3

Magnetic Anisotropy

M M A H
A A N Y
G T D S
N E T
E R E
T I R
I A E
C L S
S I
S

Maciej Urbaniak

3
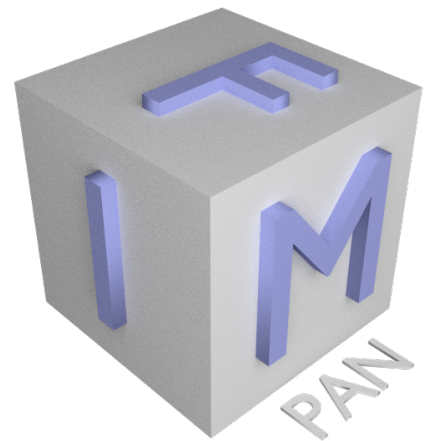
Magnetic Anisotropy

- Magnetocrystalline anisotropy

- Shape anisotropy

- Surface anisotropy

- Stress anisotropy

- Array anisotropy

Warm-up problem

Find the magnetic induction produced by a magnetized torus of revolution (major radius R, minor radius r) on a line x, y=0, when vector **M** is given by*:

$$\vec{M} = M_0 \left(\frac{-y}{\sqrt{(x^2+y^2)}}, \frac{x}{\sqrt{(x^2+y^2)}}, 0 \right)$$

(0,0,z)

The torus is symmetric about z-axis

*for the solution see last slides
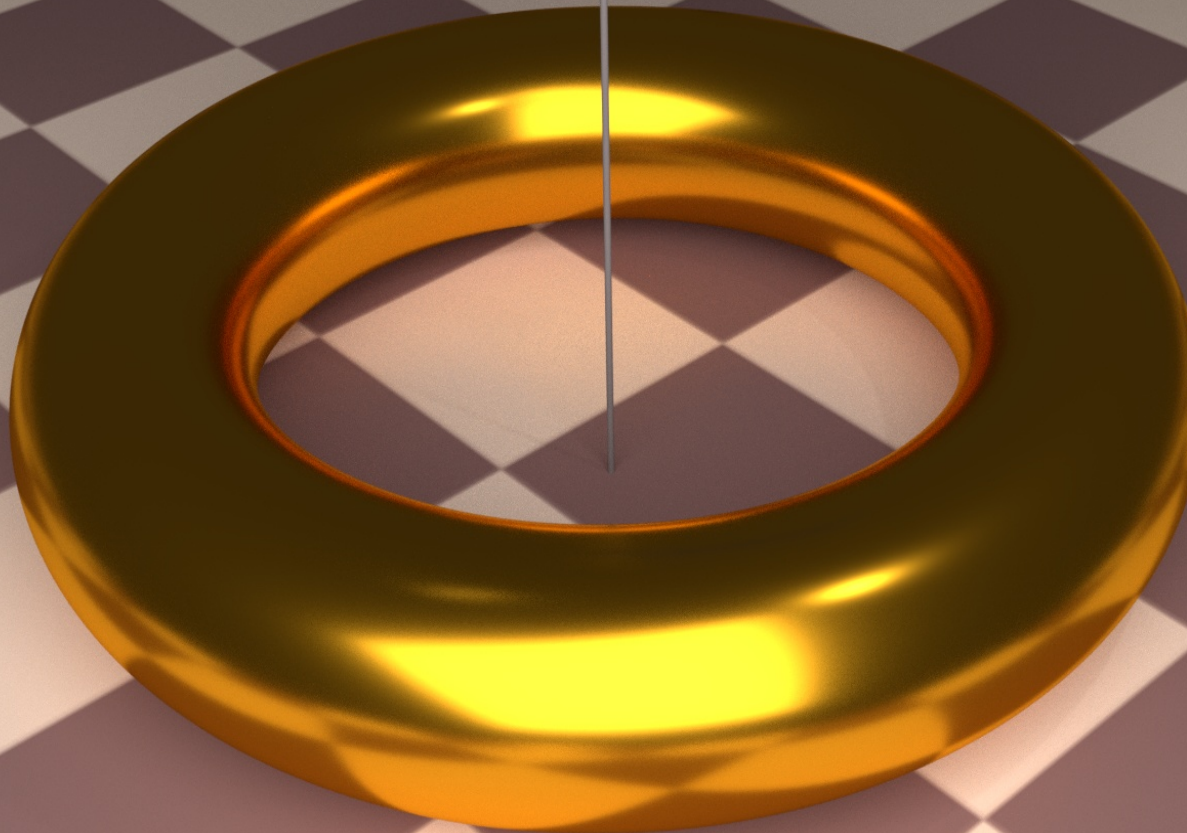
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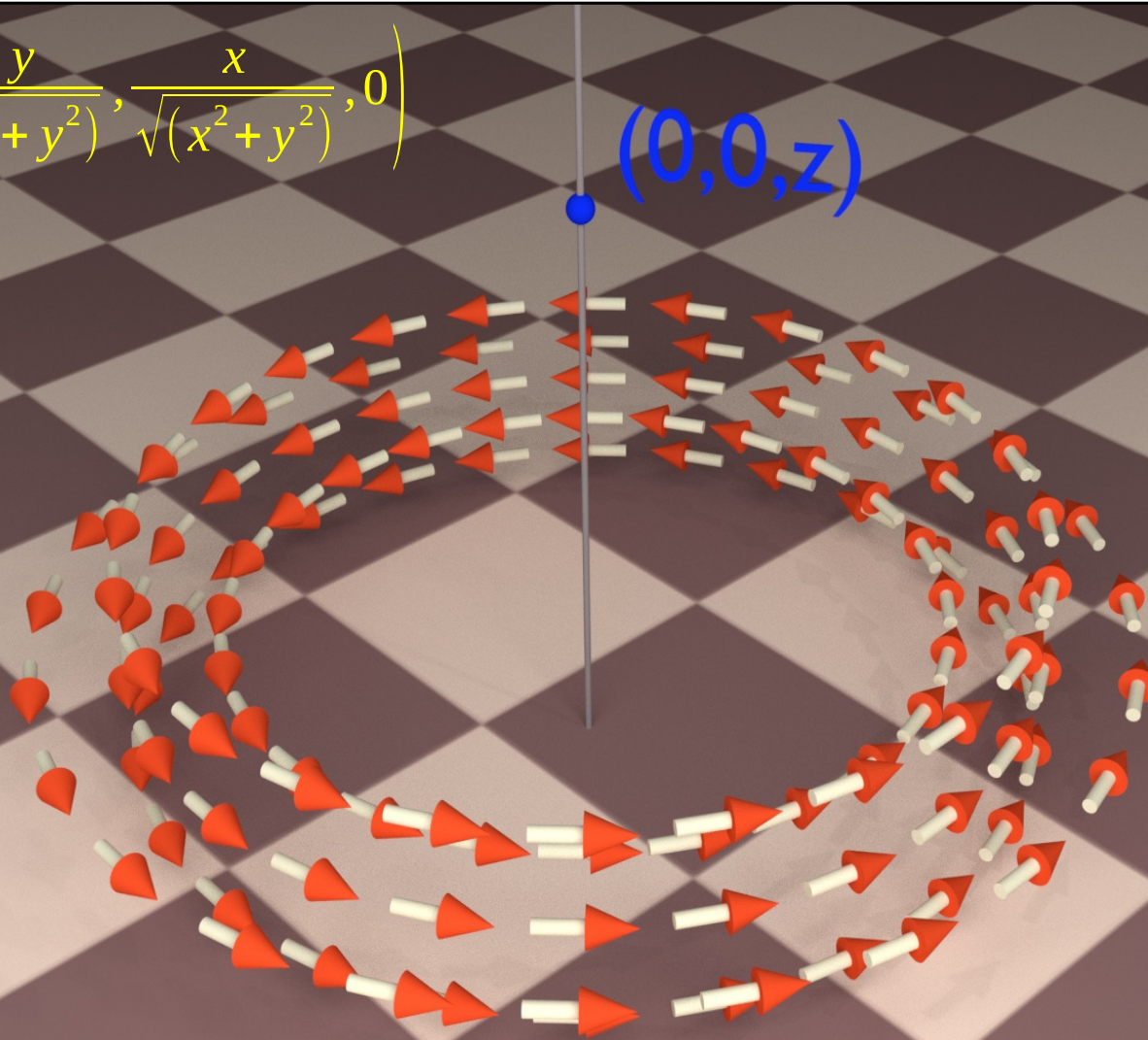
(0,0,z)

The torus is symmetric about *z*-axis

*for the solution see last slides

Pole avoidance principle*

Consider the following expression:

identity: $\nabla \cdot (f\vec{a}) = f\nabla \cdot \vec{a} + \boxed{\vec{a} \cdot \nabla f}$

$$\int \vec{B} \cdot \vec{H}\, dV = -\int \boxed{\vec{B} \cdot \nabla \phi}\, dV = -\int \left(\nabla \cdot (\phi \vec{B}) - \phi \nabla \cdot \vec{B} \right) dV\,,$$

0

which using divergence theorem transforms to:

$$\int \vec{B} \cdot \vec{H}\, dV = -\int \nabla \cdot (\phi \vec{B})\, dV = \int_S \vec{n} \cdot \phi \vec{B}\, ds$$

We know that boundary conditions require ϕ to be continuous everywhere. We assume that the surface s contains all ferromagnetic bodies (of the whole system). Outside the magnetized bodies we have:

$$\vec{B} = \mu_0 \vec{H} = -\mu_0 \nabla \phi$$

If we allow the surface to tend to infinity the $\phi\mathbf{B}$ goes to zero as r^{-3} [2] while the surface increases as r^2. Finally we have:

$$\int_{\text{all space}} \vec{B} \cdot \vec{H}\, dV = 0$$

for the field produced by finite **distribution of magnetized bodies** (no free currents).

*see A. Aharoni [2], or W. F. Brown [18]

Pole avoidance principle*

The expression for the energy of the magnetized bodies in own field is [2]:

$$E_m = -\frac{1}{2}\int_V \vec{B}\cdot\vec{M}\,dV$$

From previous slide we have:

$$\int_{Space} \vec{B}\cdot\vec{H}\,dV = \int_{Space} \mu_0\vec{H}\cdot(\vec{M}+\vec{H})\,dV = 0 \quad \rightarrow \quad \int_{Space}\mu_0 H^2\,dV = -\mu_0\int_{Space}\vec{H}\cdot\vec{M}\,dV$$

Rewriting E_m we get:

$$E_m = -\frac{1}{2}\int_V \mu_0(\vec{M}+\vec{H})\cdot\vec{M}\,dV = -\frac{1}{2}\boxed{\overset{\text{constant}}{\int_V \mu_0 M^2\,dV}} - \frac{1}{2}\int_V \mu_0\vec{H}\cdot\vec{M}\,dV$$

$$\boxed{E_m = const + \mu_0\frac{1}{2}\int_{Space} H^2\,dV}$$

- note that the integrand is never negative

- the smallest possible value for variable part of magnetostatic self energy is **zero**

- this can be achieved only when **H** is zero everywhere

- in the absence of free currents, only the magnetic charges (surface and volume) produce magnetic field strength **H**

Pole avoidance principle*

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Magnetostatic energy term leads to magnetic moments configurations with possibly small magnetic charges (pole avoidance principle)

Alternatively the magnetostatic energy term can be writte as [2]:

$$E_m = const - \frac{1}{2\mu_0} \int_{Space} B^2 \, dV$$

note that the minus sign before the integral makes the equation of little use in predicting magnetization configuration [2]: one "never" knows whether by changing orientation of some moment we can get even higher value of the integral
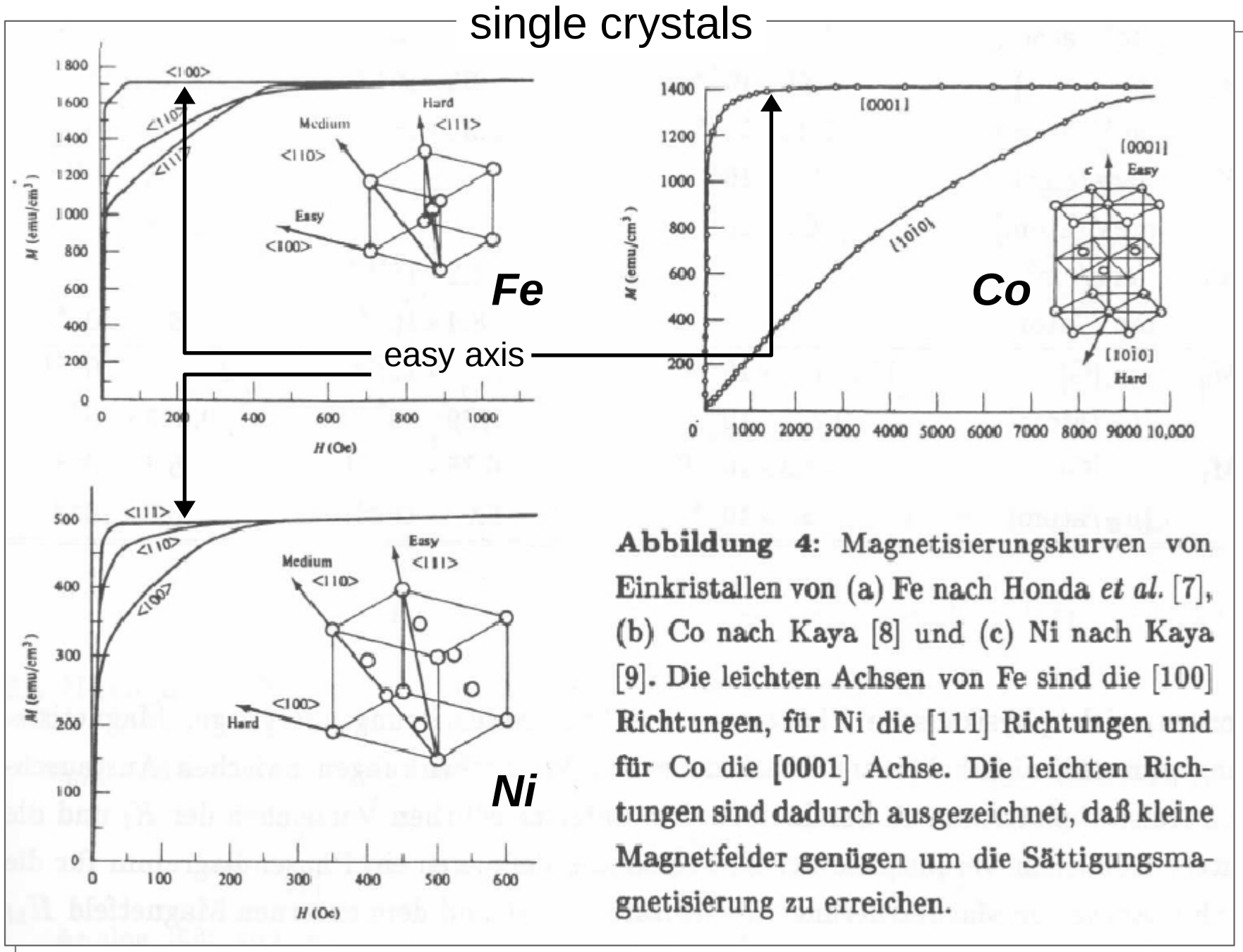
Anisotropy of hysteresis

single crystals

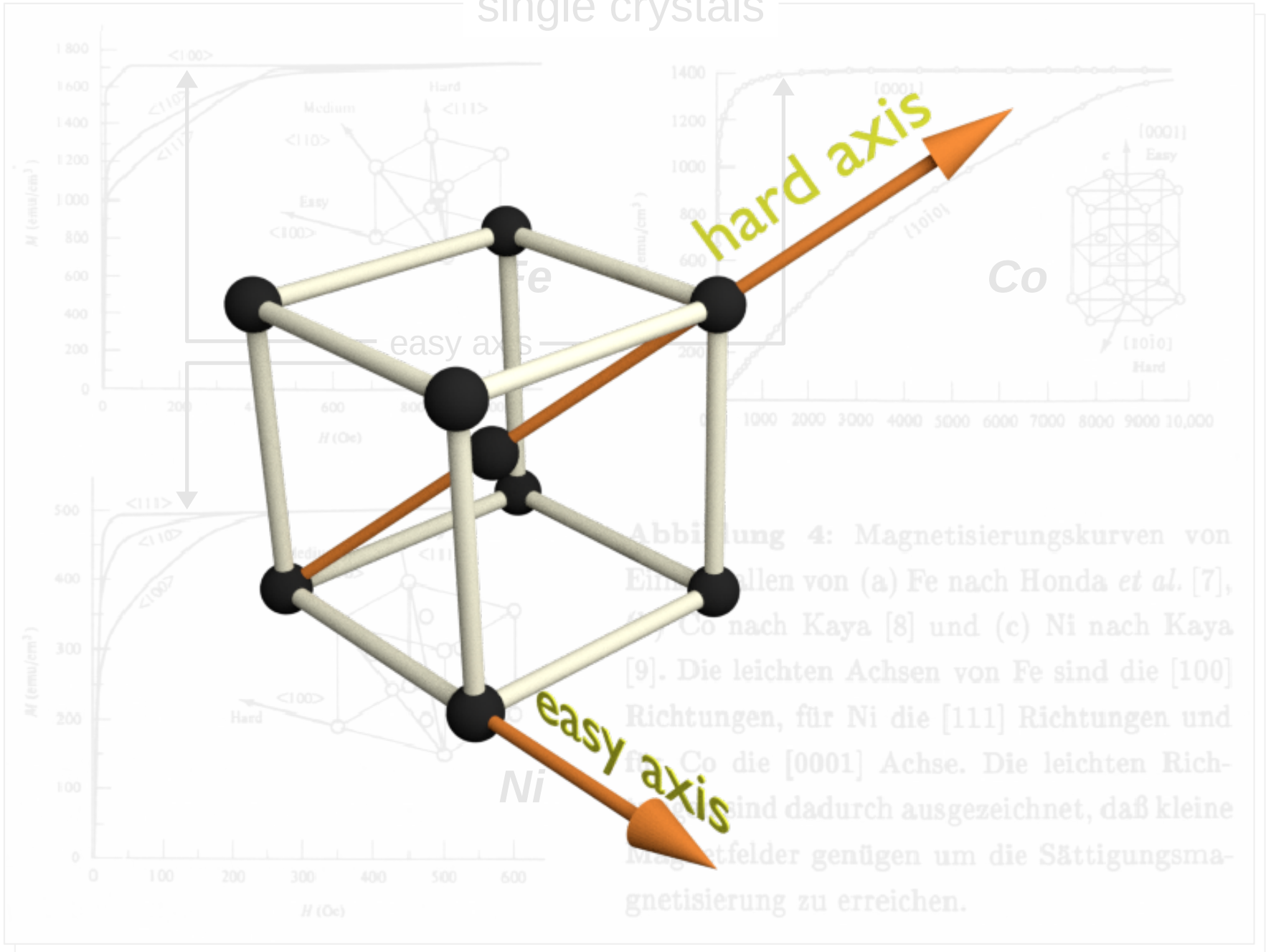**Fe**

Co

easy axis

Ni

Abbildung 4: Magnetisierungskurven von Einkristallen von (a) Fe nach Honda *et al.* [7], (b) Co nach Kaya [8] und (c) Ni nach Kaya [9]. Die leichten Achsen von Fe sind die [100] Richtungen, für Ni die [111] Richtungen und für Co die [0001] Achse. Die leichten Richtungen sind dadurch ausgezeichnet, daß kleine Magnetfelder genügen um die Sättigungsmagnetisierung zu erreichen.

