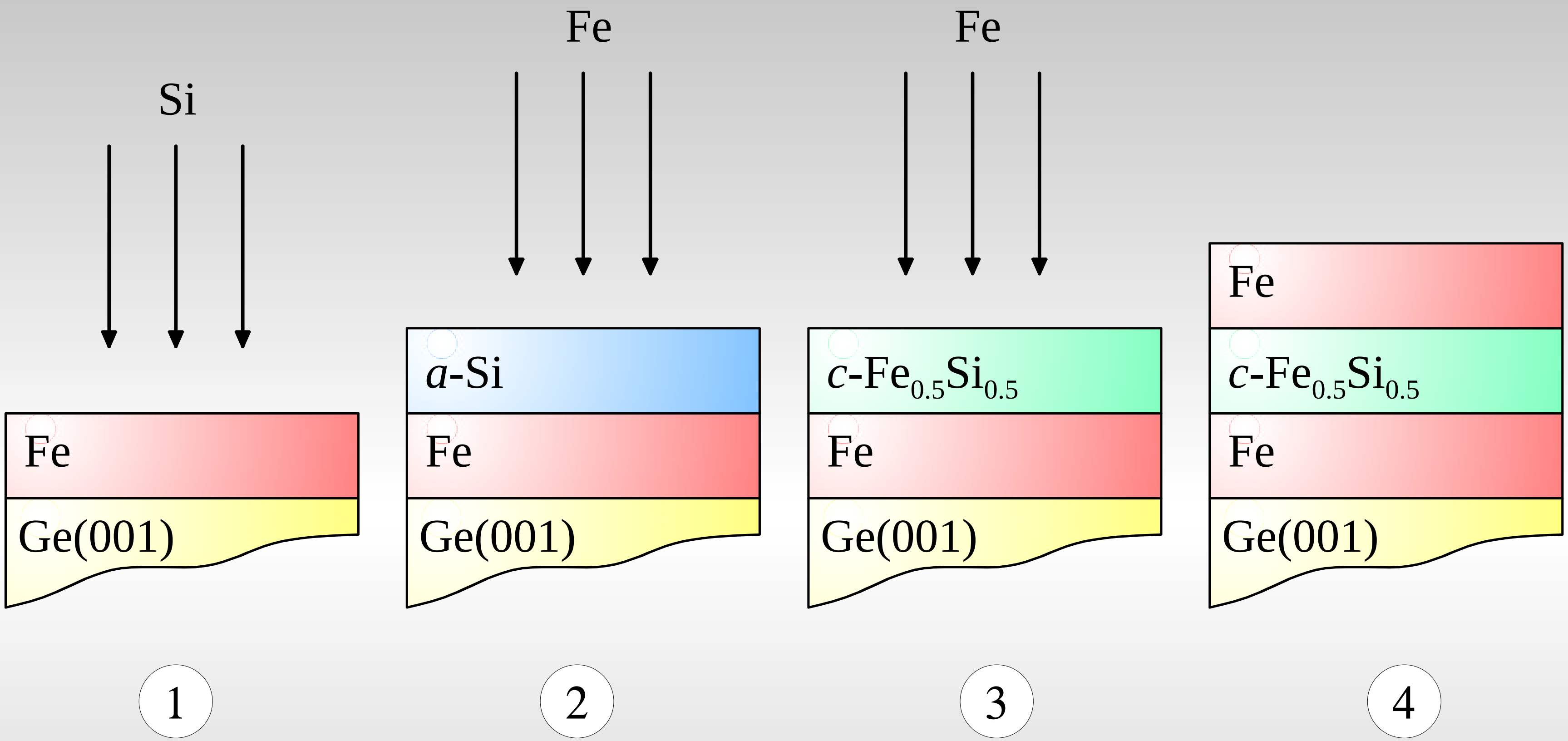
$Fe_{(1-x)}Si$ (CsCl)



G.J. Strijkers, J.T. Kohlhepp *et al.*
Phys. Rev. B 60, 9583 (1999)

Þ *c-$Fe_{(1-x)}$Si with metastable CsCl (B2) structure and x » 0.36 is formed in the spacer*

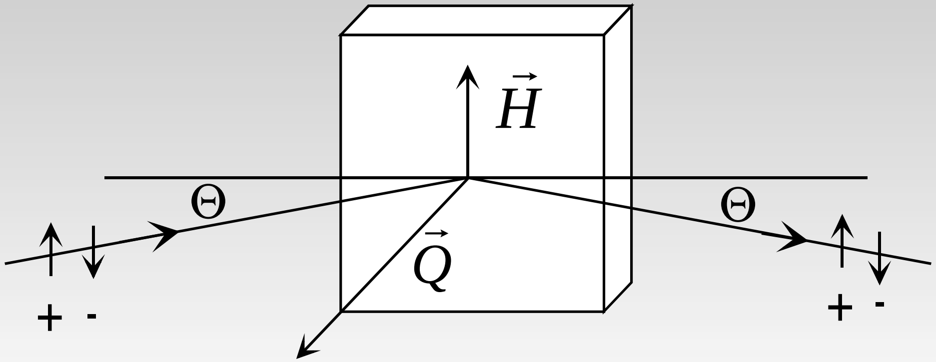
Summary: Iron-silicide formation (simplified)



$$t_{Si}\ \mathrm{Si} + 0.59 \cdot t_{Si}\ \mathrm{Fe} \rightarrow 1.06 \cdot t_{Si}\ \mathrm{Fe_{0.5}Si_{0.5}}$$