MAGNETIC MATERIALS AND HYSTERESIS

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Anisotropy of hysteresis

Fe

single crystals

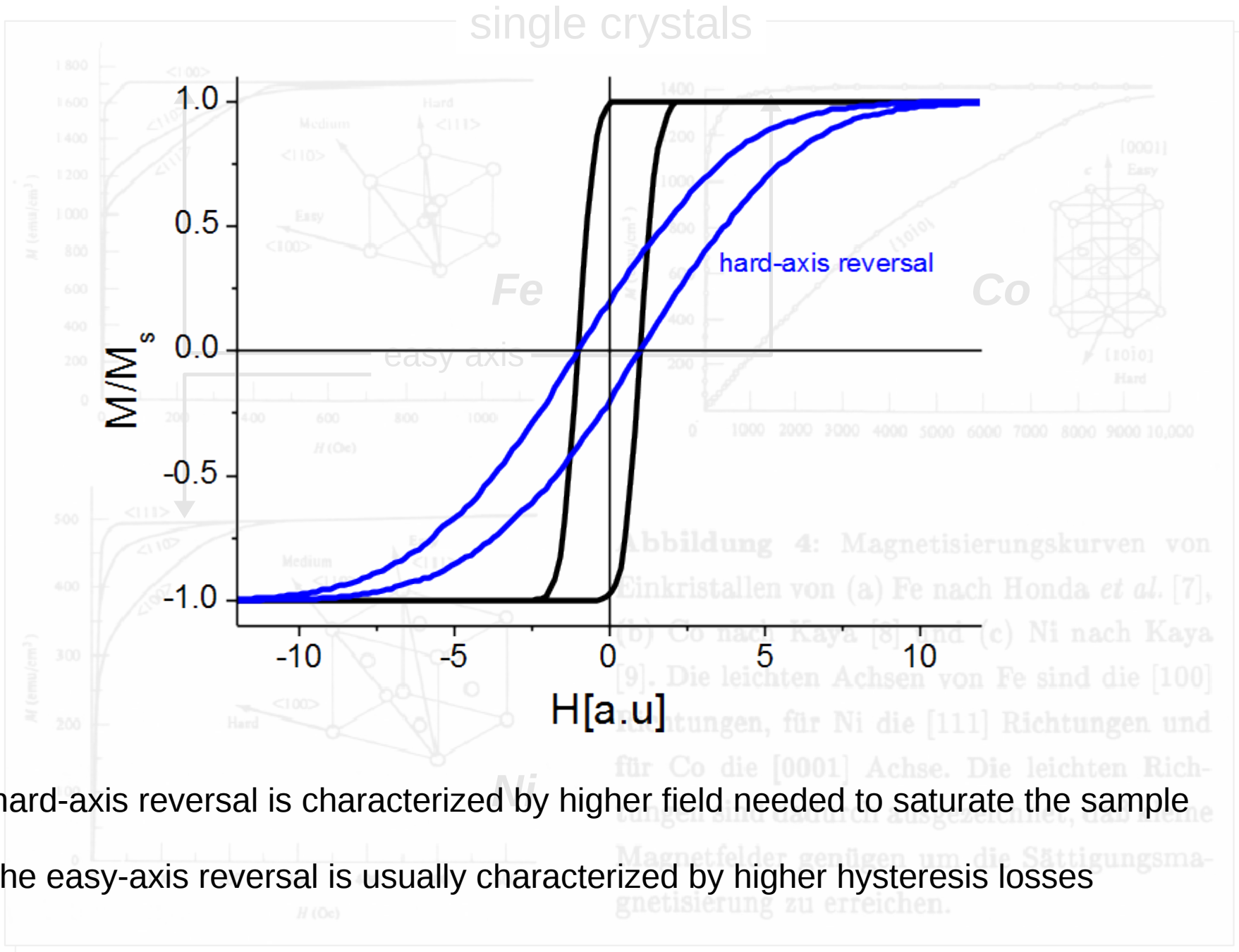hard axis

easy axis

Fe *Co* *Ni*

Abbildung 4: Magnetisierungskurven von Einkristallen von (a) Fe nach Honda *et al.* [7], (b) Co nach Kaya [8] und (c) Ni nach Kaya [9]. Die leichten Achsen von Fe sind die [100] Richtungen, für Ni die [111] Richtungen und für Co die [0001] Achse. Die leichten Richtungen sind dadurch ausgezeichnet, daß kleine Magnetfelder genügen um die Sättigungsmagnetisierung zu erreichen.

MAGNETIC MATERIALS AND HYSTERESIS

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Anisotropy of hysteresis

single crystals

Fe *Co*

hard-axis reversal

easy axis

- hard-axis reversal is characterized by higher field needed to saturate the sample

- the easy-axis reversal is usually characterized by higher hysteresis losses

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Anisotropy of hysteresis – hysteresis of a sphere

- In case of large sphere (containing many atoms) the shape of the sample does not introduce additional anisotropy
- In small clusters the magnetization reversal is complicated by the reduction of symmetry (and the increased relative contribution of surface atoms)
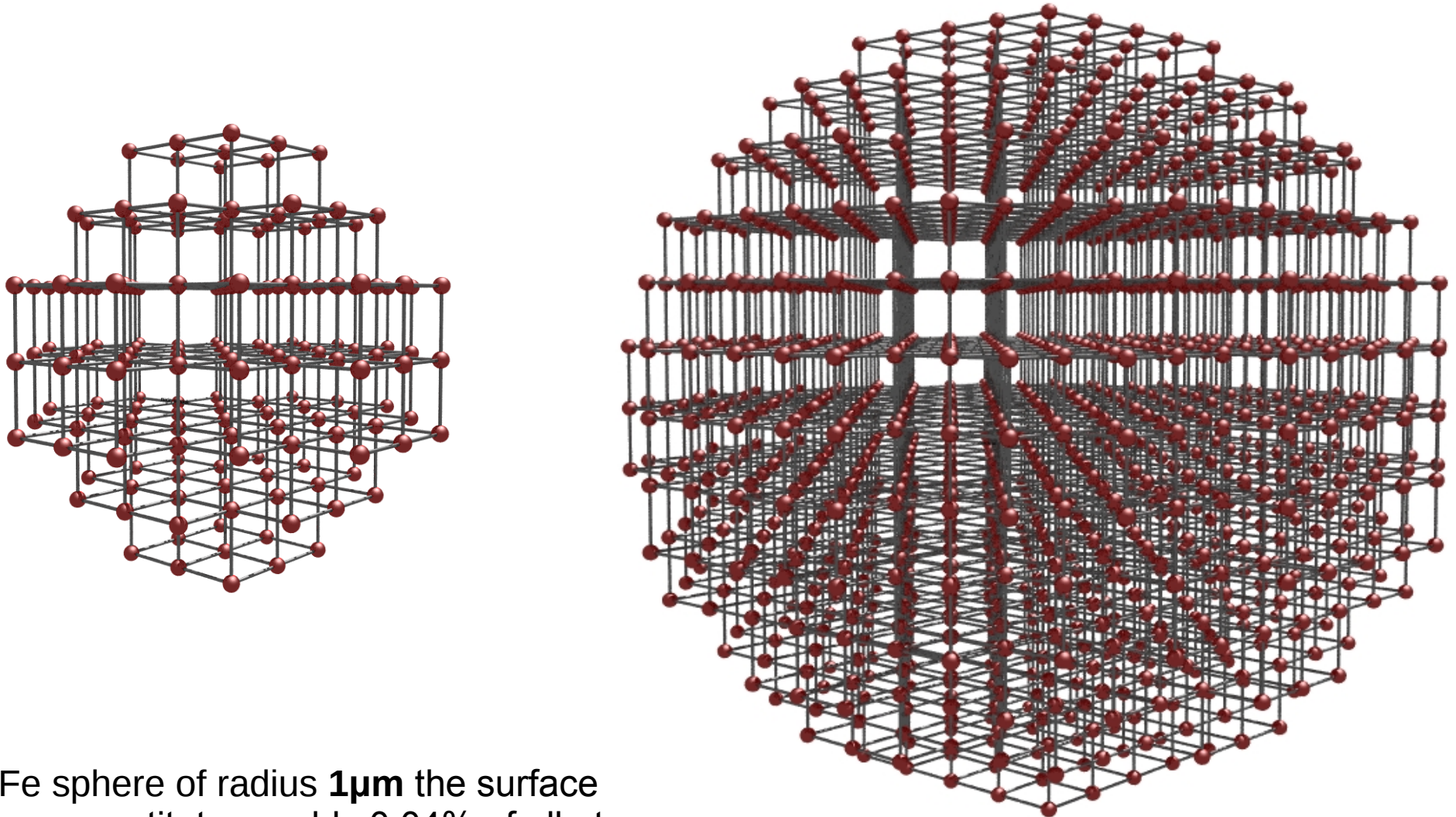
In Fe sphere of radius **1µm** the surface atoms constitute roughly 0.04% of all atoms

- In case of large sphere (containing many atoms) the shape of the sample does not introduce additional anisotropy
- In small clusters the magnetization reversal is complicated by the reduction of symmetry (and the increased relative contribution of surface atoms)
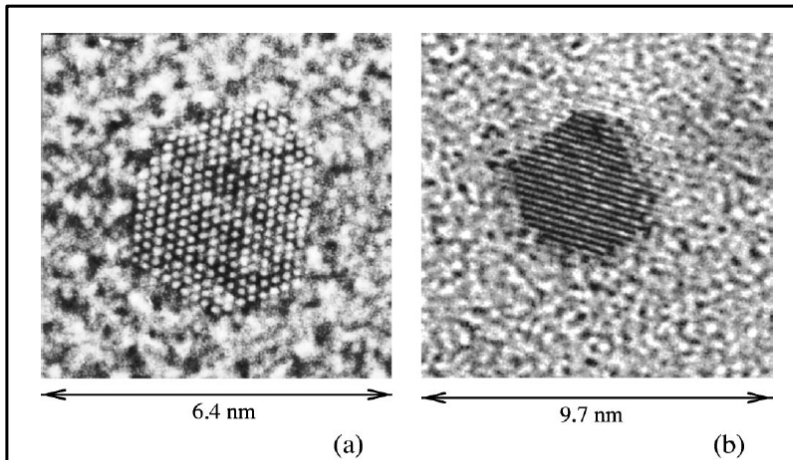
sphere-like – no breaking of crystal symmetry for high r

6.4 nm   9.7 nm

(a)   (b)

FIG. 6. (a) high-resolution transmission electron microscopy (HRTEM) observation of a cobalt cluster along a [110] direction. Interplanar distances $d_{(111)} = 2.04 \pm 0.02$ Å, $d_{(200)} = 1.77 \pm 0.02$ Å and angles correspond to bulk fcc cobalt. Moreover facet sistent with the Wulff theorem (Ref. 27). (b) HRTEM of an iron cluster along a [110] direction. The interplana $d_{(110)} = 2.01 \pm 0.03$ Å corresponds to the bulk bcc iron one is also consistent with the Wulff theorem (Ref. 27).
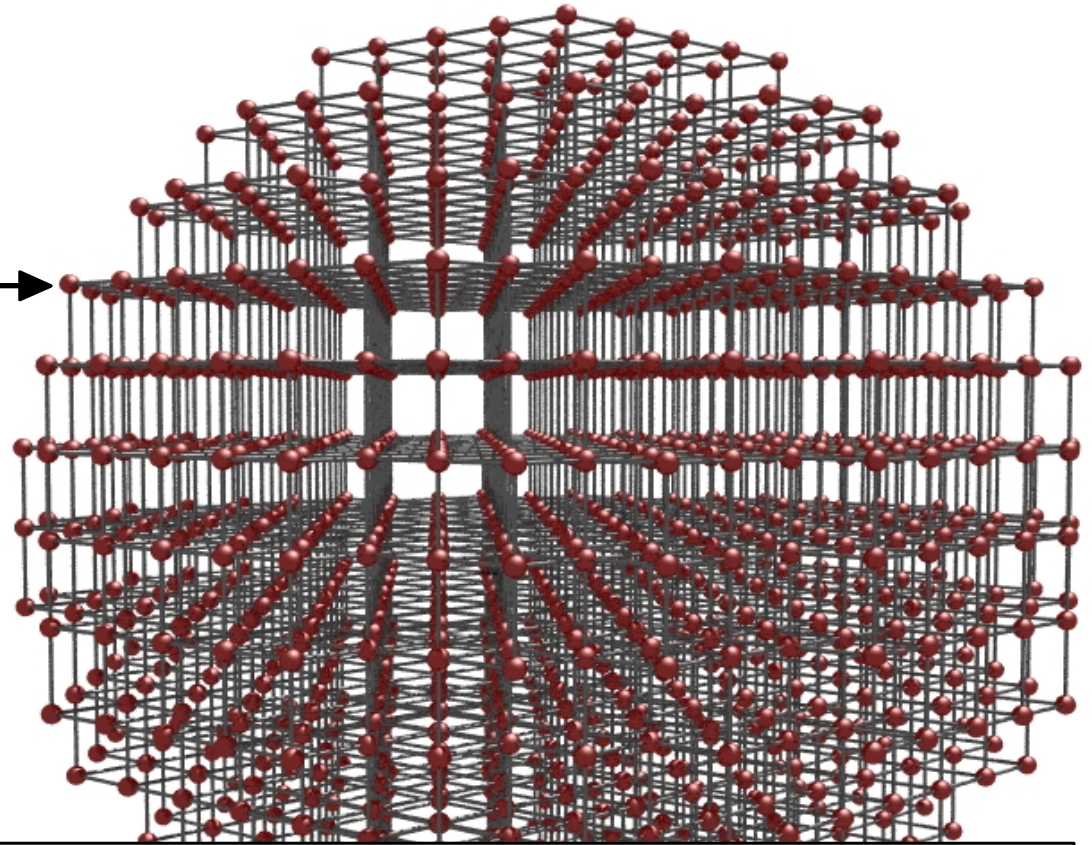
Interplanar distances $d_{(111)} = 2.04 \pm 0.02$ Å, $d_{(200)} = 1.77 \pm 0.02$ Å and angles correspond to bulk fcc cobalt. Moreover faceting is consistent with the Wulff theorem (Ref. 27). (b) HRTEM observation of an iron cluster along a [110] direction. The interplanar distance $d_{(110)} = 2.01 \pm 0.03$ Å corresponds to the bulk bcc iron one. Faceting

$$E = -\vec{m} \cdot \vec{B}$$
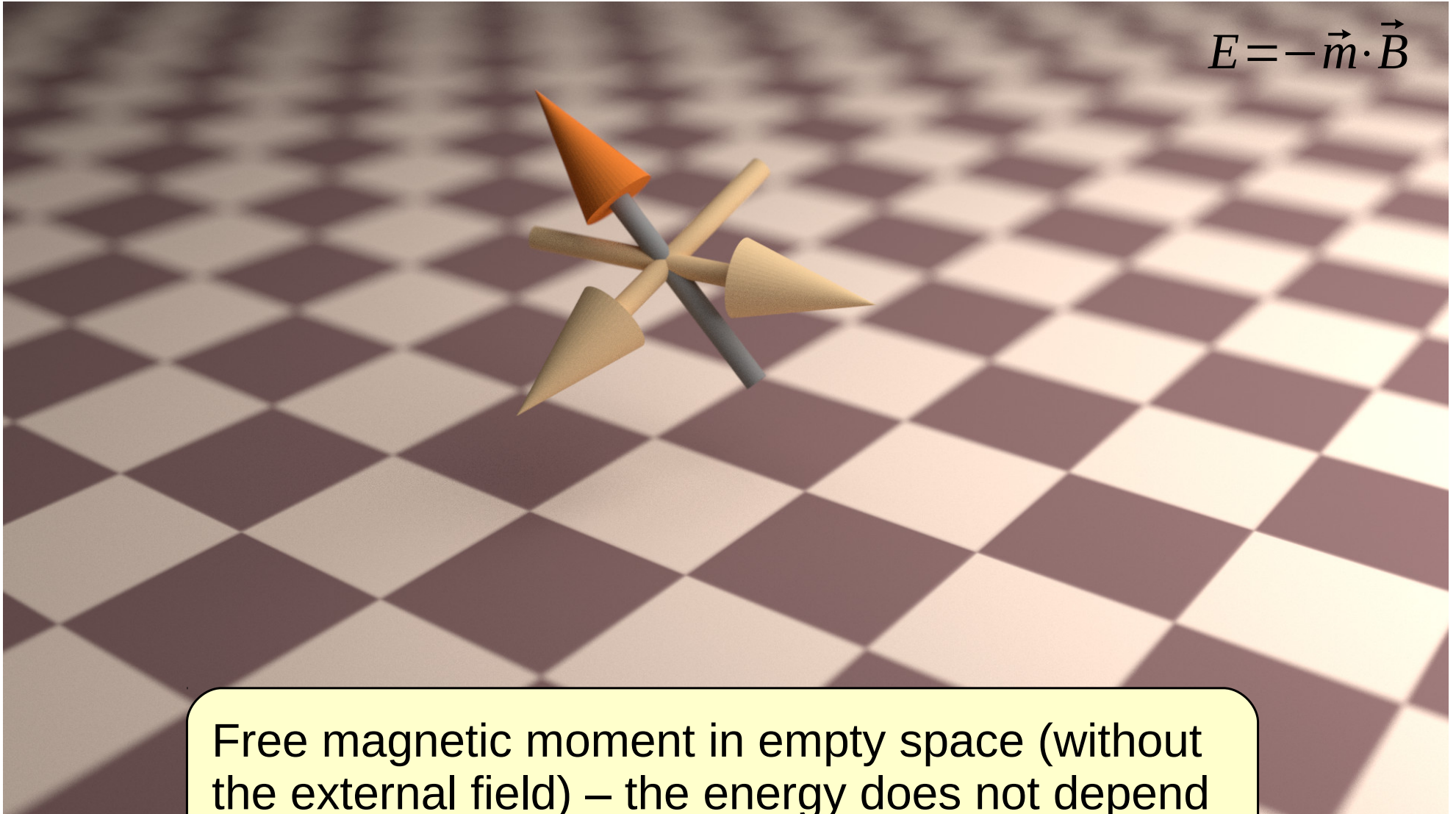
Free magnetic moment in empty space (without the external field) – the energy does not depend on the orientation of the moment

- Co atoms deposited by molecular beam epitaxy on Pt(111) surface
- Coverage less than 0.03 ML
- "The XMCD signal (Fig. 1C) is the difference between the XAS* spectra recorded for parallel and antiparallel alignment of the photon helicity with the applied field **B**. Fields of up to **7 T** were used to magnetize the sample at angles 0° and 70° with respect to the surface normal."

- The presence of Pt surface induces very high magnetic anisotropy of 9.3±1.6 meV/atom

- In SmCo$_5$ magnets the anisotropy is 0.3 meV/Co atom

It is about 6% of a latent heat of melting (243 kJ/kg [14]) of bulk Co

isolated Co adatoms
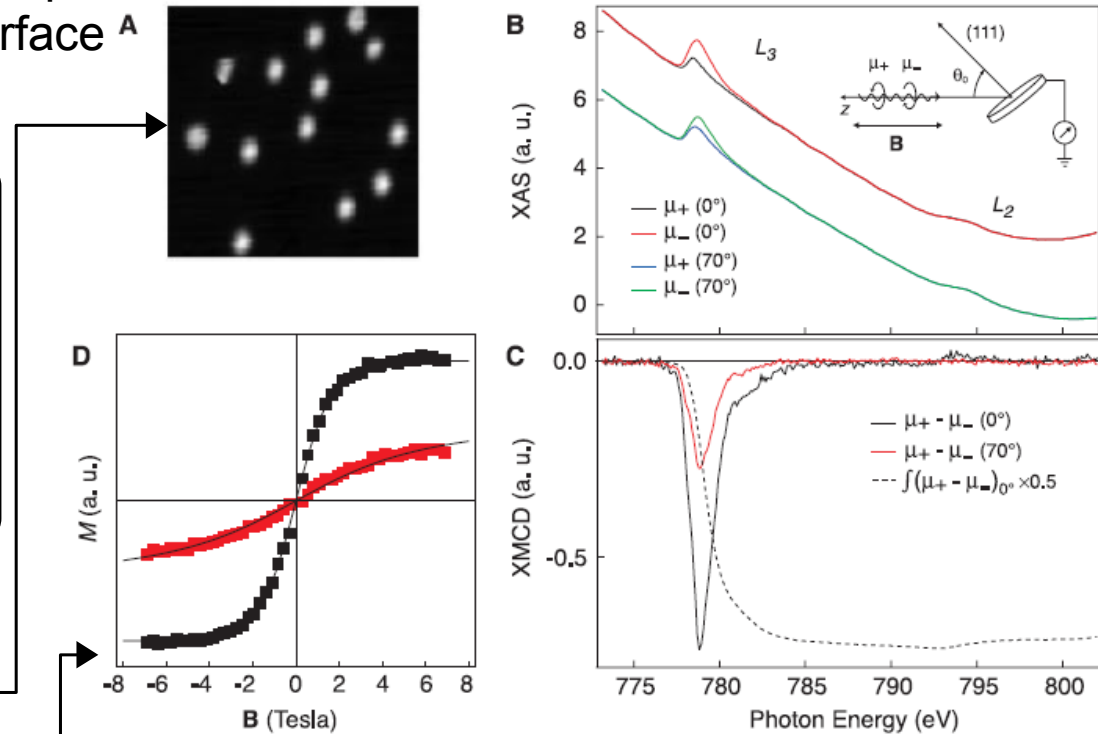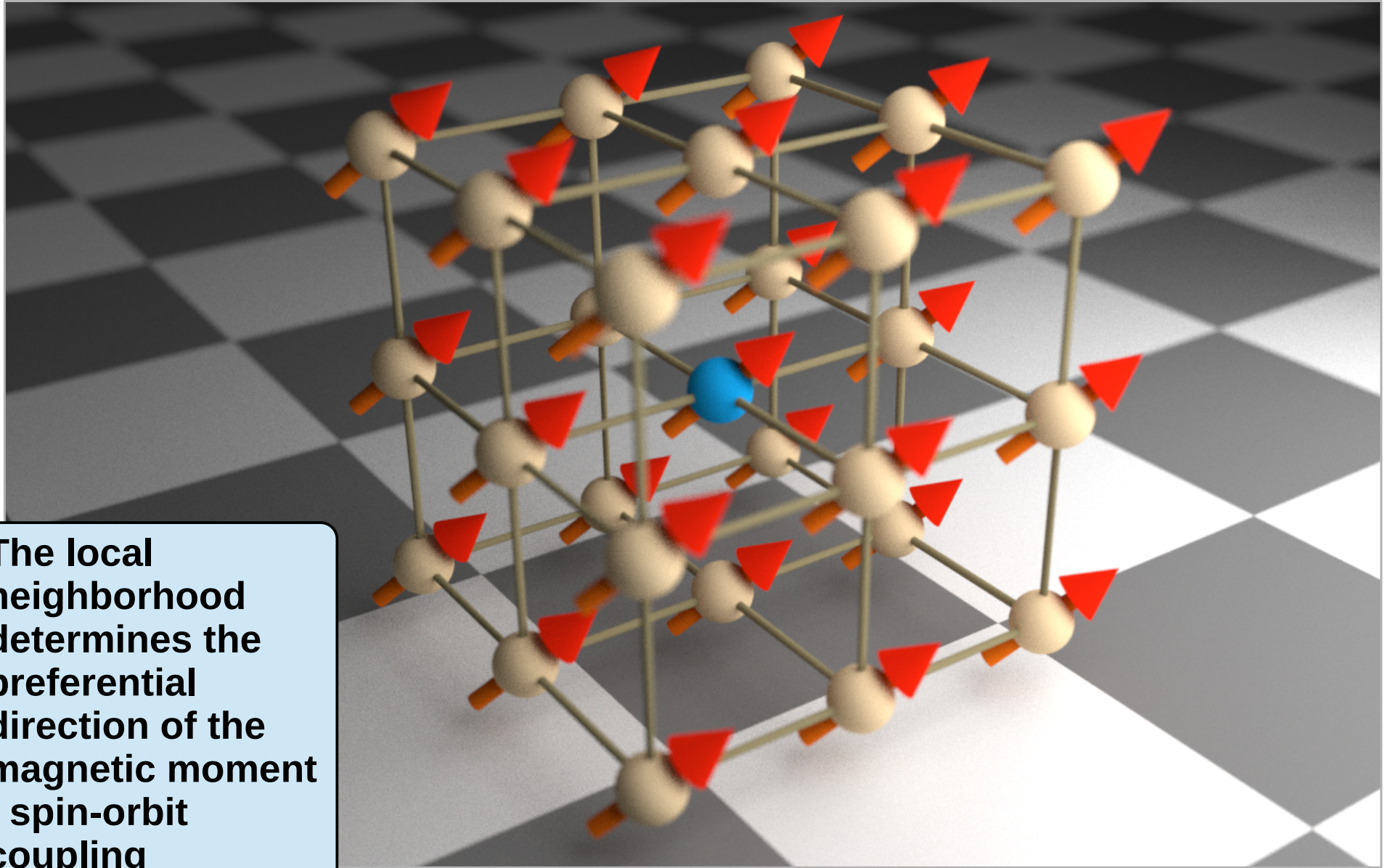
very high saturation field

Fig. 1. (A) STM image of isolated Co adatoms (bright dots) on Pt(111). The Co coverage is 0.010 ML, and the image size is 85 Å by 85 Å. (B) $L_{2,3}$ XAS spectra of isolated Co adatoms (0.010 ML) at $T = 5.5 \pm 0.5$ K, $B = 7$ T taken with parallel (μ_+) and antiparallel (μ_-) alignment of light helicity with respect to B at $\theta_0 = 0°$, 70° relative to the surface normal (inset). The spectra at 70° have been normalized to the ($\mu_+ + \mu_-$) L_3 intensity at 0° to eliminate the dependence of the electron yield on the sample orientation. (C) XMCD spectra ($\mu_+ - \mu_-$) obtained for the $\theta_0 = 0°$ and 70° magnetization directions. The dashed line is the integrated XMCD at $\theta_0 = 0°$. (D) Magnetization curves at $\theta_0 = 0°$ (black squares) and 70° (red squares) measured at $T = 5.5$ K. The points represent the peak of the L_3 XMCD intensity at 778.6 eV divided by the pre-edge intensity at 775 eV as a function of B. The difference between the $\theta_0 = 0°$ and 70° curves was checked for consistency with the XAS-normalized XMCD spectra. The solid lines are fits to the data according to Eq. 3.

P. Gambardella et al., Science **300**, 1130 (2003)

*XAS – X-ray absorption spectroscopy

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The local neighborhood determines the preferential direction of the magnetic moment - spin-orbit coupling

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Spin-orbit interaction (coupling)

- The electron is orbiting the nucleus of the +Ze charge*
- Looking at the nucleus from electron we have the magnetic field due to the motion of the nucleus. The energy of electron in that field is

$$\vec{E} = -g\,\mu_B\,m_s\,B$$

Correspondingly every electronic state splits into two (with two orientations of the spin). We assume that an electron is orbiting the nucleus in xy plane and that its instantaneous velocity is along x-direction.
The electric field of the nucleus at the place of an electron is along y-direction then

$$E_y = \frac{1}{4\pi\epsilon_0}\frac{Z\,e}{r^2}$$

From special relativity theory (A. Einstein) for the components of the magnetic field in the electron reference frame we have [16]
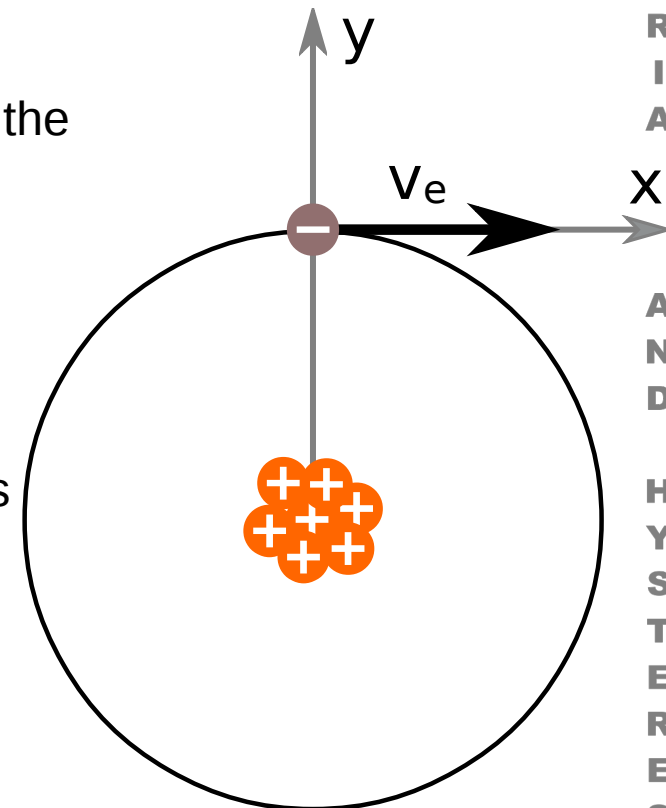
$$B_x^{\text{el(ectron)}} = B_x = 0$$

$$B_y^{\text{el}} = \frac{1}{\sqrt{1-v^2/c^2}}\left(B_y + \frac{v_e}{c^2}E_z\right) = 0 \qquad B_z^{\text{el}} = \frac{1}{\sqrt{1-v^2/c^2}}\left(B_z - \frac{v_e}{c^2}E_y\right) \approx -\frac{v_e}{c^2}E_y$$

Electron feels then the magnetic field that is oriented along z-axis
Further, the field seen by the electron can be written as

$$B^{\text{el}} = \frac{1}{c^2}\left(\vec{E}\times\vec{v}\right) = \frac{1}{mc^2}\left(\vec{E}\times\vec{p}\right) \qquad\qquad \vec{p} = \frac{m_0\vec{v}}{\sqrt{1-v^2/c^2}}$$

*the derivation is taken from *Einführung in die Quantenmechanik* (Physik IV), ETH Zurich [13]

Spin-orbit interaction (coupling)

Inserting the above calculated magnetic field into the expression for energy yields

$$\Delta E_{spin-orbit} = -g\mu_B m_s B = -g\mu_B m_s \frac{1}{mc^2}(\vec{E}\times\vec{p}) = -g\mu_B m_s \frac{1}{mc^2}\left(\boxed{\frac{1}{4\pi\epsilon_0}\frac{Ze}{r^2}}\frac{\vec{r}}{r}\times\vec{p}\right)$$
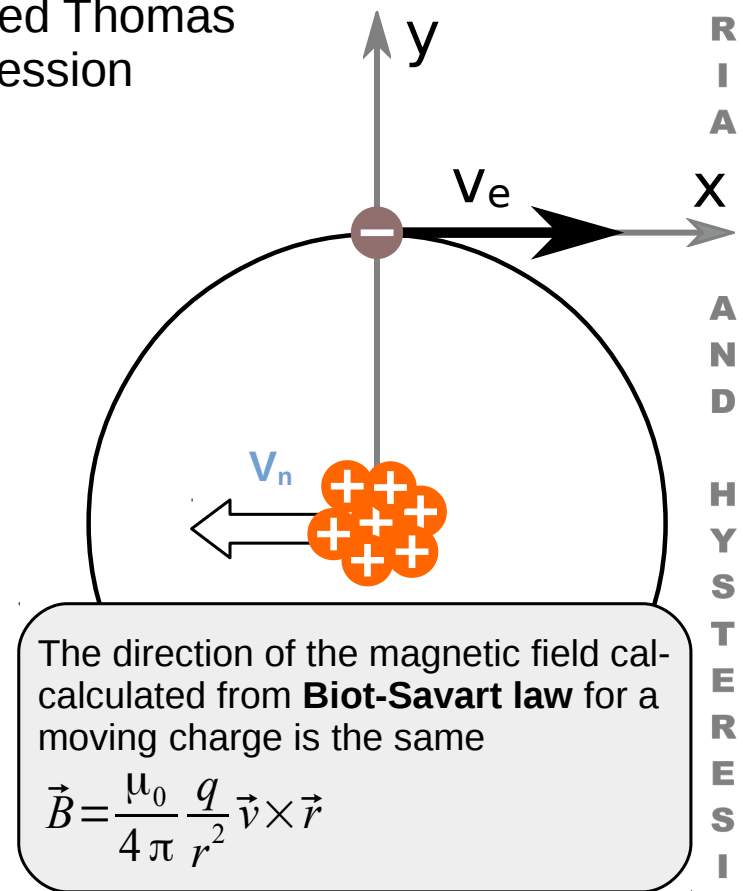
this give the appropriate direction of electric field

$$\Delta E_{spin-orbit} = -g\mu_B m_s \frac{1}{mc^2}\left(\left[\frac{1}{4\pi\epsilon_0}\frac{Ze}{r^3}\right]\vec{r}\times\vec{p}\right) = -g\mu_B m_s \frac{1}{mc^2}\left(\left[\frac{1}{4\pi\epsilon_0}\frac{Ze}{r^3}\right]\vec{L}\right)$$

angular momentum

More exact calculations require taking into account the so called Thomas precession* – this leads to factor ½ which leads to "final" expression

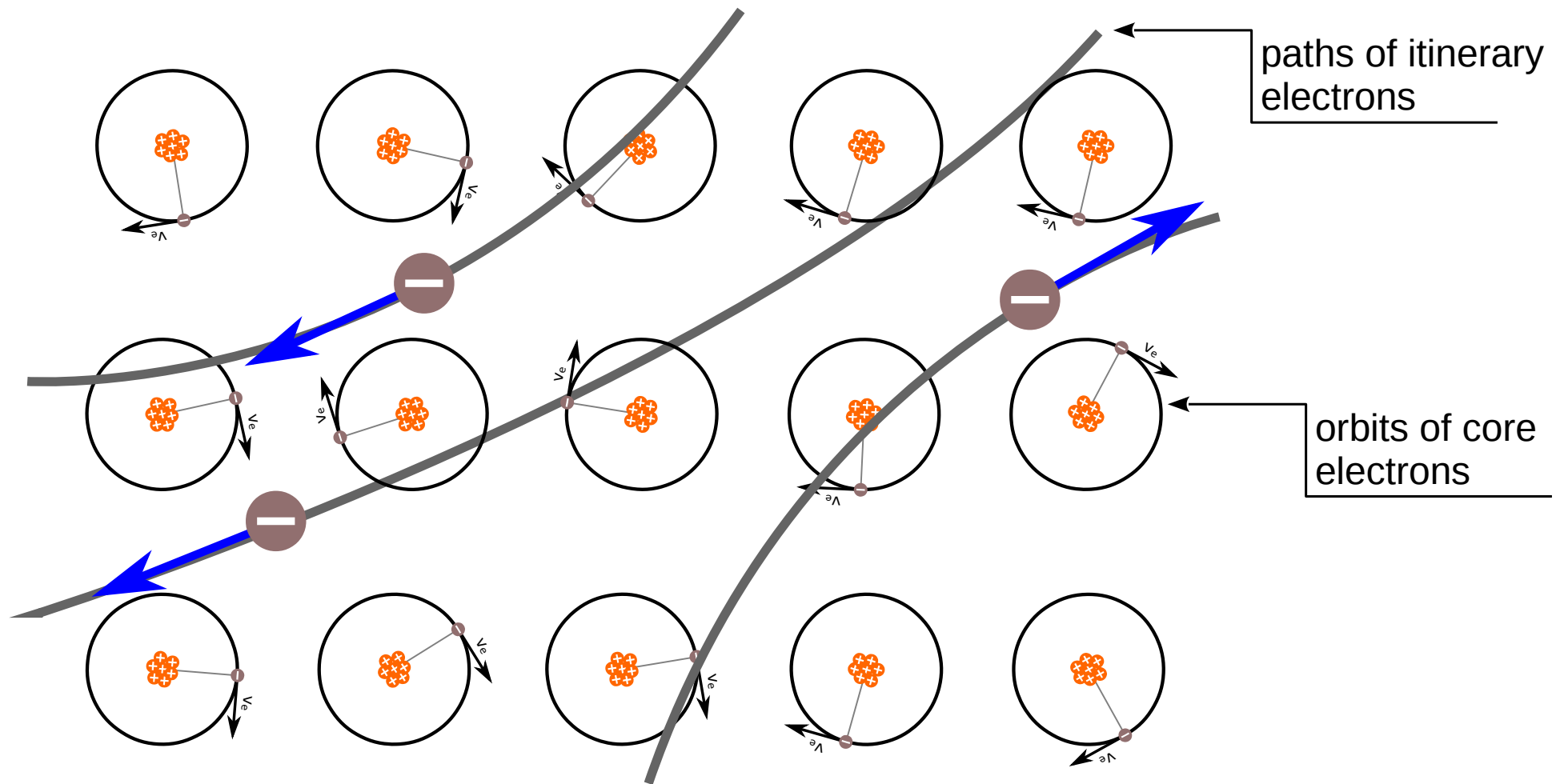$$\Delta E_{spin-orbit} = -\frac{g}{2}\mu_B \frac{1}{mc^2}\frac{1}{4\pi\epsilon_0}\frac{Ze}{r^3}\vec{L}$$