Magnetic Properties

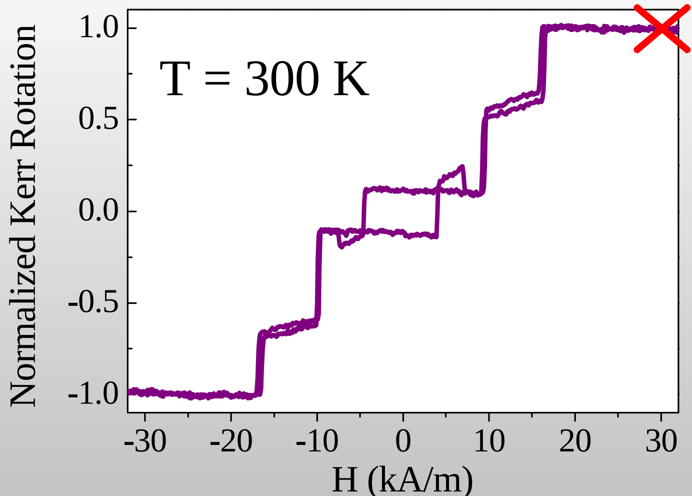
Spin Polarized Neutron Reflectometry:



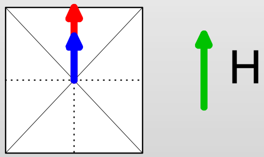
$$\left|\vec{Q}\right| = \frac{4p}{l}\sin\Theta$$

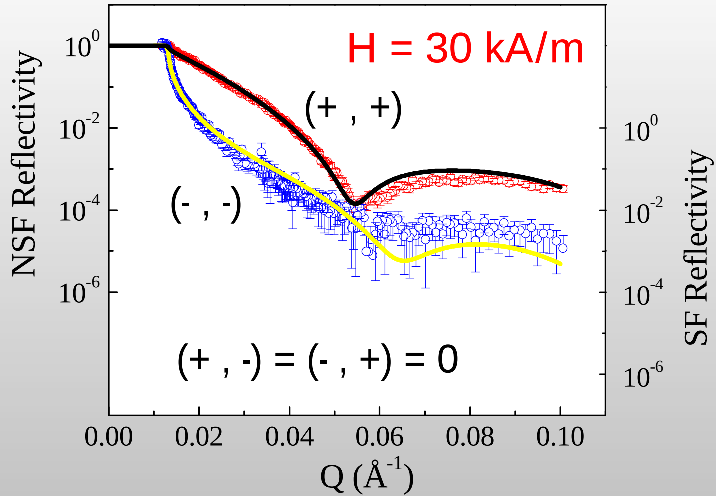
(+ , +) ; (- , -) : Non Spin Flip (NSF) Reflectivity
(+ , -) ; (- , +) : Spin Flip (SF) Reflectivity

Ge(001) / 60 Å Fe / 14 Å Si / 45 Å Fe / 40Å Si



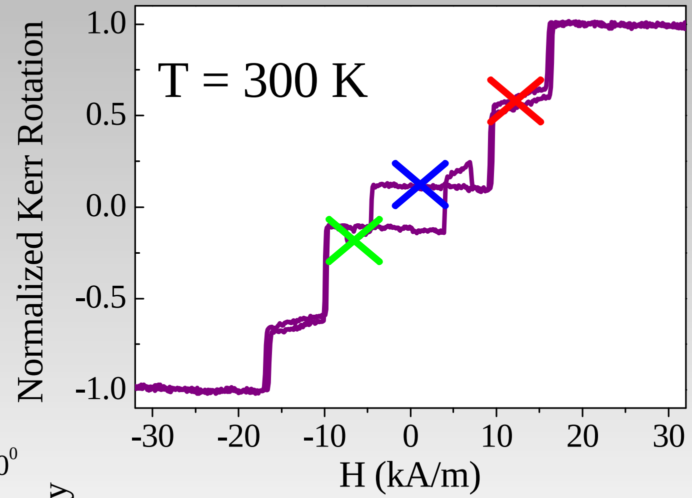
Saturation:



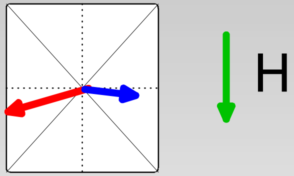


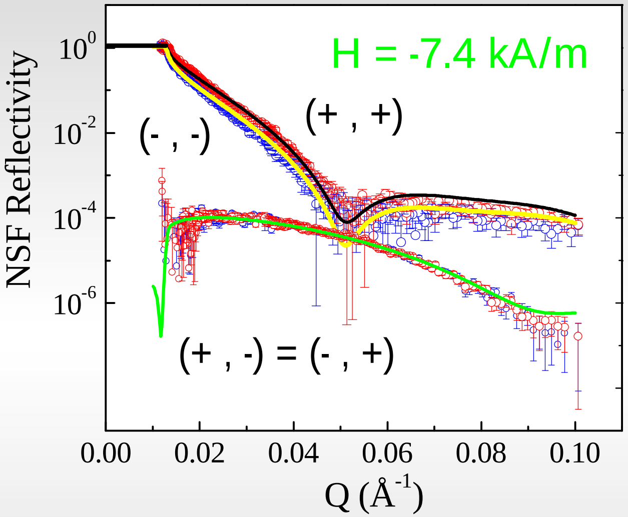
cNM

Magnetization reversal details at RT:

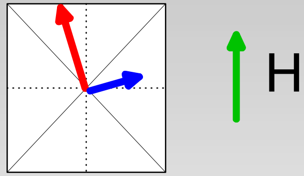


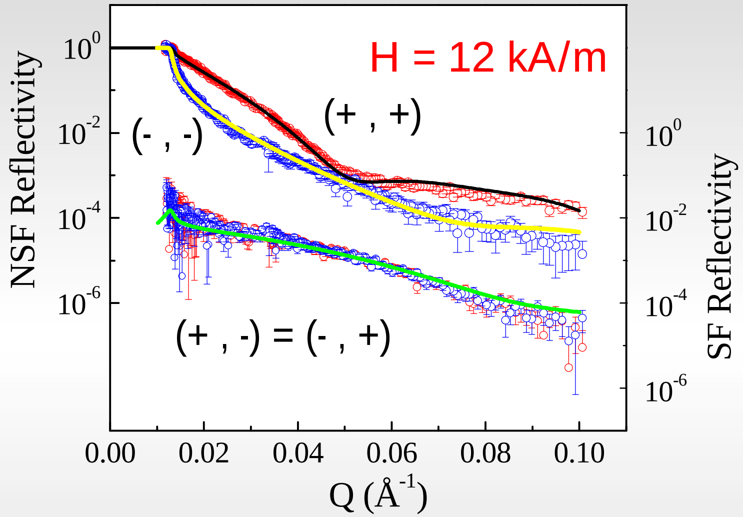
Spin flop:



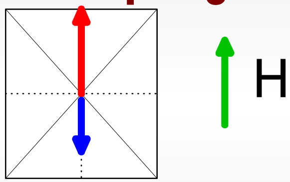


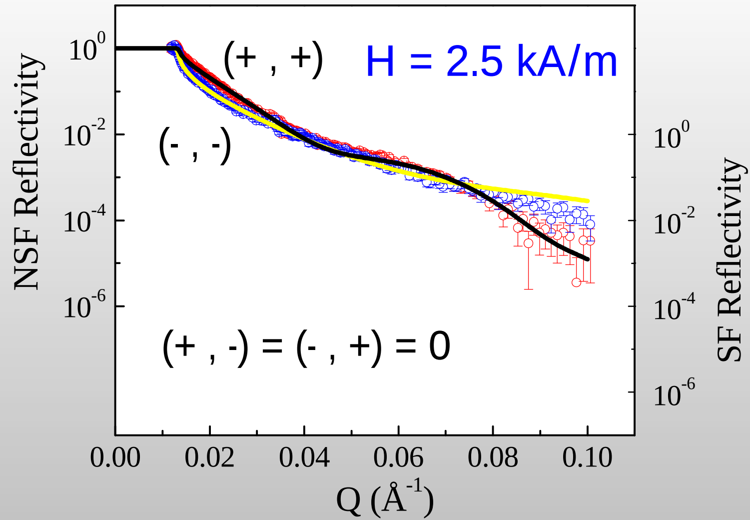
90 deg coupling:



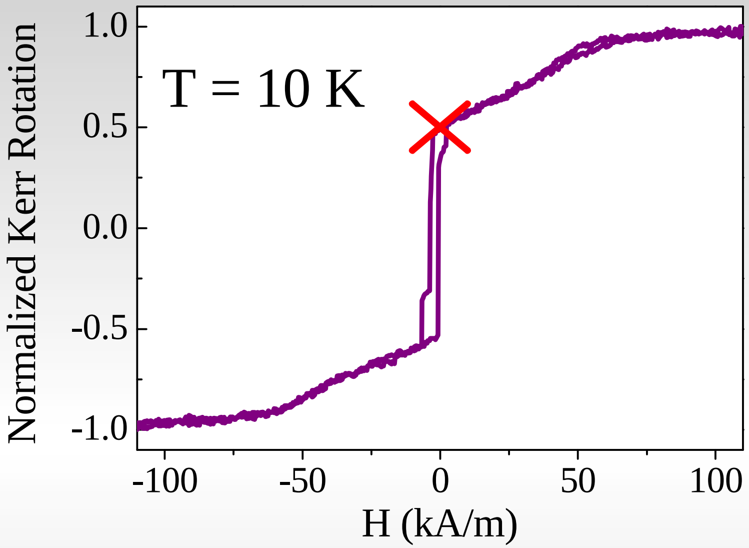


AF coupling:

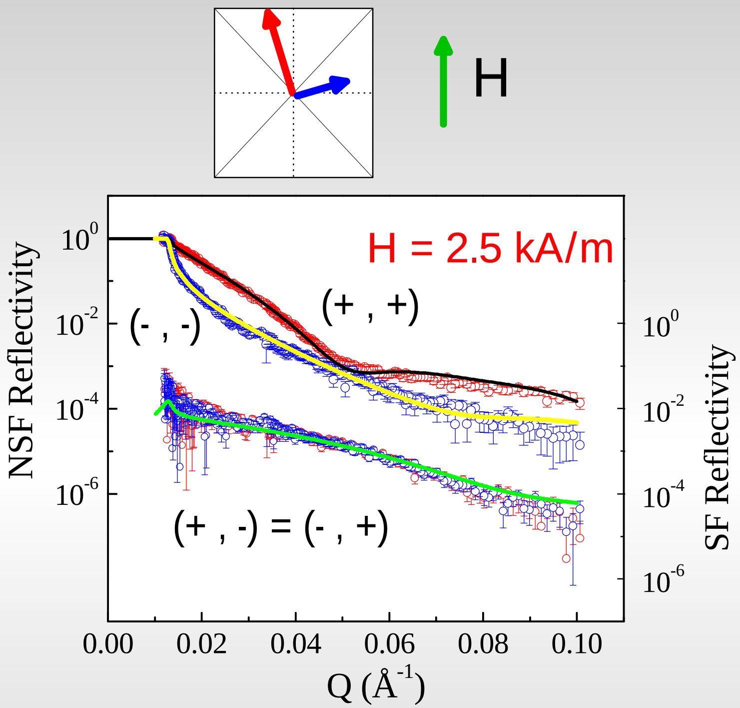




Magnetization reversal details at low T:



90 deg coupling:

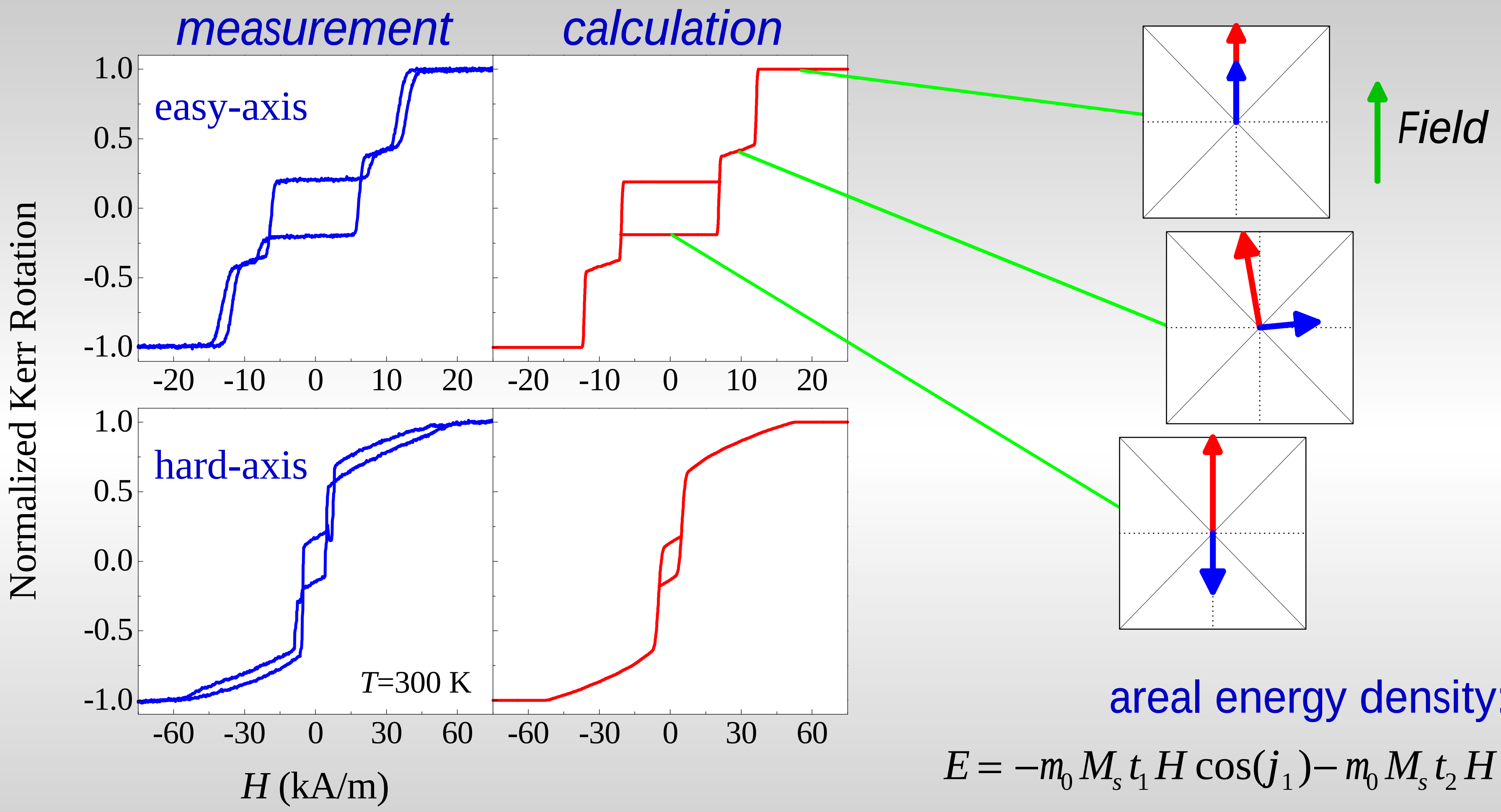


Þ ***biquadratic coupling dominates at low T***

R.W.E. van de Kruijs, J.T. Kohlhepp *et al.*
Phys. Rev. B (2002), accepted

Magnetization loops and simulation (1)

Ge(001) / 115Å Fe / 13.7 Å Si / 90Å Fe / 30Å Si



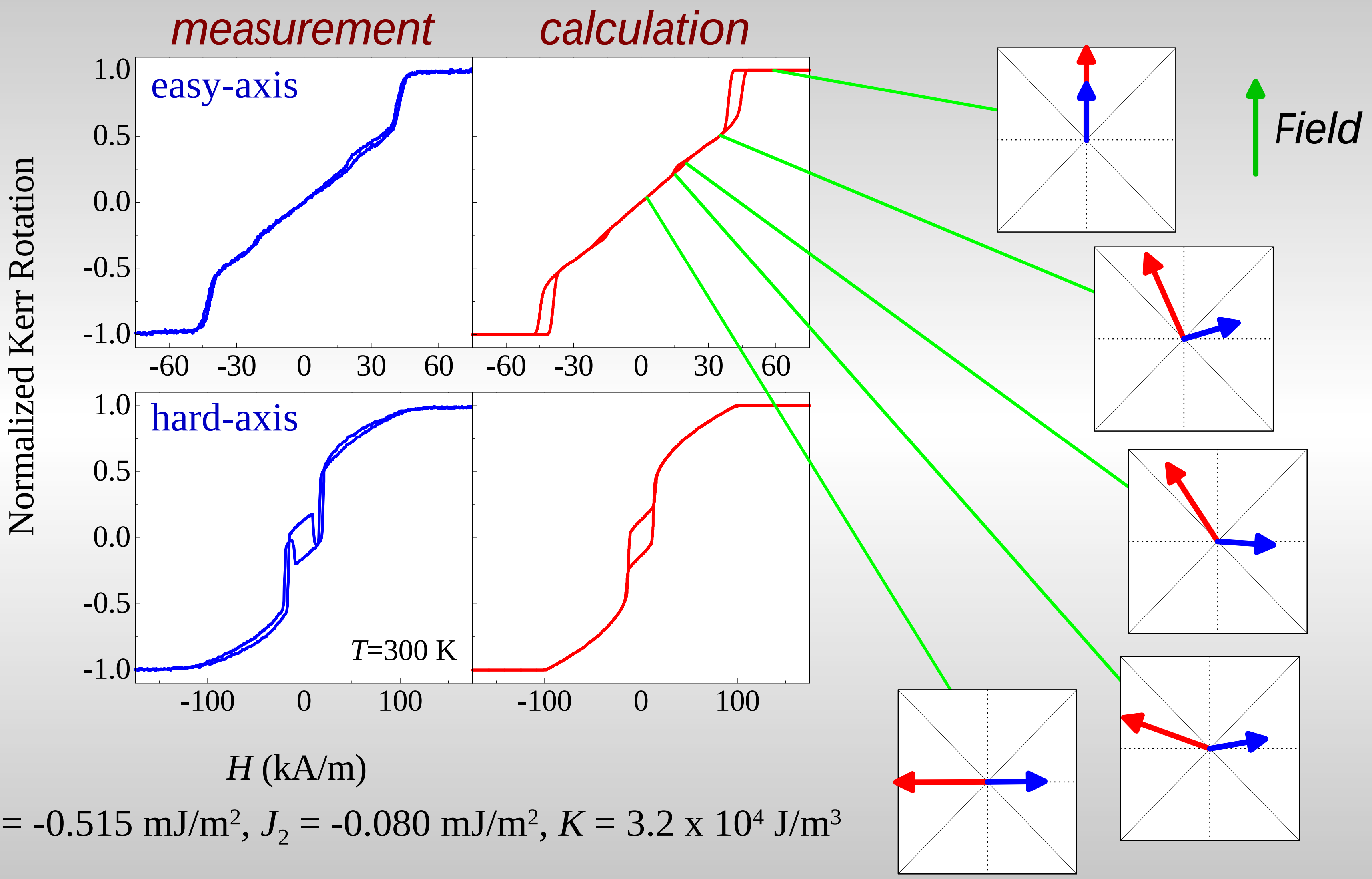
J_1 = -0.160 mJ/m², J_2 = -0.028 mJ/m², K = 3.2 x 10⁴ J/m³