- note that spin-orbit coupling is proportional to Z

- ...and to orbital moment of an electron

The direction of the magnetic field cal-calculated from **Biot-Savart law** for a moving charge is the same

$$\vec{B} = \frac{\mu_0}{4\pi}\frac{q}{r^2}\vec{v}\times\vec{r}$$

*the derivation assumed that electron moves along straight line [13]

Spin-orbit interaction (coupling)

- **In a crystal** conducting electrons move in the average electric field of the atom cores and other electrons
- The core electrons that remain in the vicinity of the nucleus experience strong electric fields and, provided that the orbit is not centrosymmetric, they experience strong spin-orbit coupling (please see movies at https://staff.aist.go.jp/v.zayets/spin3_32_SpinOrbit.html)

paths of itinerary electrons

orbits of core electrons

Spin-orbit interaction (coupling)

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- The magnetic fields due the core electron movement can be huge [15]:

Linear velocity of an electron rotating around a nucleus is **~$2.1*10^6$ m/s**
The electric field experienced by an electron in the vicinity of nucleus (calculated for 1s orbital of hydrogen atom) is roughly **$5*10^{11}$ V/m**
The effective magnetic field of the spin-orbit interaction is about **12 T**

For comparison we [15] estimate the effective field in devices in which we try to influence the behavior of itinerant electrons applying external electric fields
The maximal electron velocity (saturation velocity, maximal drift speed) **~$1*10^7$ m/s**
The maximal available electric field (limited by breakdown voltage of the materials), for GaAs or Si it is roughly **$5*10^7$ V/m**
The effective magnetic field of the spin-orbit interaction is about **$5*10^{-4}$ T** (about tenfold strength of the earth magnetic field)

Spin-orbit interaction (coupling) – dependence on a atomic number

The SO coupling depends indirectly on the charge of the nucleus (Z)
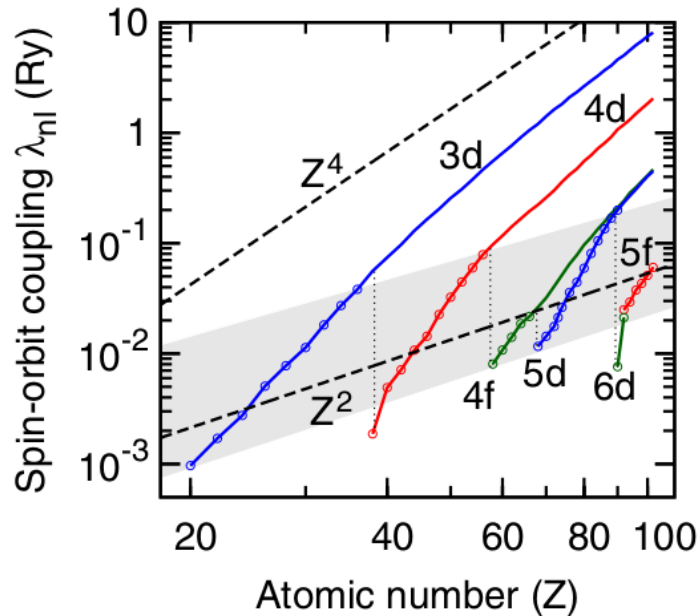The dependence is different for different series

FIG. 1. (Color online) Dependence of the spin-orbit coupling strength λ_{nl} for atoms as a function of the atomic number Z. The calculated results of Herman and Skillman [24] using the Hartree-Fock method (colored lines) are compared to the hydrogenic Z^4 dependence, which is computed from Eq. (4) for the 3d series (upper dashed line). For the *outermost* electrons (indicated by the circles and the shaded area), which are the relevant electrons in the solid, the quantum numbers nl change with Z and the spin-orbit interaction increases much more slowly, following roughly the Landau-Lifshitz Z^2 scaling [lower dashed line, calculated from Eq. (5) with $A = 0.10$].

- The Z^4 dependence for SO in central field (near core electrons) comes from perturbative correction [18]:

$$H_{so}(r) = \frac{1}{2\,m^2\,c^2} \frac{\partial V(r)}{\partial r} \vec{L} \cdot \vec{S}$$

$$E_{nl} = E^0_{nl} + F(l,j)\,Z^4$$

- The Z^2 dependence is more relevant for solids
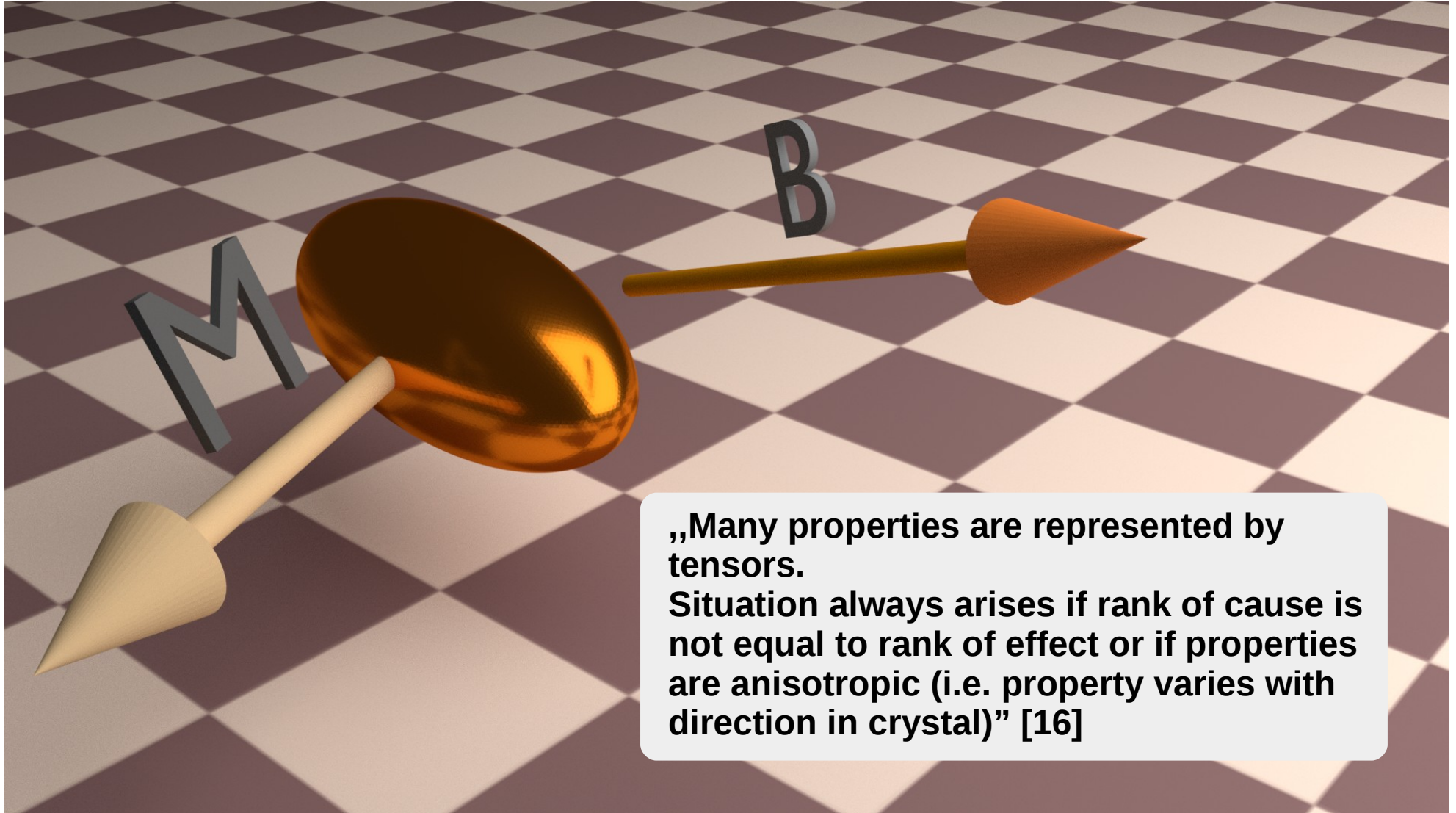
,,Many properties are represented by tensors.
Situation always arises if rank of cause is not equal to rank of effect or if properties are anisotropic (i.e. property varies with direction in crystal)" [16]

In magnetism a **magnetic susceptibility tensor** is one of the important exemples:
the direction of magnetic moment (in macrospin approximation) is not in general parallel to the direction of the external magnetic field

- For all practical purposes the atomic magnetic moments of a macroscopic homogeneous magnetic *sphere* behave as if placed in infinite crystal of the *same shape*.

A. Aharoni: "in ferromagnetism there is no physical meaning to the limit of an infinite *crystal without a surface*" [2]

- We do not know *a priori* the dependence of the energy of the crystal on the orientation of magnetic moment of the sample.
- It can be shown [1] that energy density related to the orientation of magnetic moment in a crystal structure can be expanded into power series of direction cosines relative to the crystal axes:

$$E_{crystal}(\vec{M}) = b_0 + \sum_{i=1,2,3} b_i \alpha_i + \sum_{i,j=1,2,3} b_{ij} \alpha_i \alpha_j + \sum_{i,j,k=1,2,3} b_{ijk} \alpha_i \alpha_j \alpha_k + ... \tag{1}$$
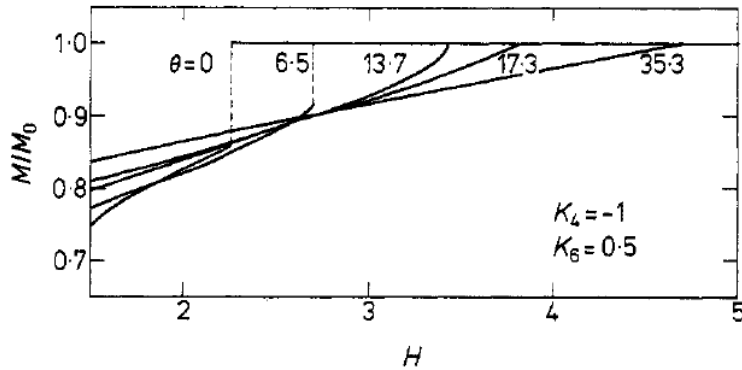
$\alpha_1,\ \alpha_2,\ \alpha_3$ - direction cosines of magnetization

$(\alpha_1, \alpha_2, \alpha_3) = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$ $\theta,\ \phi$ - polar and azimuthal angles

- The experience shows that it is enough to use very limited number of expansion terms to describe the magnetic systems – the usual limit are sixth order anisotropy constants

- An example of the use of sixth order anisotropy constants for hysteresis description:

Figure 3. Magnetisation curves calculated for $\theta = 0°, 6·5°, 13·7° (\simeq \theta_T), 17·3°$ and $35·3°$ [110]. The parameters K_4 and K_6 are phenomenological and not directly related to $DyAl_2$.

To see qualitatively that a sixth-order anisotropy term may indeed increase the discontinuity and the tricritical angle θ_T, consider the classical mean field energy

$$E = -\mathbf{H} \cdot \frac{\mathbf{M}}{M_0} + K_4(M_x^4 M_y^4 + M_z^4)/M_0^4 + K_6[M_x^6 + M_y^6 + M_z^6$$

$$- \tfrac{15}{4}(M_x^4 M_y^2 + M_y^4 M_x^2 + M_z^2 M_y^4 + M_y^2 M_z^4 + M_z^2 M_x^4$$

$$+ M_x^2 M_z^4)]/M_0^6$$

where K_4 and K_6 are phenomenological anisotropy constants. We have calculated magnetisation curves by minimising E with respect to $\mathbf{M}$ for various directions of $\mathbf{H}$. In figure 3 are shown calculated magnetisation curves with $K_4 = -1$ and $K_6 = 0·5$. The discontinuity for $\theta = 0$ is 15% which corresponds to the situation for $DyAl_2$ at $T \simeq 20$ K.

B. Barbara et al., J. Phys. C: Solid State Phys. 11 L183 (1978)

Magnetic anisotropy

- Intrinsic symmetries of the physical properties reduce the number of independent components of anisotropy tensors.
- The energy of the system is the same for both opposite orientations of magnetic moment. From Eq. (1) we have:

$$\sum_{i=1,2,3} b_i \alpha_i = \sum_{i=1,2,3} b_i(-\alpha_i) \quad for \quad all \quad \alpha_i \quad \Rightarrow \quad b_1 = b_2 = b_3 = 0$$

- The magnetocrystalline anisotropy energy may not depend on odd powers of direction cosines α. Consequently all odd rank tensors in the expansion (1) are identically null [1].

the same energy

$$E_a(\vec{M}) = E_a(-\vec{M})$$

*rank of a tensor – number of its indices
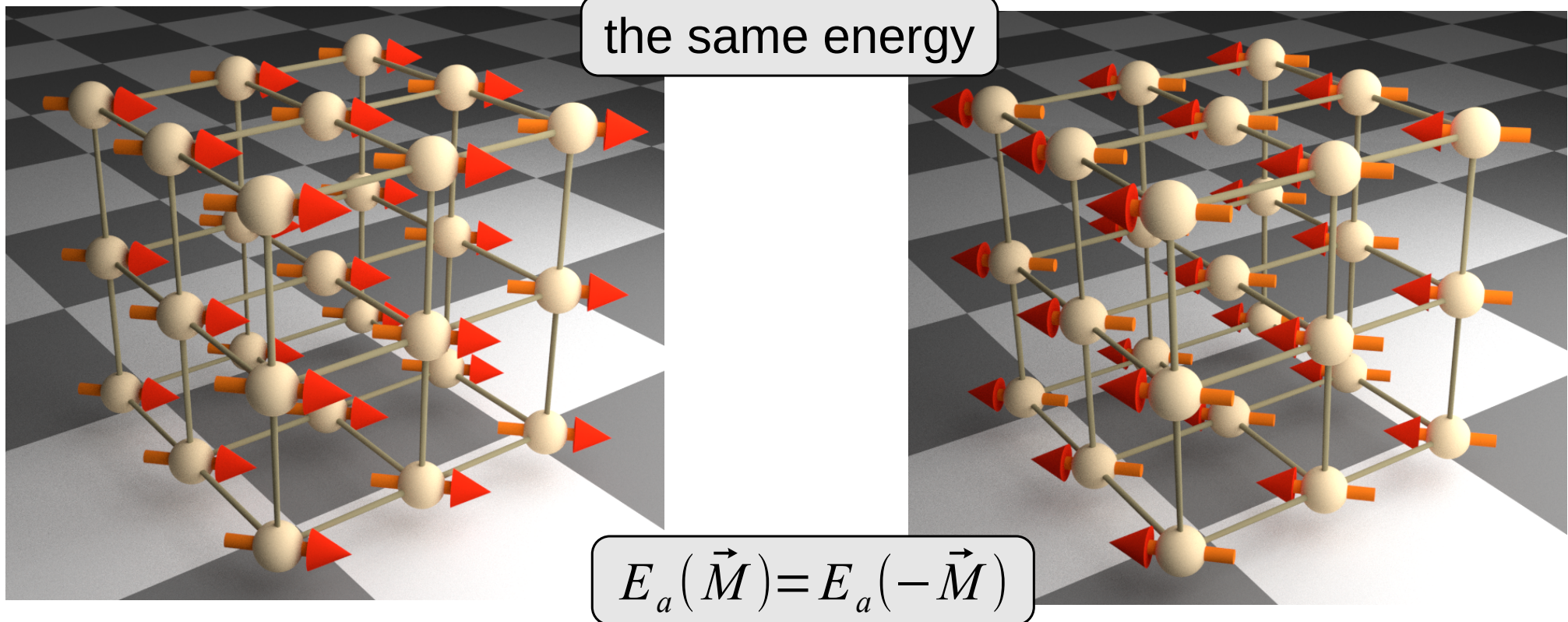
Magnetic anisotropy - symmetry of crystals

- **Neumann's Principle:**

The symmetry elements of any physical property of crystal must include all the symmetry elements of the point group* of the crystal.

- Consider a cubic crystal system with a 3-fold rotation axis [111] and the first nonvanishing anisotropy tensor (second rank):

$$b_{ij} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix}$$

> Transpose of a matrix – switches rows and column indices
>
> $$[M^T]_{ij} = M_{ji}$$

- The transformation matrix corresponding to that rotation is:

$$M = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Note: isometries (angles and distances preserved) of R^3 space are described by square matrices for which an inverse of a matrix is equal to its transpose:
$$M^T = M^{-1}$$

and coordinates transform according to the following rule:
$$a'_i = \sum_j M_{ij} a_j$$

- **Voigt's Principle:**

The conditions of Neumann's principle are fulfilled if the physical property of the crystal is described by the tensor which is invariant under point symmetry operations which leave the crystal unchanged

- It follows that the physical property tensor must fulfill the condition $b = M^T b M$ for all symmetry operations of the point group.

*A point group is a group of symmetry operations all of which leave at least on point unmoved.

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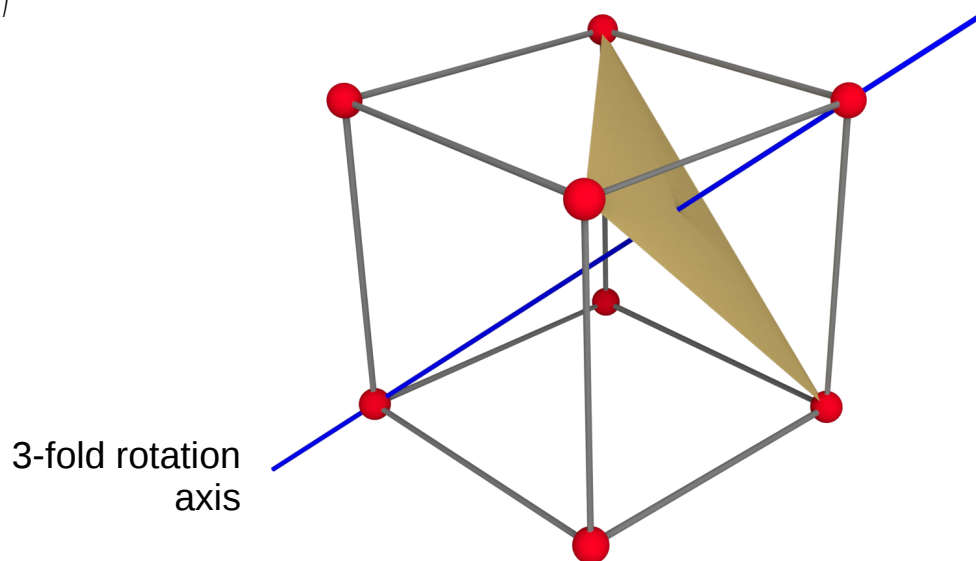> Transpose of a matrix – switches rows and column indices
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3-fold rotation axis

Magnetic anisotropy - symmetry of crystals

- From Voigt's principle it follows for tensor b:

$$b = M^T b M$$

$$b_{ij} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \begin{bmatrix} b_{22} & b_{23} & b_{21} \\ b_{32} & b_{33} & b_{31} \\ b_{12} & b_{13} & b_{11} \end{bmatrix}$$

rotation by 120Deg about [111] direction

effect of the rotation of the crystal on tensor b_{ij}

- Comparing the elements of both (identical) tensors we get:

$b_{11} = b_{22}$	$b_{12} = b_{23}$	$b_{13} = b_{21}$
$b_{21} = b_{32}$	$b_{22} = b_{33}$	$b_{23} = b_{31}$
$b_{31} = b_{12}$	$b_{32} = b_{13}$	$b_{33} = b_{11}$

$$b_{11} = b_{22} = b_{33} = a$$
$$b_{21} = b_{32} = b_{13} = b$$
$$b_{31} = b_{12} = b_{23} = c$$

- The invariance in respect the 120 Deg rotation leaves only **3 independent components**:

$$b_{ij} = \begin{bmatrix} a & c & b \\ b & a & c \\ c & b & a \end{bmatrix}$$

Magnetic anisotropy - symmetry of crystals

$$b = M^T b M$$

- We apply the same procedure again, but this time with other symmetry element of cubic crystal, namely 90Deg rotation around z-axis:

$$b_{ij} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{bmatrix} a & c & b \\ b & a & c \\ c & b & a \end{bmatrix} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{bmatrix} a & -b & c \\ -c & a & -b \\ b & -c & a \end{bmatrix}$$

rotation by 90Deg about [001] direction

effect of the rotation of the crystal on tensor b_{ij}

- Comparing the elements of the first row of both (identical) tensors we get:

$$c = -b, \quad b = c \quad \Rightarrow \quad b = c = 0$$

- It follows that the second rank tensor consistent with the above two symmetry operations possesses **one independent component**:

$$b_{ij} = \begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix}$$

- Similar analysis can be performed for other tensors in the expansion (1):

$$E_{crystal}(\vec{M}) = b_0 + \sum_{i=1,2,3} b_i \alpha_i + \sum_{i,j=1,2,3} b_{ij} \alpha_i \alpha_j + \sum_{i,j,k=1,2,3} b_{ijk} \alpha_i \alpha_j \alpha_k + \dots \quad (1)$$

- Inserting tensor b into the third term of expansion (1) we get:

$$\sum_{i,j=1,2,3} b_{ij}\alpha_i\alpha_j = a(\alpha_1^2 + \alpha_2^2 + \alpha_3^2) = a$$ - independent of the orientation of magnetic moment

$\alpha_1\alpha_2, \alpha_1\alpha_3$, etc. terms are not present because of $b_{ij}=0$ for $j \neq i$

- In cubic system there are no second order terms in the expansion of energy in directional cosines [1].
- Using similar procedure we obtain the complete expression for the energy contribution related to the orientation of magnetic moment in cubic system [1]:

$$E_{crystal}(\vec{M}, T) = K_0(T) + K_1(T)(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + K_2(T)\alpha_1^2\alpha_2^2\alpha_3^2$$

-the coefficients K_0, K_1 … are the linear combinations of tensor components b_{11}, b_{1111}, b_{111111} etc. [4].

- For other crystal systems the similar procedure is employed to obtain the $E_{crystal}(M,T)$ expressions.
- For hexagonal crystals the energy can be expressed as [1]:

$$E_{crystal}(\vec{M}, T) = K_0(T) + K_1(T)(\alpha_1^2 + \alpha_2^2) + K_2(T)(\alpha_1^2 + \alpha_2^2)^2 + \ldots$$

which is usually expressed, using trigonometric identities, as:

$$E_{crystal}(\vec{M}, T) = K_0(T) + K_1(T)\sin^2\theta + K_2(T)\sin^4\theta + \ldots \qquad (2)$$

angle with respect to easy axis

$$\alpha_1^2 + \alpha_2^2 = \sin^2\theta\cos^2\phi + \sin^2\theta\sin^2\phi = \sin^2\theta$$

- Inserting tensor b into the third term of expansion (1) we get:

$$\sum_{i,j=1,2,3} b_{ij}\alpha_i\alpha_j = a(\alpha_1^2 + \alpha_2^2 + \alpha_3^2) = a$$ - independent of the orientation of magnetic moment

- In cubic system there are no second order terms in the expansion of energy in directional cosines [1].
- Using similar procedure we obtain the complete expression for the energy contribution related to the orientation of magnetic moment in cubic system [1]:

$$E_{crystal}(\vec{M},T) = K_0(T) + K_1(T)(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + K_2(T)\alpha_1^2\alpha_2^2\alpha_3^2$$

-the coefficients K_0, K_1 … are the linear combinations of tensor components b_{11}, b_{1111}, b_{111111} etc. [4].

- The terms of the type α_i^4 are omitted since because of the identity [4,5]:

$$2(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + \alpha_1^4 + \alpha_2^4 + \alpha_3^4 = 1$$

they can be incorporated into K_0, K_1 terms.

- The terms of the type α_i^6 can be similarly replaced by $\alpha_i^2\alpha_j^2$ and $\alpha_1^2\alpha_2^2\alpha_3^2$ terms [6].

Magnetic anisotropy - symmetry of crystals

- Number of independent components of the (second rank) tensor depends on the crystal symmetry

- In crystals of cubic system there is one independent component of the tensor.

- Hexagonal systems are characterized by two independent components of the second rank tensors.

Оптическая класси-фикация	Системы	Характеризующая симметрия *	Вид характеристической поверхности и ее ориентация	Число независимых коэф-фициентов	Тензор, приведенный к осям принятой ориентации **
Изотропная среда	Куби-ческая	Четыре оси третьего порядка	Сфера	1	$\begin{bmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{bmatrix}$
Одно-осные кри-сталлы	Тетраго-нальная / Гексаго-нальная / Триго-нальная	Одна ось четвертого порядка / Одна ось шестого порядка / Одна ось третьего порядка	Поверхность вращения вокруг главной оси симметрии x_3 (z)	2	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
Дву-осные кри-сталлы	Орто-ромбиче-ская	Три взаимно перпендику-лярные оси второго порядка; осей высшего порядка нет	Произвольная поверхность второго порядка с осями x_1, x_2, x_3, параллельными осям второго порядка x, y, z	3	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
	Моно-клинная	Одна ось вто-рого порядка	Произвольная поверхность второго поряд-ка с одной осью x_2, параллель-ной оси вто-рого порядка y	4	$\begin{bmatrix} S_{11} & 0 & S_{31} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & S_{33} \end{bmatrix}$
	Три-клинная	Центр симме-трии или от-сутствие сим-метрии	Произвольная поверхность второго поряд-ка. Положение относительно кристаллогра-фических осей не фиксировано	6	$\begin{bmatrix} S_{11} & S_{12} & S_{31} \\ S_{12} & S_{22} & S_{23} \\ S_{31} & S_{23} & S_{33} \end{bmatrix}$

* Оси симметрии могут быть поворотными или инверсионными; см. также стр. 335.
** Ориентация осей x_1, x_2, x_3 поверхности второго порядка по отношению к кри-сталлографическим осям x, y, z и элементам симметрии указана в табл. 4. Добавочные замечания о выборе систем координат см. в приложении 3.

image source: Дж. Най Физические Свойства Кристаллов, Издательство МИР 1967
or see original version: J. F. Nye, Physical Properties of Crystals

Magnetic anisotropy – energy surfaces

- *Energy surface* – the distance from origin along the given direction is proportional to magnetocrystalline energy of the crystal with magnetization along that direction.
- We start from the expression of the magnetocrystalline energy for cubic crystals:

$$E_{crystal}(\vec{M}, T) = K_0(T) + K_1(T)(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2) + K_2(T)\alpha_1^2 \alpha_2^2 \alpha_3^2 + ...$$

- For K_0=1, K_1=0 and K_2=0 we have isotropic energy surface:
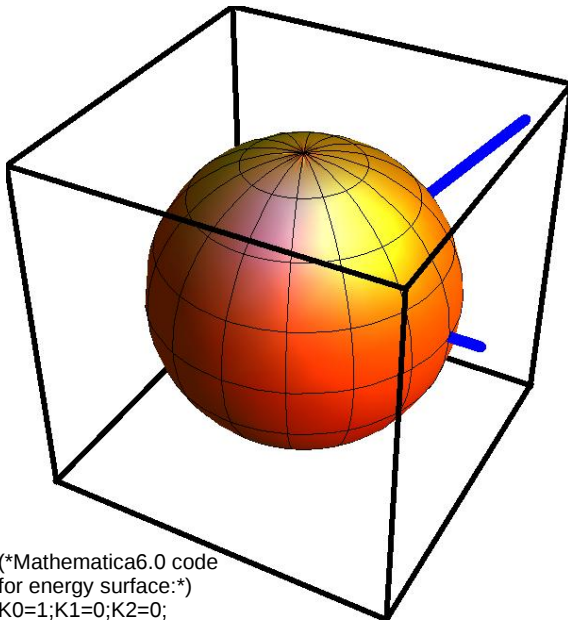
- Energy does not depend on the orientation of the magnetic moment

- The magnetization reversal (hysteresis) itself does not depend on K_0 but to show the difference between the cases of K_1>0 and K_1<0 we need a reference level – the surface of the sphere (r=K_0).

```
(*Mathematica6.0 code
for energy surface:*)
K0=1;K1=0;K2=0;
a1=Sin[teta] Cos[fi];
a2=Sin[teta] Sin[fi];
a3=Cos[teta];
Energy=K0+K1(a1^2 a2^2+a3^2 a2^2+a1^2 a3^2)+K2(a1^2 a2^2  a3^2);
xsurface=Energy a1;
ysurface=Energy a2;
zsurface=Energy a3;
obrazek=ParametricPlot3D[{xsurface,ysurface,zsurface},{fi,0,2\[Pi]},{teta,-\[Pi],\[Pi]},PlotStyle->{Orange,Specularity[White,10]},
ImageSize->600,PlotRange->{-1.2,1.2},Axes->None,AxesLabel->{X,Y,Z},BoxStyle->Directive[Thickness[0.01],Black]];
osdiag=Line[{{0,0,0},{1,1,1}}];
osx=Line[{{0,0,0},{1.2,0,0}}];
moment=Sphere[{1,1,1},1];
obrazekwy=Show[obrazek,Graphics3D[{Blue,Thickness[0.02],osx}],Graphics3D[{Blue,Thickness[0.02],osdiag}]]
```
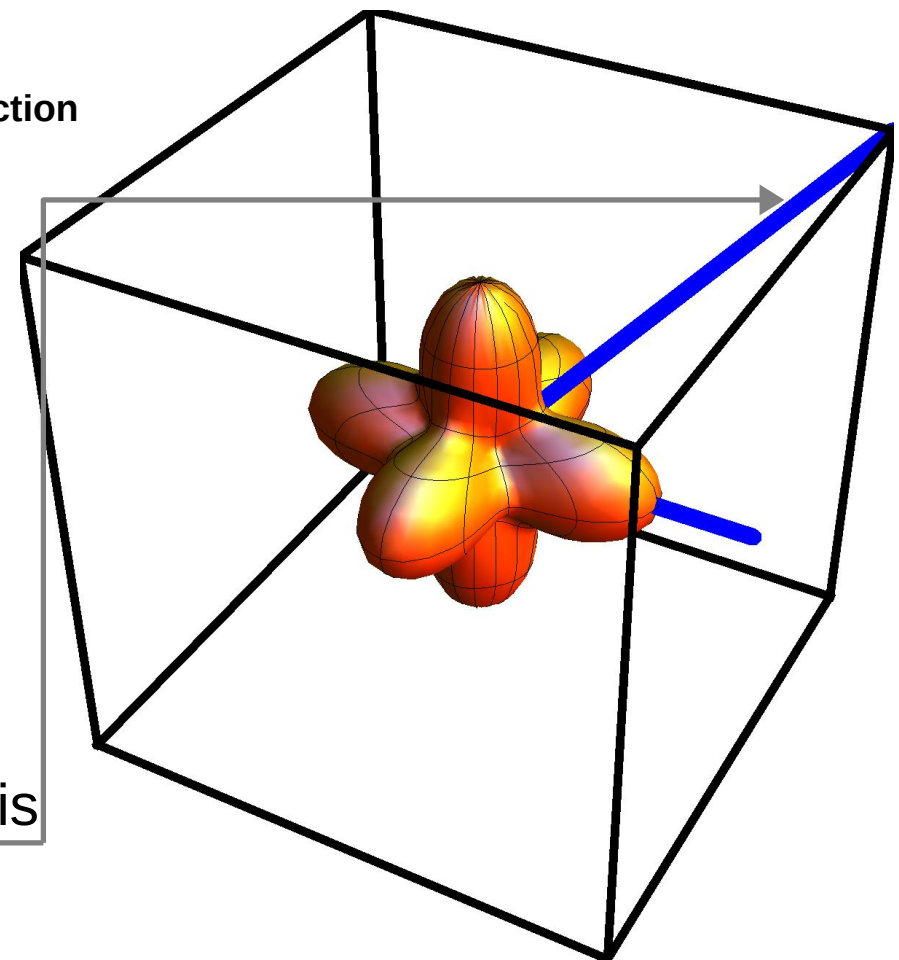
Magnetic anisotropy – energy surfaces

- Cubic crystals magnetocrystalline energy surfaces* for different anisotropy coefficients:

[111] direction

[100] direction

easy axis
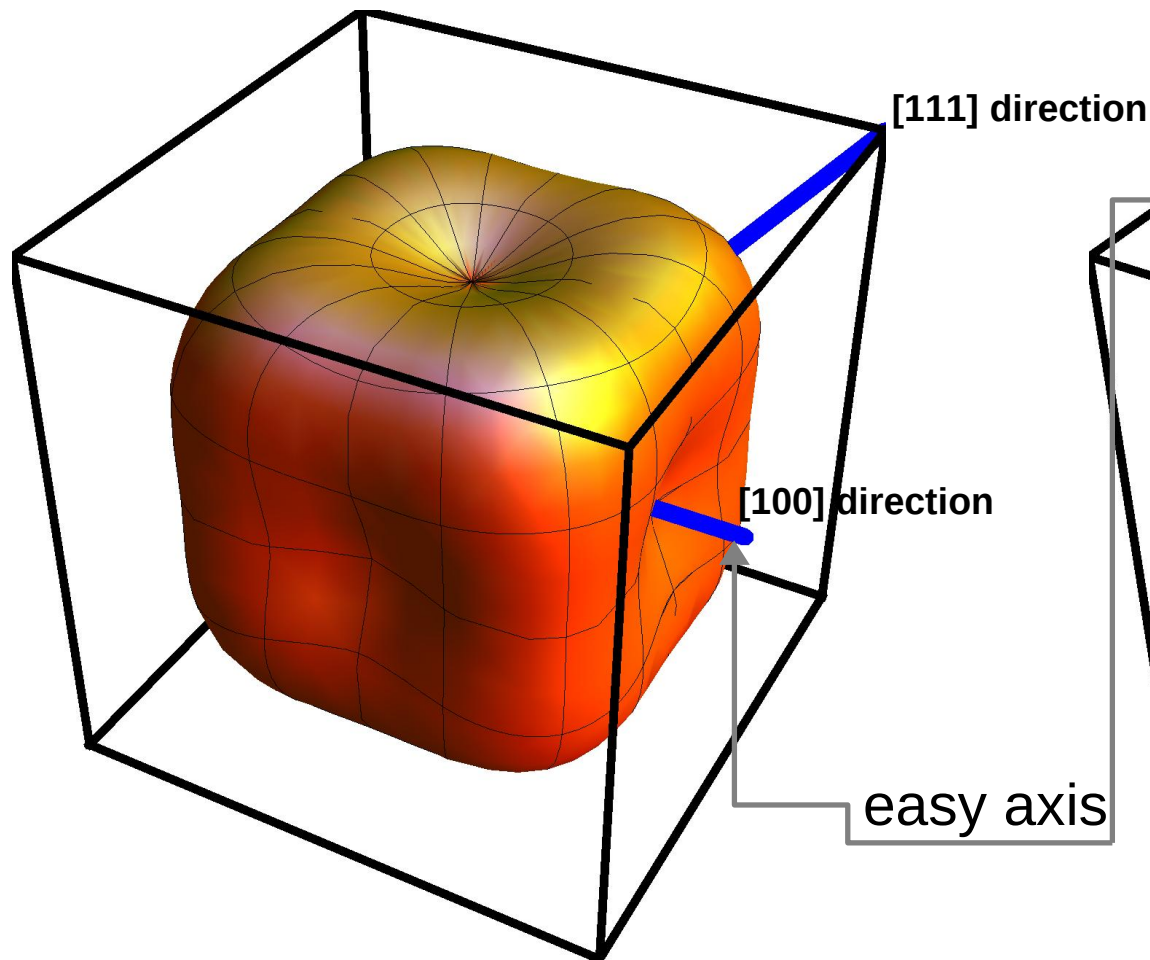
energy surface for $K_0=1$, **$K_1=2$** and $K_2=0$