areal energy density:

$$E = -\mu_0 M_s t_1 H \cos(\varphi_1) - \mu_0 M_s t_2 H \cos(\varphi_2)$$
$$+ K t_1 \cos^2(\varphi_1)\sin^2(\varphi_1) + K t_2 \cos^2(\varphi_2)\sin^2(\varphi_2)$$
$$- J_1 \cos(\varphi_1 - \varphi_2) + J_2 \cos^2(\varphi_1 - \varphi_2)$$

Magnetization loops and simulation (2)

Ge(001) / 115Å Fe / 12.4 Å Si / 90Å Fe / 30Å Si

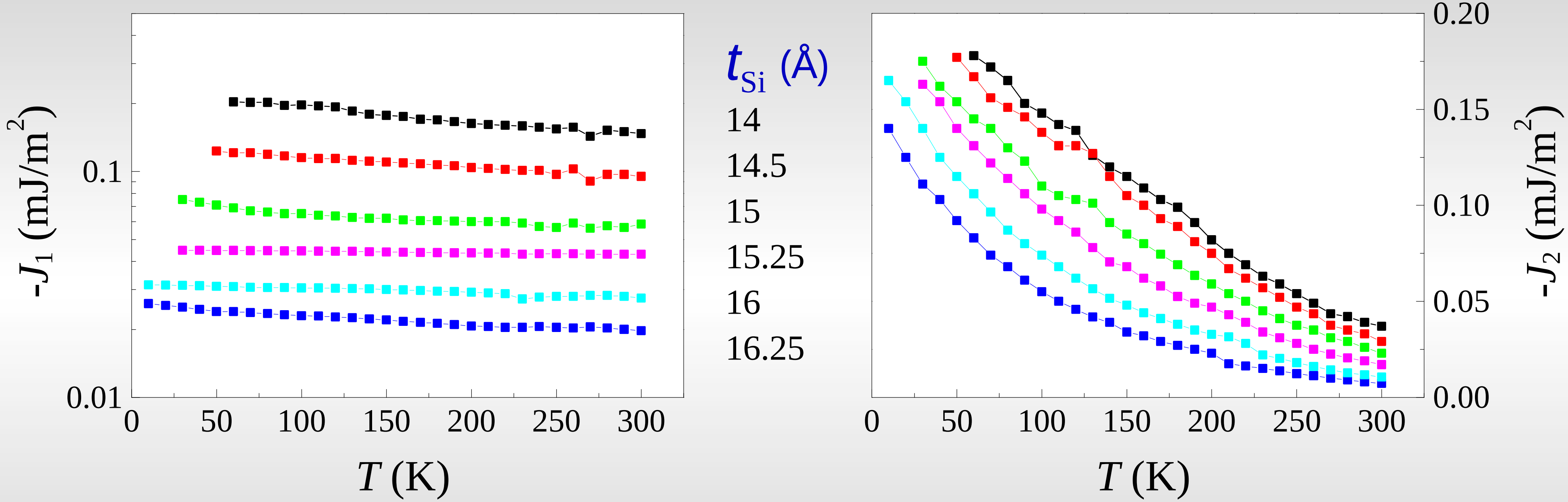


J_1 = -0.515 mJ/m², J_2 = -0.080 mJ/m², $K = 3.2 \times 10^4$ J/m³

Temperature dependence of coupling strengths

Ge(001) / 60Å Fe / t Si / 45Å Fe / 30Å Si

bilinear coupling | *biquadratic coupling*



↑ decreasing weakly with temperature

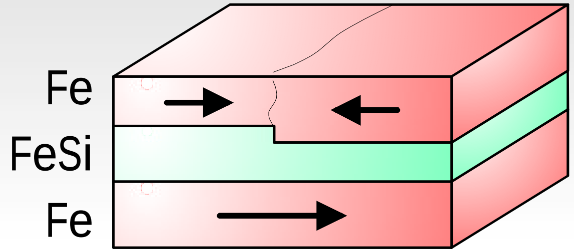
↑ strong temperature dependence

Possible origins of strong biquadratic coupling

✗ - intrinsic higher order term $J_2(T) \propto 2\, J_1(T)$

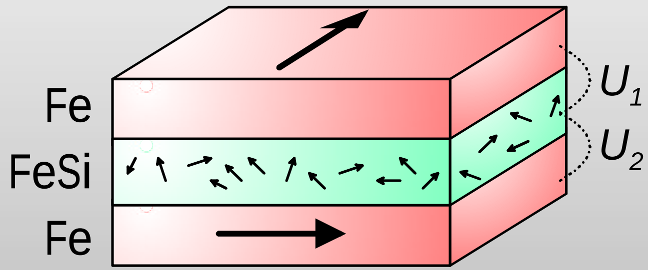
✗ - thickness fluctuations $J_2(T) \propto (J_1(T))^2$