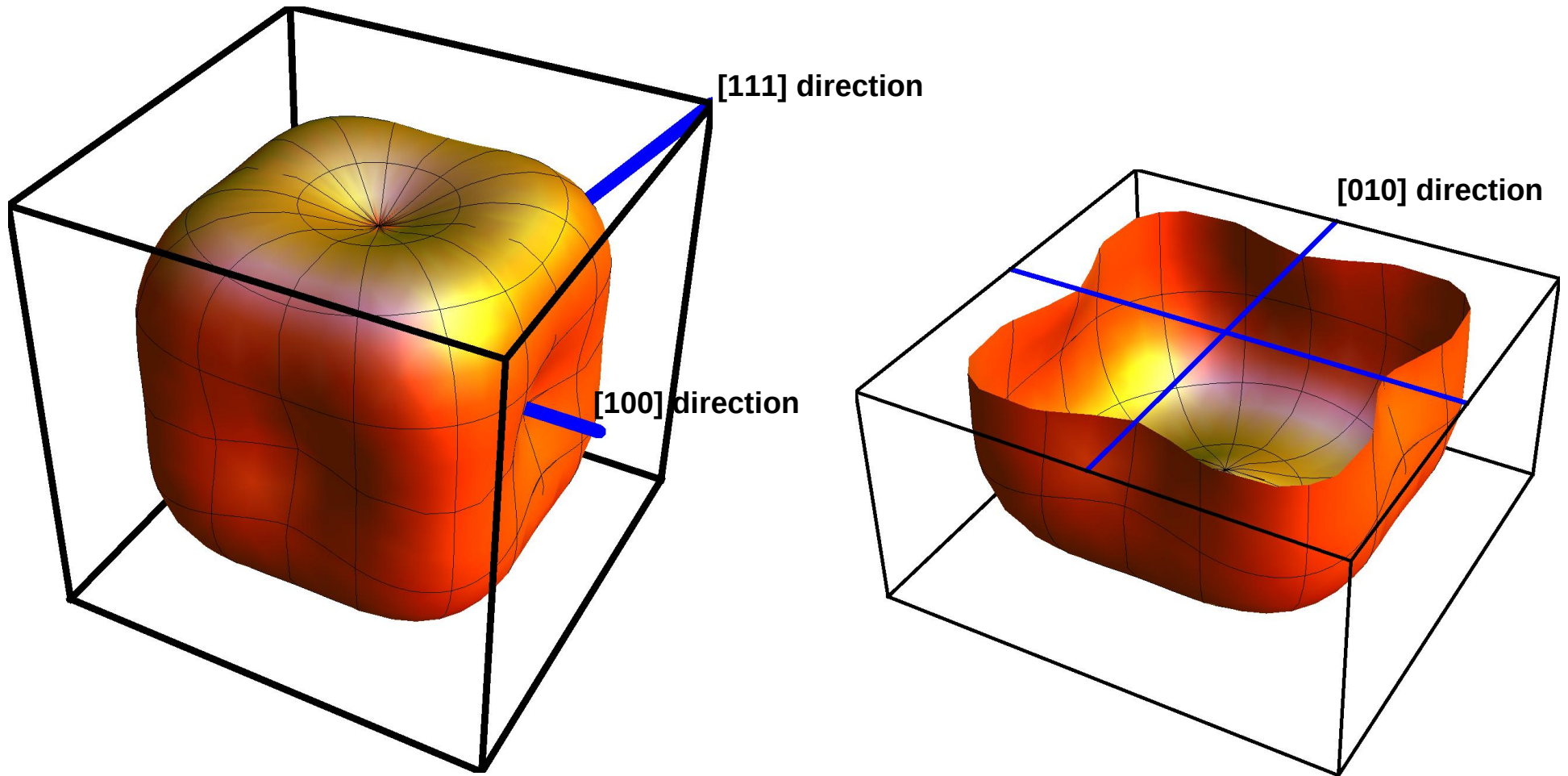typical for bcc cubic crystals (Fe)

*both images have the same scale

energy surface for $K_0=1$, **$K_1=-2$** and $K_2=0$

typical for fcc cubic crystals (Ni)

Magnetic anisotropy – energy surfaces

- Cubic crystals magnetocrystalline energy surfaces* for different anisotropy coefficients:

[111] direction

[100] direction

[010] direction

energy surface for $K_0=1$, **$K_1=2$** and $K_2=0$

typical for bcc cubic crystals (Fe)

*both images have the same scale

Magnetic anisotropy – energy surfaces

- Hexagonal crystals magnetocrystalline energy surfaces:

$$E_{crystal}(\vec{M}) = K_0 + K_1 \sin^2\theta + K_2 \sin^4\theta$$

[001] direction
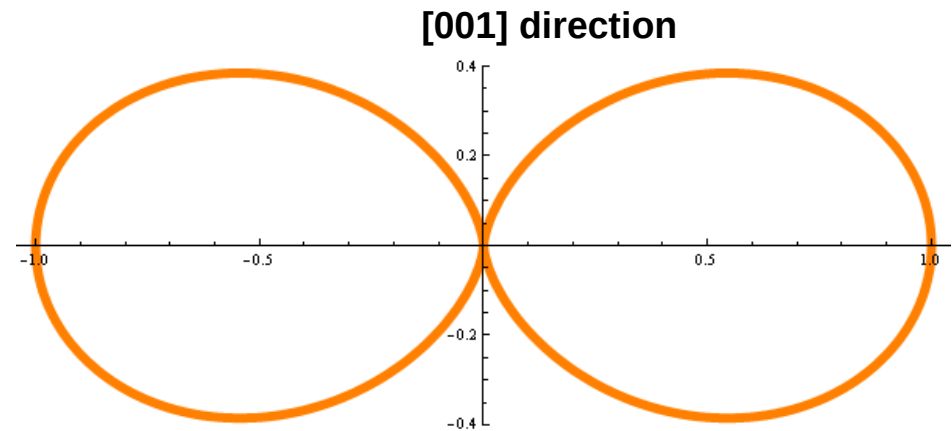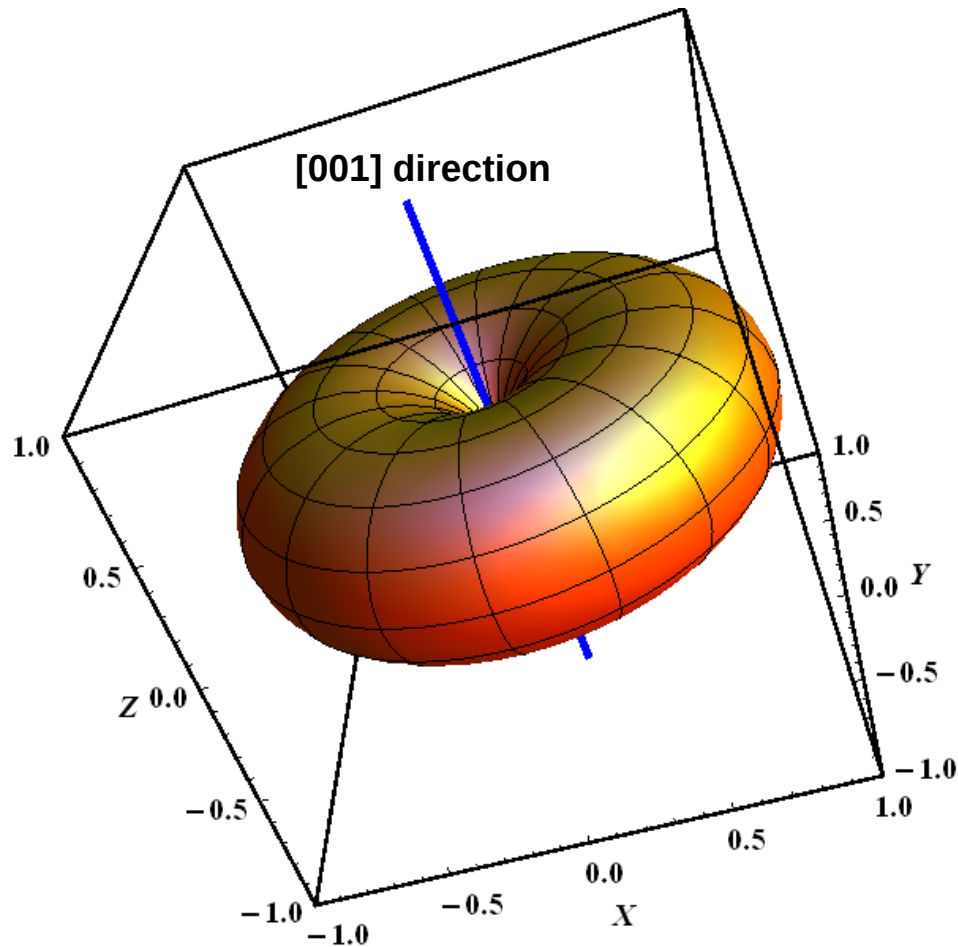
[001] direction

energy surface for $K_0=0$, **K_1=-1** and $K_2=0$

typical for hcp cobalt crystals

[0,0,1] - easy direction

Energy surfaces – the influence of the external field

- Cubic crystals magnetocrystalline energy surfaces for different values of the external field applied along [111] direction*:

H=1

field direction

H=0

H=0.5

H=1.5
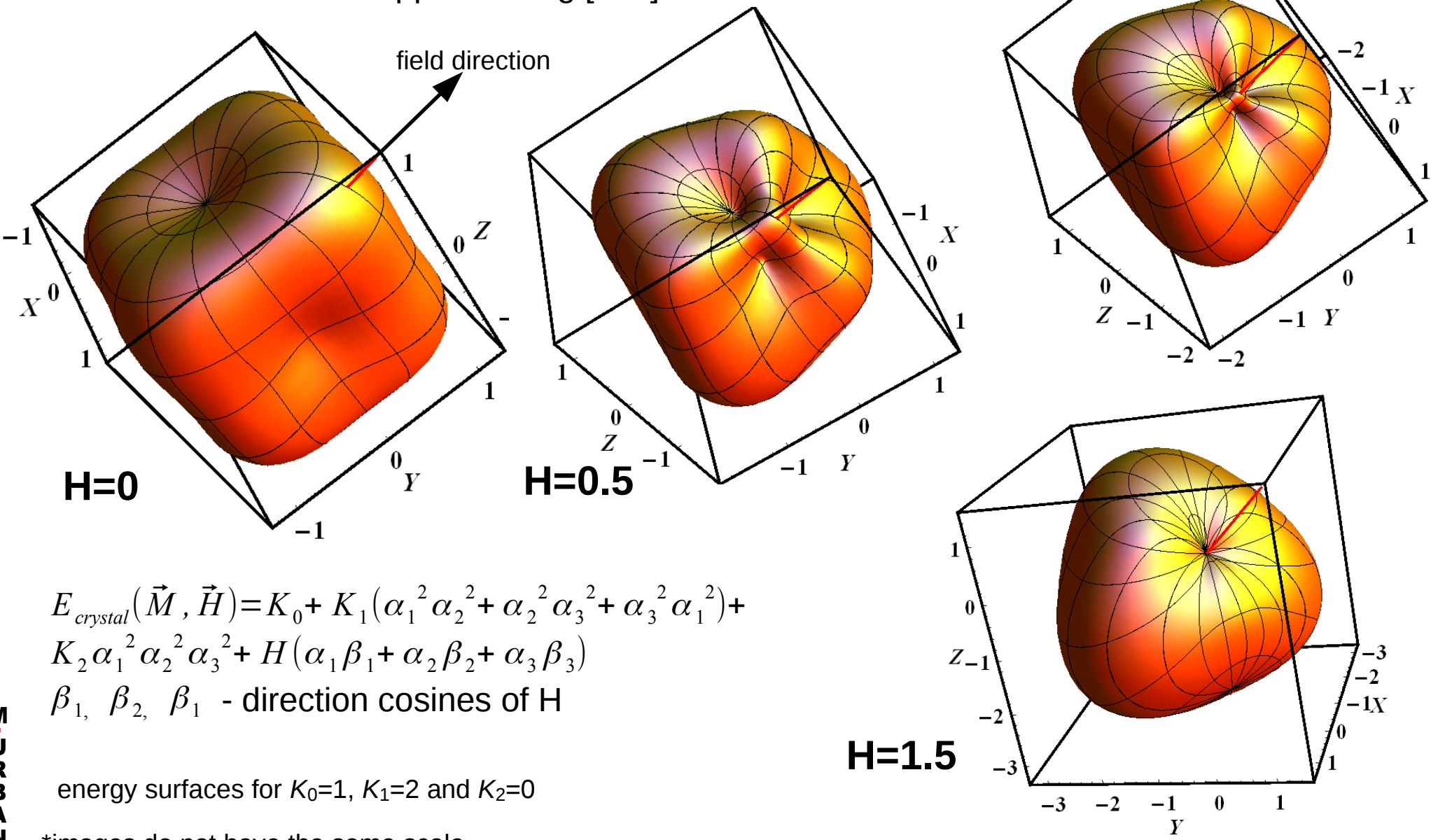
$$E_{crystal}(\vec{M},\vec{H}) = K_0 + K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) +$$
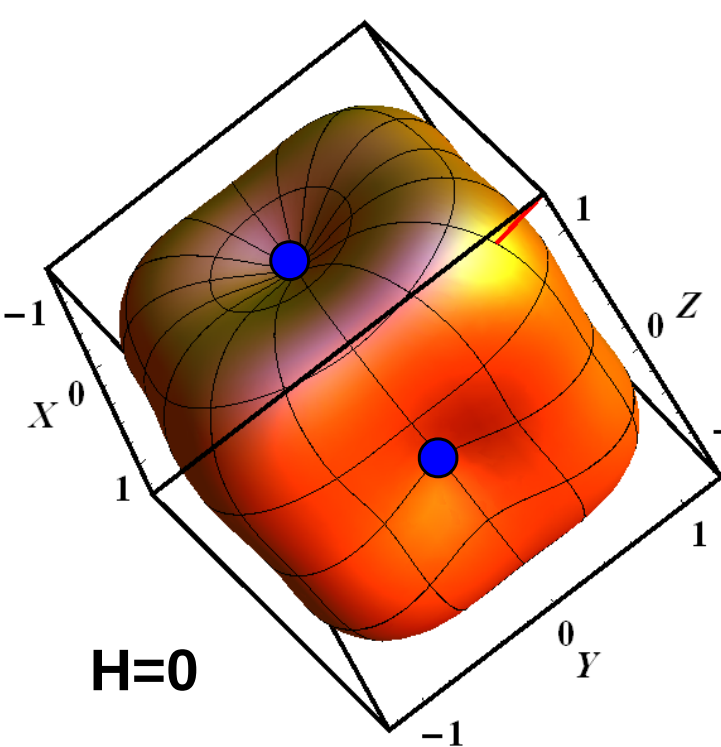$$K_2\alpha_1^2\alpha_2^2\alpha_3^2 + H(\alpha_1\beta_1 + \alpha_2\beta_2 + \alpha_3\beta_3)$$
$$\beta_1, \ \beta_2, \ \beta_1 \ \text{- direction cosines of H}$$

energy surfaces for $K_0 = 1$, $K_1 = 2$ and $K_2 = 0$

*images do not have the same scale

Energy surfaces – the influence of the external field

- Cubic crystals magnetocrystalline energy surfaces for different values of the external field applied along [111] direction*:

H=1

H=0

H=0.5

H=1.5
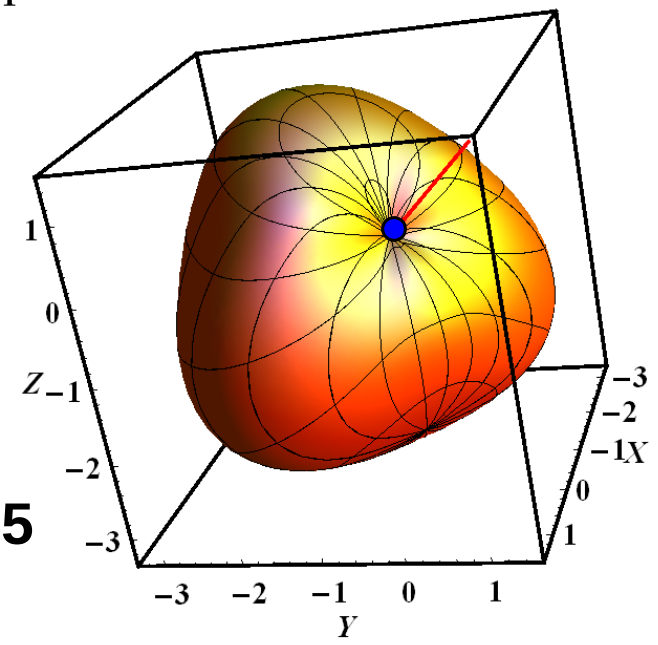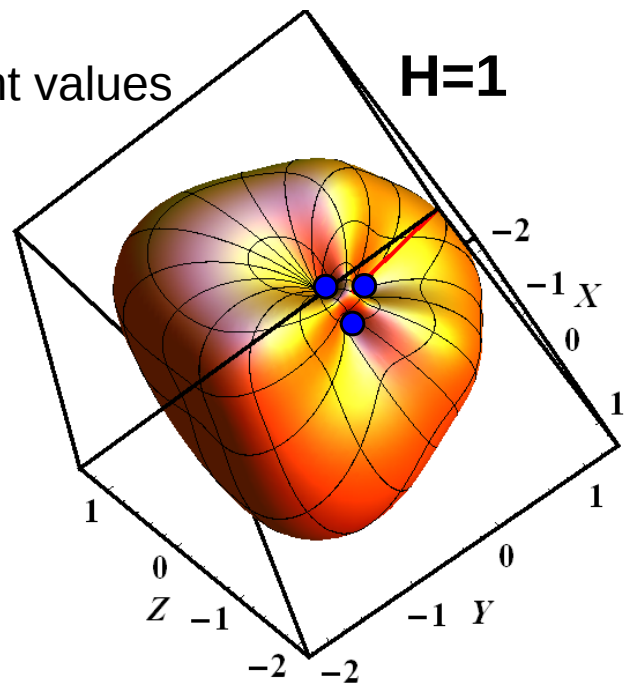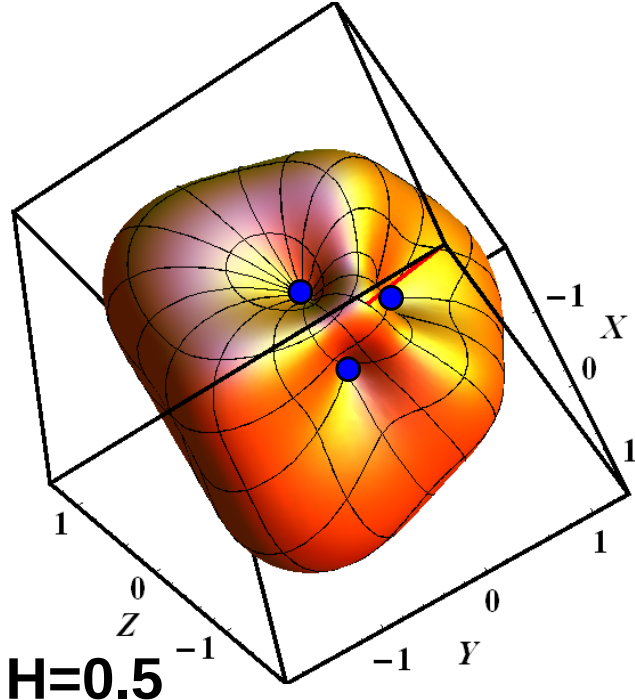
- with increasing field **H** the number of local minima decreases

- above saturation there is only **one** local minimum

energy surfaces for $K_0=1$, $K_1=2$ and $K_2=0$

*images do not have the same scale

Anisotropy constants of ferromagnetic elements

- Bulk magnetocrystalline anisotropy constants of basic ferromagnetic elements at 4.2K [1]:

	Fe (bcc)	Co (hcp)	Ni (fcc)
K_1 [J/m^3]	54800	760000	-126300
[meV/atom]	4.02×10^{-3}	5.33×10^{-2}	-8.63×10^{-3}
K_2 [J/m^3]	1960	100500	57800
[meV/atom]	1.44×10^{-5}	7.31×10^{-3}	3.95×10^{-3}

- Magnetocrystalline anisotropy of permalloy ($Ni_{81}Fe_{19}$):

$K \approx 0$ kJ/m^3

- Magnetocrystalline anisotropy of rare-earth magnets [3]:

YCo_5 $K \approx 5.5 \times 10^6$ J/m^3

$SmCo_5$ $K \approx 7.7 \times 10^6$ J/m^3

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Mixed anisotropies

- Consider the crystal in which two uniaxial anisotropies are present together [3]. We limit our discussion to second order terms [see Eq.(2)]:

$$E_A = K_0 + K_A \sin^2\theta, \qquad E_B = K_0 + K_B \sin^2(90-\theta) = K_0 + K_B \cos^2\theta$$