J.C. Slonczewski, Phys. Rev. Lett. 67, 3172 (1991)



✓ - loose spins, strong temperature dependence of J_2

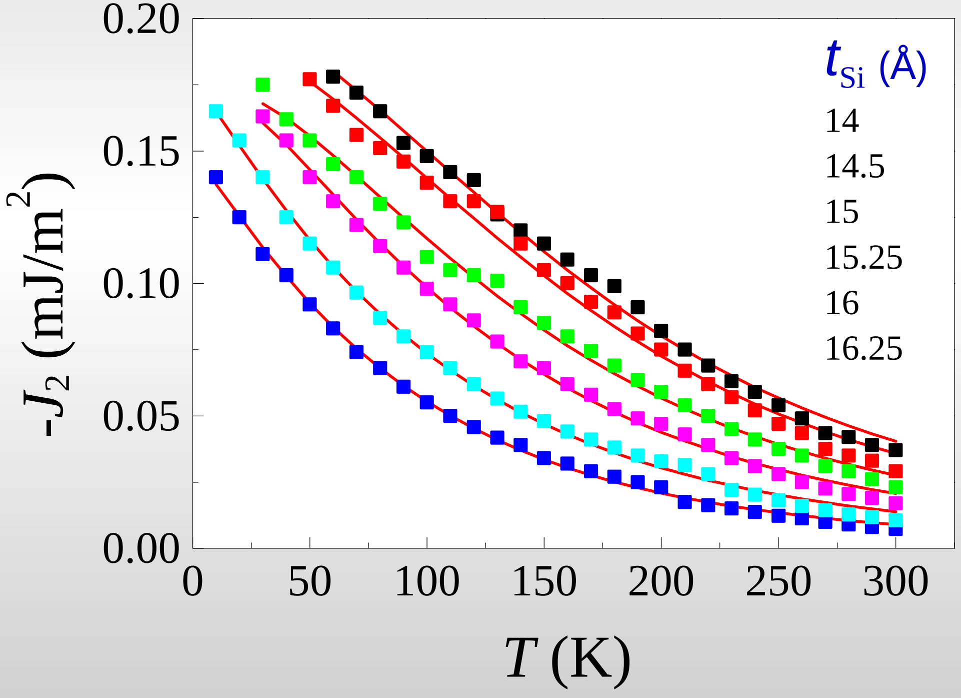
J.C. Slonczewski, J. Appl. Phys. 73, 5957 (1993)



Loose spins model

- strong temperature dependence of the biquadratic coupling can be described with the loose spins model

Ge(001) / 60Å Fe / t Si / 45Å Fe / 30Å Si



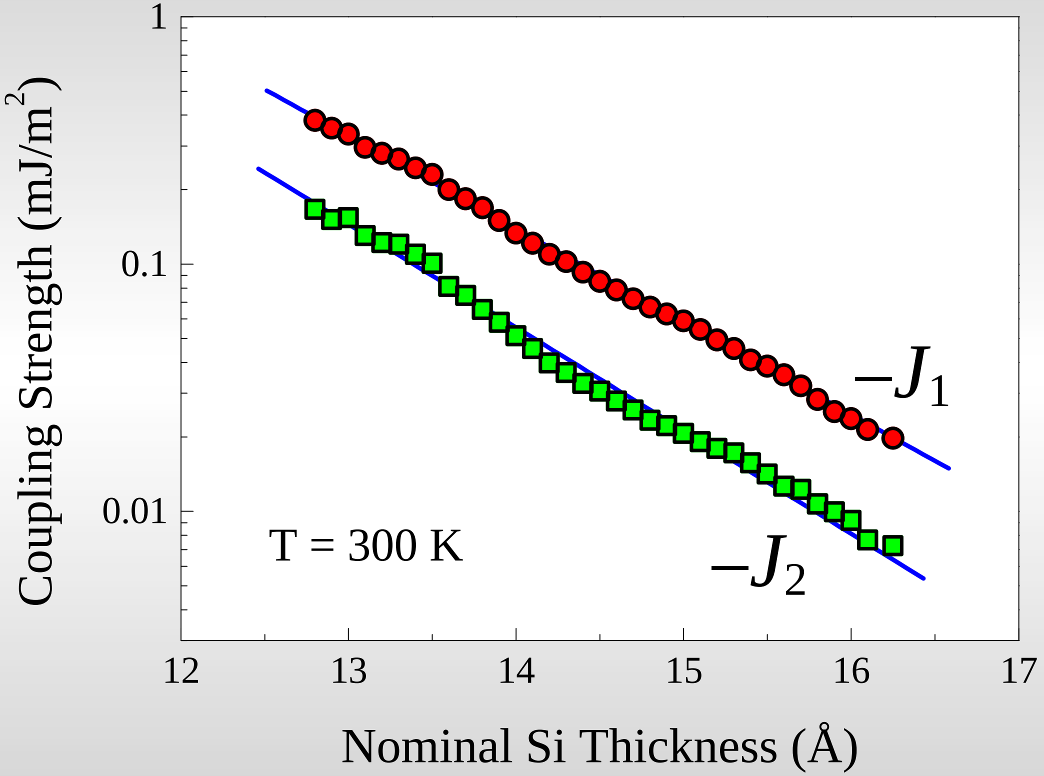
- concentration of 1% loose spins in the spacer
- interaction potentials $U_1 = U_2$
- interaction potential $U/k_B \approx$ 200 - 340 K

G.J. Strijkers, J.T. Kohlhepp *et al.*
J. Appl. Phys. 87, 5452 (2000)

Qualitative proof of loose spins model

- bilinear and biquadratic coupling constants should have the same thickness dependence because of the identical interaction potential !