- The total energy of the moment is:

$$E_{total} = K'_0 + K_A \sin^2\theta + K_B \cos^2\theta$$
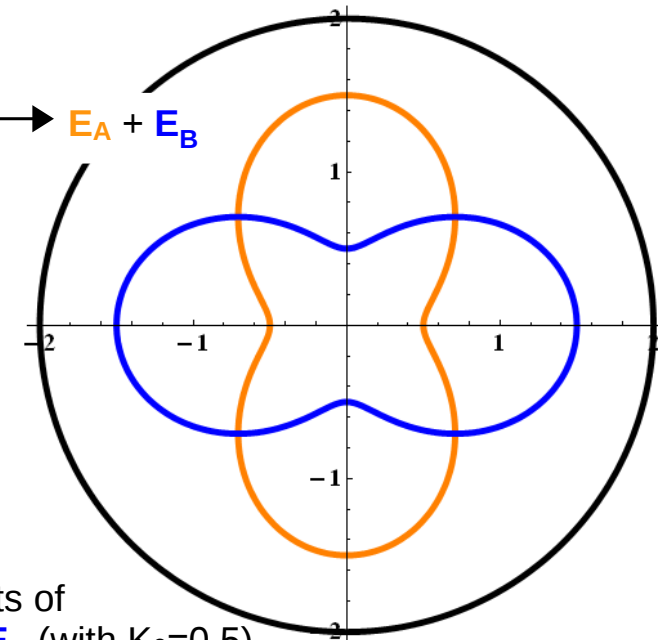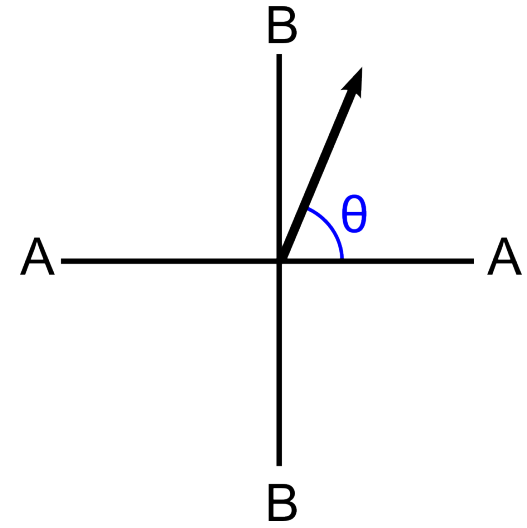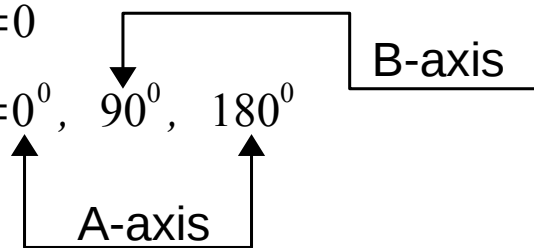
- If $K_A = K_B$ the energy is independent of θ:

$$E_{total} = K'_0 + K_B(\sin^2\theta + \cos^2\theta) + (K_A - K_B)\sin^2\theta = K'_0 + K_B$$

> Two equal uniaxial anisotropies at right angle are not equivalent to biaxial anisotropy.

- If K_A and K_B are not equal the equilibrium angle is given by:

$$\frac{\partial E_{total}}{\partial\theta} = \frac{\partial}{\partial\theta}(K_A - K_B)\sin^2\theta = \frac{\partial}{\partial\theta}(K_A - K_B)\left(\frac{1-\cos(2\theta)}{2}\right) =$$

$$(K_A - K_B)\sin(2\theta) = 0$$

B-axis

- Solutions are $\theta = 0^0, \ 90^0, \ 180^0$

A-axis

$E_A + E_B$

Polar plots of
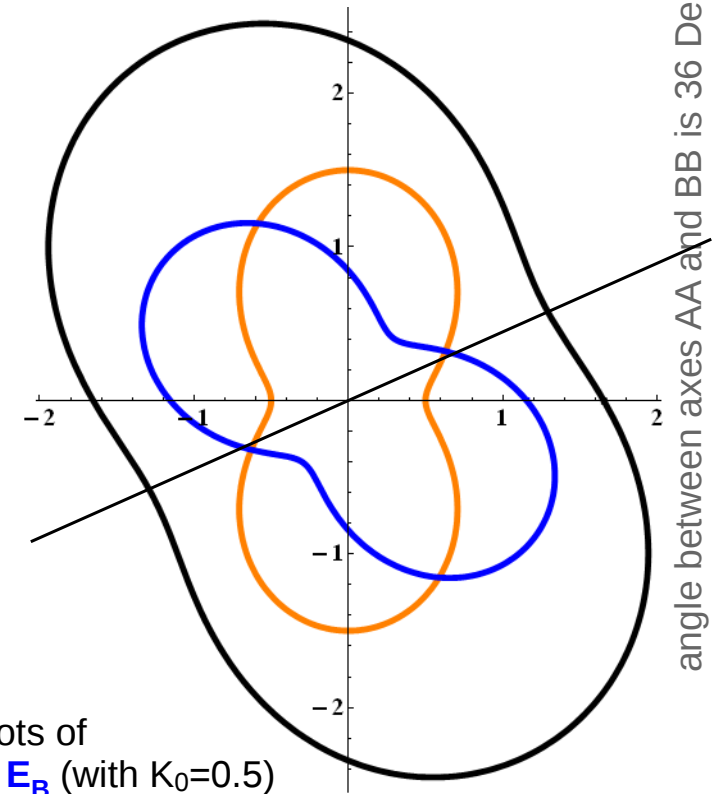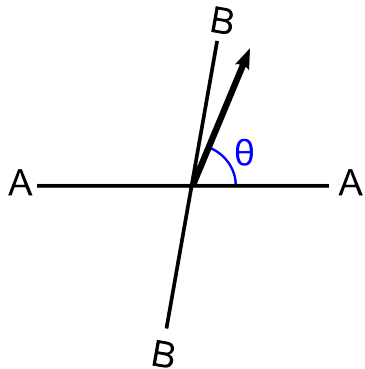E_A and E_B (with $K_0 = 0.5$)

Mixed anisotropies

- From the second derivative (must be positive for minimum) we obtain [3]:

$$\frac{\partial^2 E_{total}}{\partial \theta^2} = 2(K_A - K_B)\cos(2\theta) \quad \Rightarrow$$

$K_A > K_B$	$K_A < K_B$
Easy axis – θ=0 Deg	Easy axis – θ=90 Deg

The direction of easy magnetization is not along some axis lying between AA and BB axes but is along the axis pertaining to higher anisotropy.

- Case of the two uniaxial anisotropies which are not perpendicular:

-in case of anisotropies of equal strength the resultant easy axis CC lies midway between axes AA and BB

-otherwise the CC axes makes smaller angle with axis pertaining to stronger anisotropy

Polar plots of **E_A** and **E_B** (with K₀=0.5)

$$E_A \quad and \quad E_B \quad (with \ K_0=0.5)$$

angle between axes AA and BB is 36 Deg

Microscopic mechanism of magnetocrystaline anisotropy

- The spin of electron interacts with the crystal structure via spin orbit coupling

  - the moment of a spin (red arrow) is strongly coupled to the electron cloud (blue orbitals) – spin orbit coupling
  - when external magnetic field rotates the spin the electron "attempts" cloud follows but its energy depends on the orientation relative to neighboring atoms/orbitals
  - if the orbitals overlap there is additional energy due to coulomb repulsion (on the other hand it can lower the energy of repulsion between ions) -   **IT IS A QUALITATIVE DESCRIPTION**!

overlap
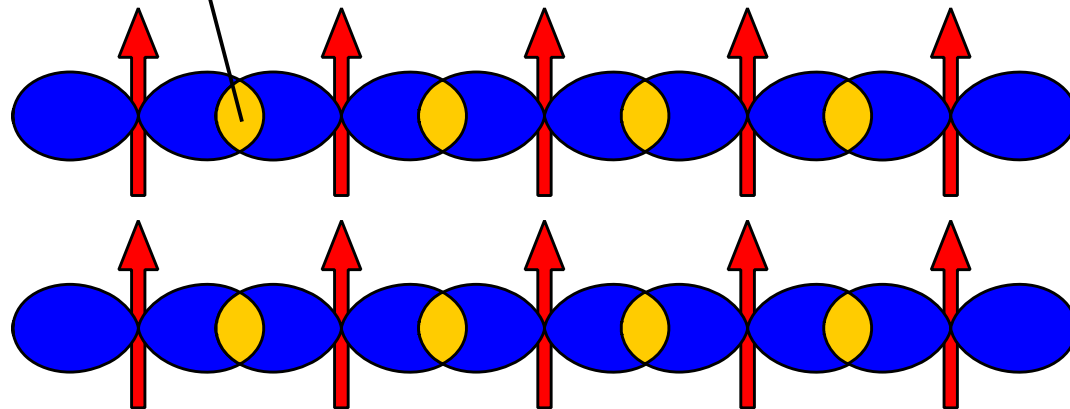
Higher energy
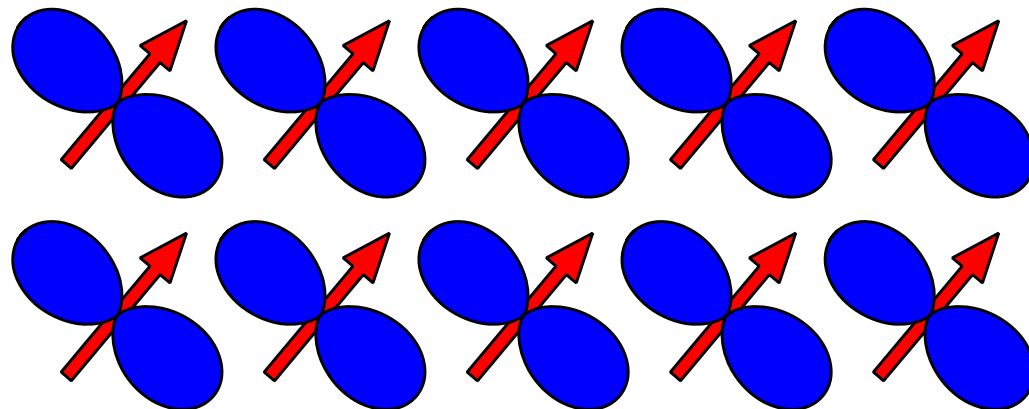
small overlap   **Lower energy**

- Due to spin-orbit coupling different orientations of electron spins correspond to different orientations of **atomic orbitals** relative to crystal structure

- As a consequence some orientations of the resultant magnetic moment are energetically favorable – **easy directions**.

Stoner-Wohlfarth model*

- Describes magnetization reversal in **single domain** magnetic particles/films
- The reversal is characterized by the orientation of single magnetic moment
- The anisotropy may be of magnetocrystalline, shape etc. origin
- For the uniaxial anisotropy case the energy can be described as (compare magnetocrystalline anisotropy energy expression for hexagonal system) [8]:
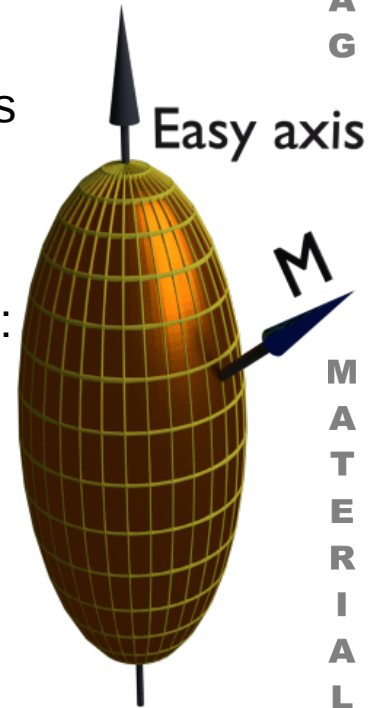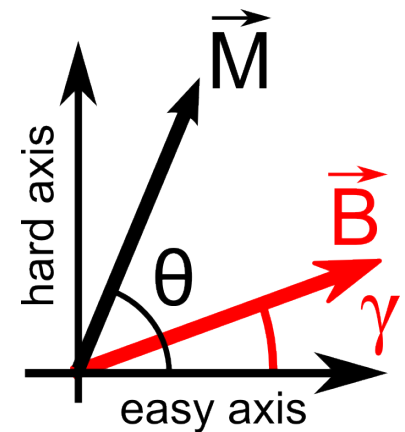
$$E_{total} = K_0 + K_1 \sin^2\theta - \vec{B}\cdot\vec{M} = K_0 + K_1\sin^2\theta - M\,B\cos(\gamma-\theta)\ **$$

Zeeman energy

- The energy landscape for different values of **B** ($K_0=0, K_1=1, M=1, \gamma=30^0$):


direction of the applied field
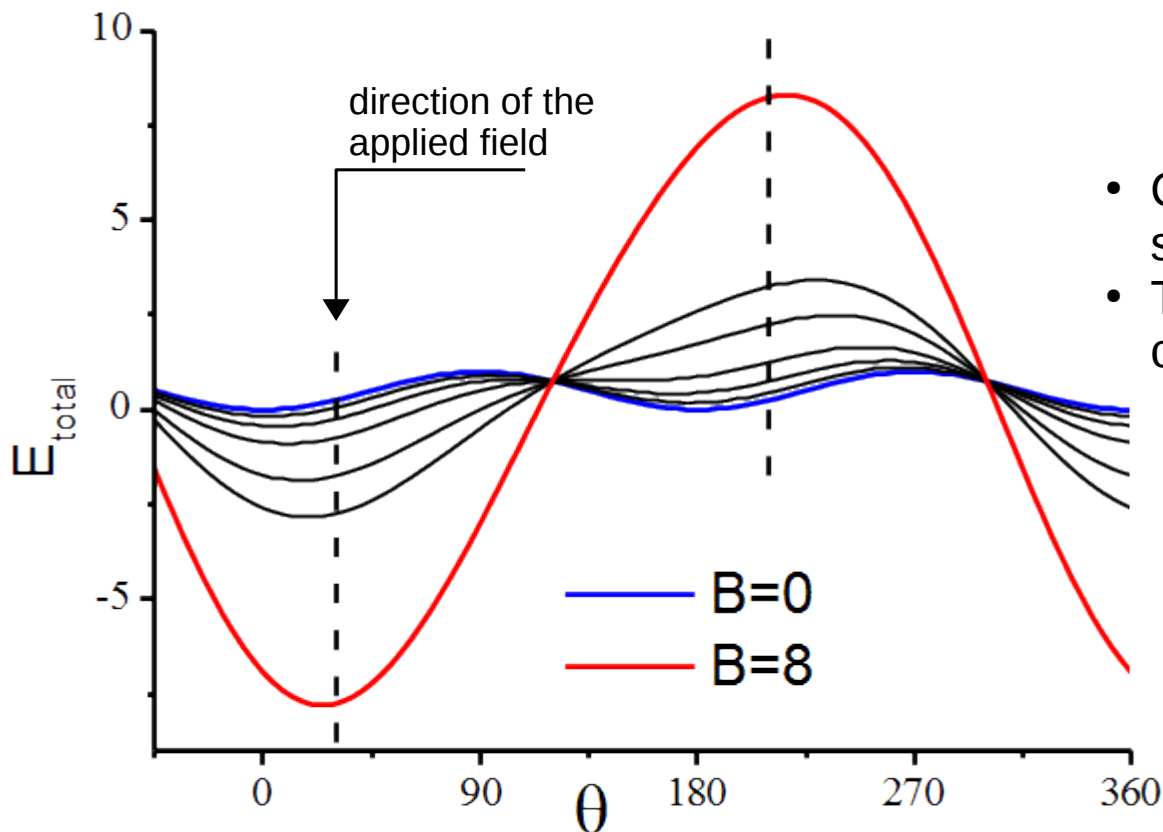
- On increasing the field the minima shift toward its direction
- The angle antiparallel to field corresponds to absolute maximum

B=0

B=8

*some times called macrospin model ** this expression is for a unit volume of the material: M:=MV [Am²], K=KV [J]

Stoner-Wohlfarth model

- The dependence *angle(field)* obtained from the energy landscapes of the previous slide gives hysteresis loops:
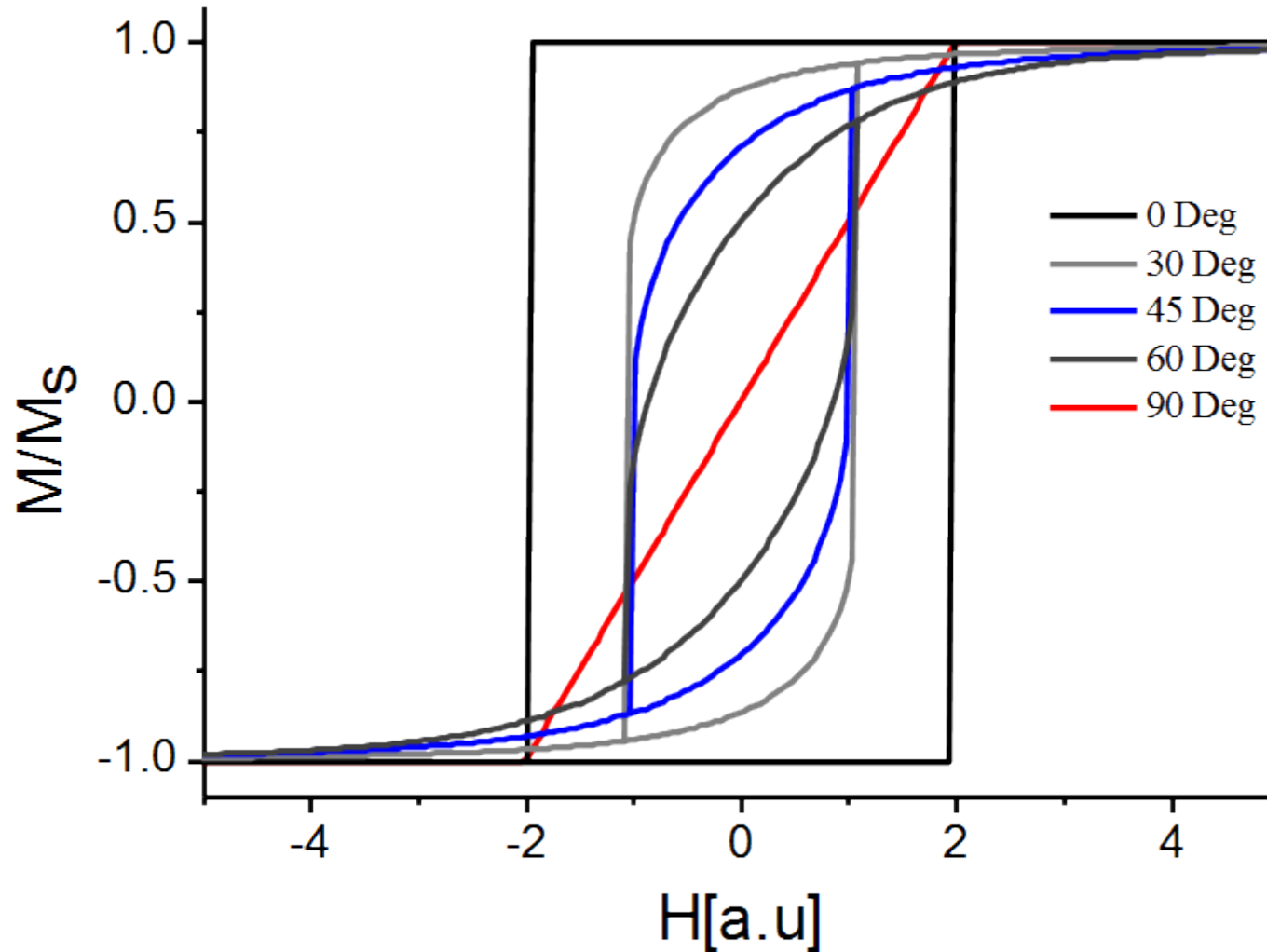
- For field applied along easy-axis the reversal is completely irreversible