Ge(001) / 60Å Fe / t Si / 45Å Fe / 30Å Si



- indeed both J_1 and J_2 decay exponentially with the spacer thickness with approximately the same decay length λ

Quantitative proof of loose spins model

- theoretical intrinsic J_1 under the assumption that loose spins are located at midplane:

$$J_1(t_{\mathrm{Si}}, 0\,\mathrm{K}) = a^{-2}\, e^{-t_{\mathrm{Si}}/2l}\, U(t_{\mathrm{Si}})$$

lattice constant (a) — interlayer coupling decay length (l)

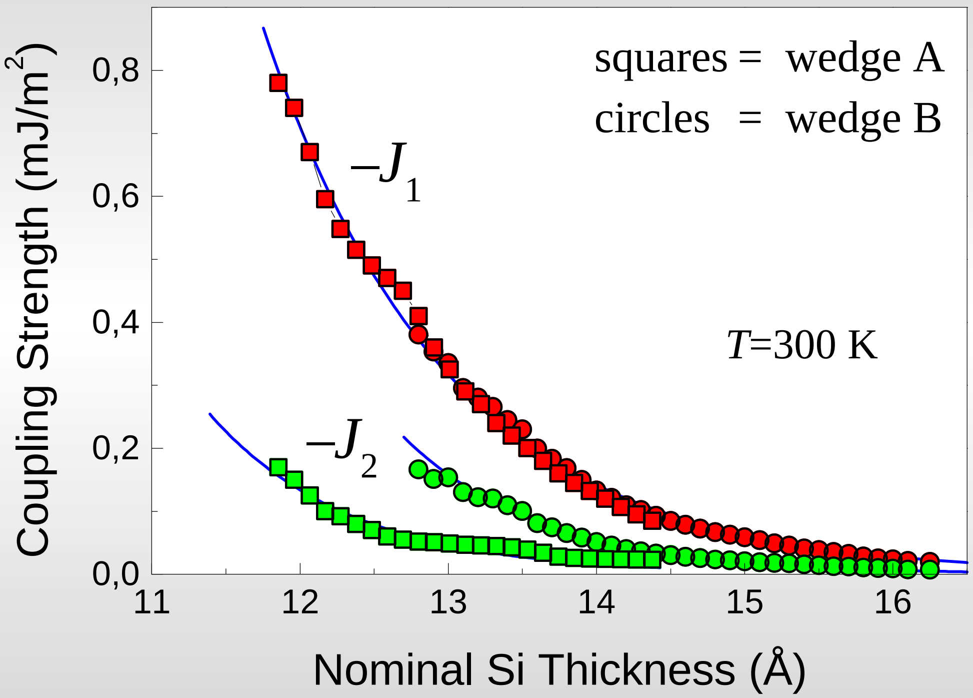
t_{Si} (Å)	J_1(calc) (mJ/m^2)	J_1(exp) (mJ/m^2)
14.25	0.104 ± 0.018	0.126 ± 0.010
15.00	0.072 ± 0.009	0.075 ± 0.008
15.25	0.058 ± 0.011	0.046 ± 0.004
16.00	0.035 ± 0.008	0.033 ± 0.005
16.25	0.028 ± 0.005	0.025 ± 0.003

G.J. Strijkers, J.T. Kohlhepp *et al.*
Phys. Rev. Lett. 84, 1812 (2000)

- good agreement between experimental and calculated values for J_1; but this is only correct if there is no bilinear loose spin contribution !

Is there a bilinear loose spin contribution ?

- Apparently not !
  In slightly different prepared samples (different concentrations of loose spins in the FeSi spacer) $J_1(t_{Si})$ is unchanged but $J_2(t_{Si})$ varies:



- J_1 is apparently the only contribution to the overall bilinear coupling; virtually no bilinear loose spin contribution is observed !

Conclusions

- in MBE-grown Fe/Si/Fe trilayers a is maintained throughout the stack;
  a crystalline iron-silicide with a *metastable CsCl structure* is formed in the spacer layer
- the magnetization behavior can be fully understood and described with bilinear and biquadratic coupling constants
- the *biquadratic* coupling in Fe/Si/Fe is caused by loose spins in the FeSi spacer layer

J_1 and J_2 are caused by the same interaction potential !

- virtually no *bilinear loose spin* contribution is observed