- For field applied perpendicularly to EA direction the reversal is completely reversible

- For field applied in arbitrary direction magnetization is "partly reversible and partly irreversible" [9]

Stoner-Wohlfarth model

- *Hard axis reversal*. We can rewrite the expression for the total energy using components of the field parallel (B_x) and perpendicular (B_y) to easy axis [9]:

$$E_{total}=K_0+ K_1\sin^2\theta - M B\cos(\gamma-\theta)=K_0+ K_1\sin^2\theta - B_x M_x - B_y M_y=$$
$$K_0+ K_1\sin^2\theta - B_x M\cos(\theta)-B_y M\sin(\theta)$$

- Energy becomes minimum at a specific angle which can be determined setting:

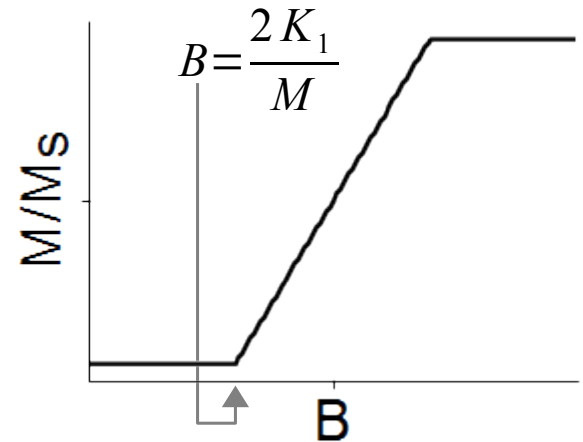$$\frac{\partial E_{total}}{\partial\theta}=2K_1\sin\theta\cos\theta + B_x M\sin(\theta)-B_y M\cos(\theta)=0$$

- With $\alpha=\dfrac{2K_1}{M}$ this can be written as:

$$\alpha\sin\theta\cos\theta + B_x\sin(\theta)-B_y\cos(\theta)=0 \quad \text{or} \quad \boxed{\frac{B_y}{\sin(\theta)}-\frac{B_x}{\cos(\theta)}=\alpha}$$

- If field is applied perpendicularly to EA we have ($B_x=0$, $B_y=B$):

$$\sin(\theta)=\frac{B}{\alpha}$$ proportional to $\vec{M}$ component parallel to $\vec{B}$

$B=\dfrac{2K_1}{M}$

(M/Ms vs B graph)

If field is applied perpendicularly to the easy axis the component of magnetization parallel to the field is a linear function of the external field up to saturation which happens at*:

$$B_S=\frac{2K_1}{M}$$

$B[1T=\frac{kg}{s^2 A}]$

$[\frac{K}{M}=\frac{J/m^3}{A/m}=\frac{J}{A\cdot m^2}=\frac{kg\cdot m\cdot m\,h^2}{A\cdot m^2}=\frac{kg}{s^2\cdot A}=1T]$

*in practical applications K[Jm⁻³], M[Am⁻¹]

*in practical applications K[Jm^{-3}], M[Am^{-1}]

Stoner-Wohlfarth model – astroid* curve

- Depending on the value of the external field there may one or two equilibrium orientations of magnetic moment. For a given field orientation the two minima collapse to one when [9]:

$$\frac{\partial^2 E_{total}}{\partial \theta^2} = 0$$

one of the minima ceases to exist

$$\frac{\partial E_{total}}{\partial \theta} = \alpha \sin\theta \cos\theta + B_x \sin(\theta) - B_y \cos(\theta) = 0$$

- From the expression for derivative of energy (previous slide) we have: From previous slide:

$$\frac{\partial^2 E_{total}}{\partial \theta^2} = \alpha(\cos^2\theta - \sin^2\theta) + B_x \cos(\theta) + B_y \sin(\theta) = 0$$

$$\alpha = \frac{B_y}{\sin(\theta)} - \frac{B_x}{\cos(\theta)}$$

$$\frac{\partial^2 E_{total}}{\partial \theta^2} = \cos^2\theta \sin^2\theta \left(\frac{B_y}{\sin^3(\theta)} + \frac{B_x}{\cos^3(\theta)} \right) = 0$$

- We are looking for the solution of the set (the first and the second derivatives equal to 0):

$$\alpha = \frac{B_y}{\sin(\theta)} - \frac{B_x}{\cos(\theta)} \quad , \quad \frac{B_y}{\sin^3(\theta)} + \frac{B_x}{\cos^3(\theta)} = 0$$

$$\alpha + \frac{B_x}{\cos(\theta)} = \boxed{\frac{B_y}{\sin(\theta)}} \quad , \quad \frac{B_y}{\sin(\theta)} \frac{1}{\sin^2(\theta)} + \frac{B_x}{\cos^3(\theta)} = 0$$

- By a direct substitution of the first equation into the second we get:

$$B_x = -\alpha \cos^3\theta , \quad B_y = \alpha \sin^3\theta$$

- Introducing reduced fields ($b_x = \frac{B_x}{\alpha} = -\cos^3\theta$) it may be written as:

$$\boxed{b_x^{2/3} + b_y^{2/3} = 1} \quad = \cos^2\theta + \sin^2\theta \quad \underline{\text{equation of astroid}}$$
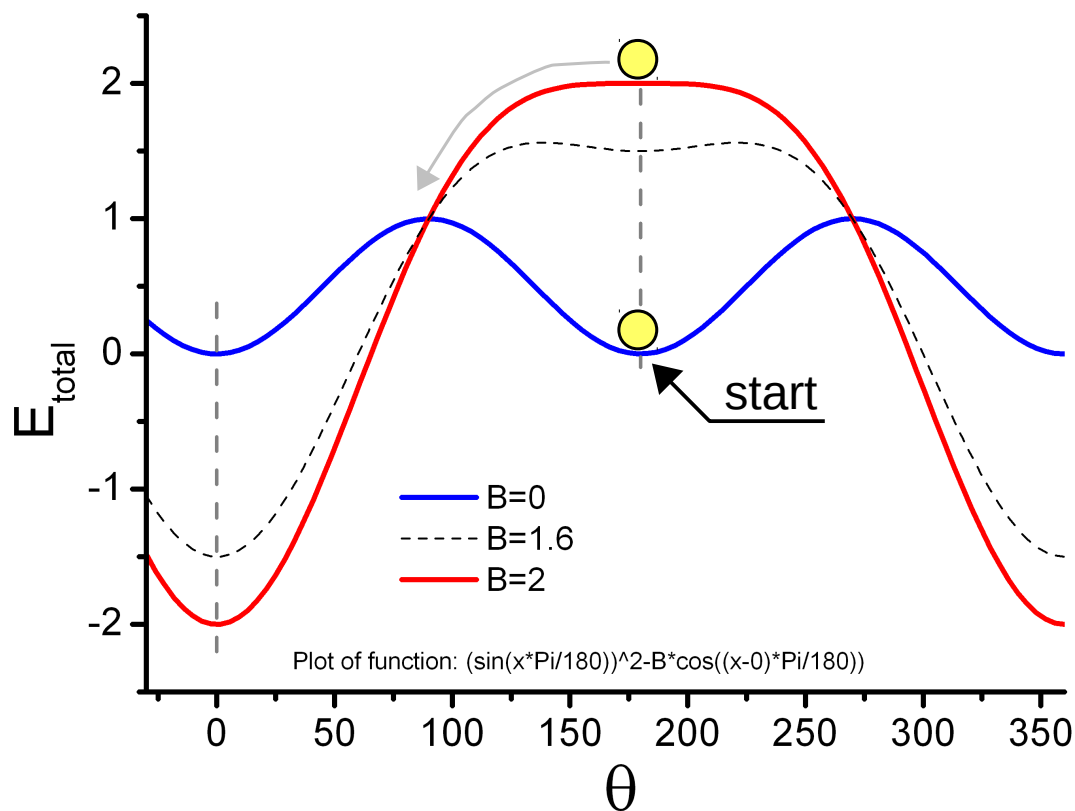
* it happens people call it „asteroid" [S.U. Jen and C.C. Liu, Journal of Applied Physics 115, 013909 (2014)]

Stoner-Wohlfarth model – astroid curve

- Stoner-Wohlfarth astroid separates region, in (bx,by) plane, with two minima of energy from that with only one minimum*
- When the external field is changed so that the astroid is crossed the discontinuous changes of the orientation of magnetization can take place


inside: two minima
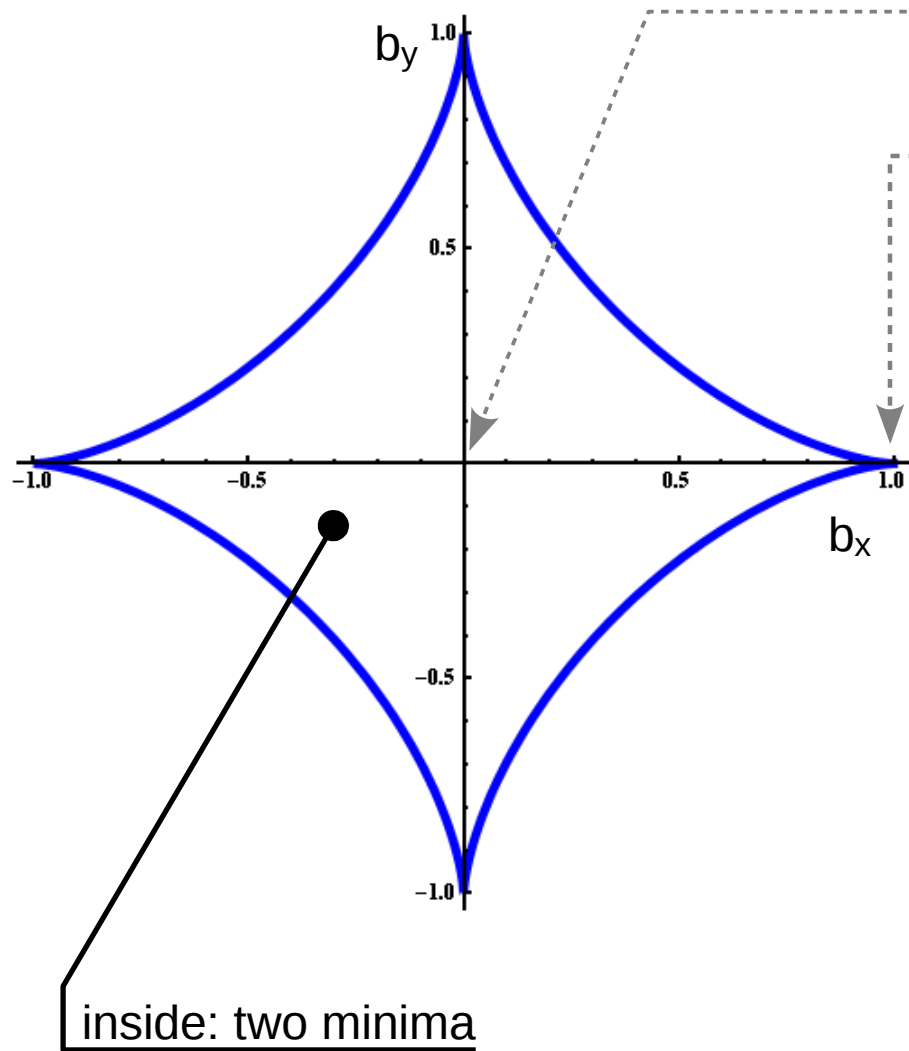
- we start with magnetic moment pointing in negative direction (180 Deg, parallel to easy axis) and zero applied field
- we increase then the field (parallel to easy axis) into positive values and the minimum at 180 Deg becomes less deep
- finally, at B=2 (b_x=1), the 180 Deg orientation ceases to be a minimum (first and second derivatives are zero – we cross Stoner-Wohlfart astroid) and we end up with a single minimum at 0 Deg – magnetic moment switches to that minimum

Plot of function: (sin(x*Pi/180))^2-B*cos((x-0)*Pi/180))

B=0
B=1.6
B=2

E_{total}

θ

start

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Stoner-Wohlfarth model – astroid curve

- Stoner-Wohlfarth astroid separates region, in (bx,by) plane, with two minima of energy from that with only one minimum*
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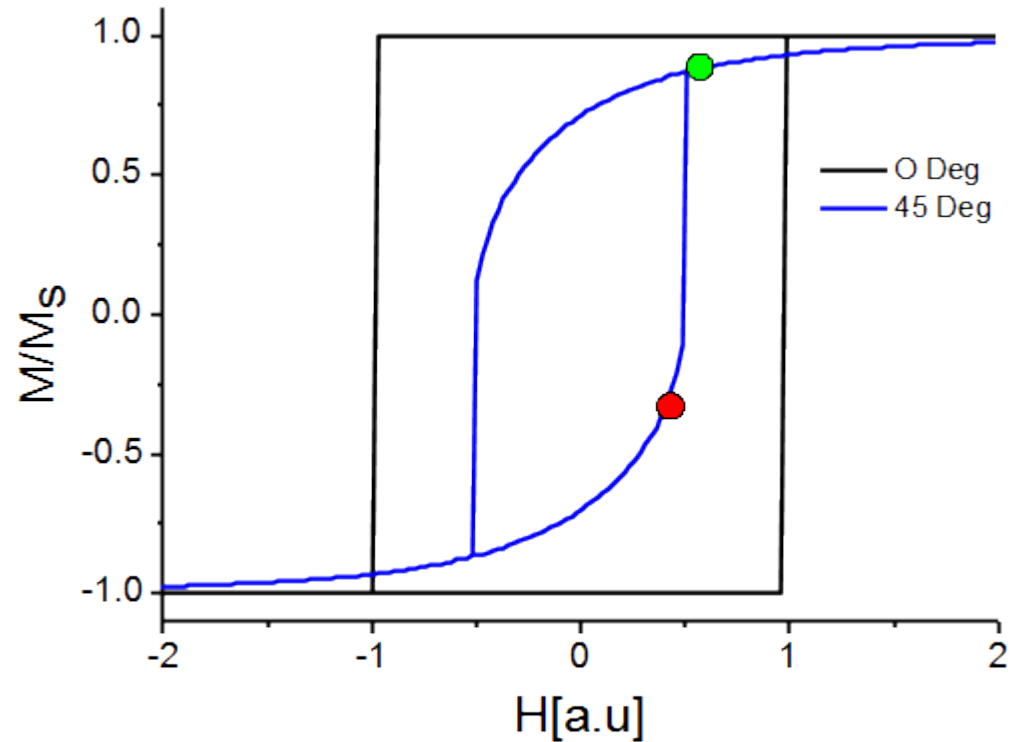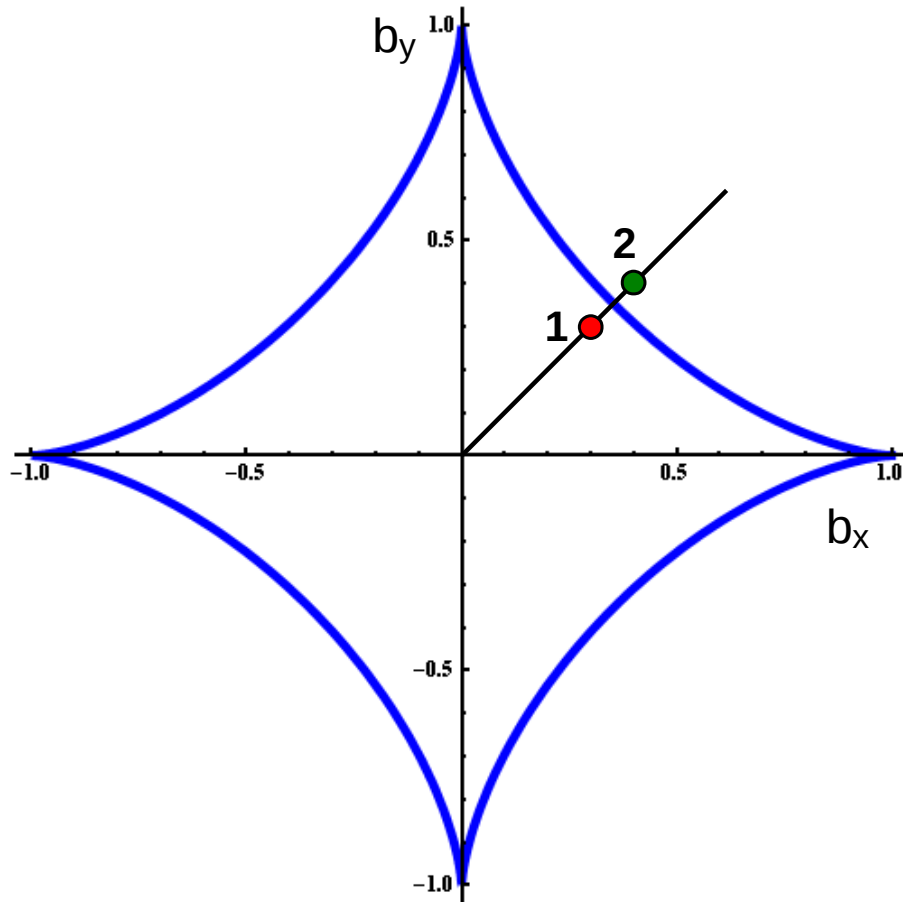
Stoner-Wohlfarth model – astroid curve

- Stoner-Wohlfarth astroid separates region, in $\mu_0(h_x, h_y)$ plane, with two minima of energy from that with only one minimum


**Temperature dependence of the switching fields of a 3 nm Co cluster**

$T_B \approx 14$ K

$\Delta t \approx 1$ s

0.04 K, 1 K, 2 K, 4 K, 8 K, 12 K

$S \approx 1000$

PRL 86, 4676 (2001)
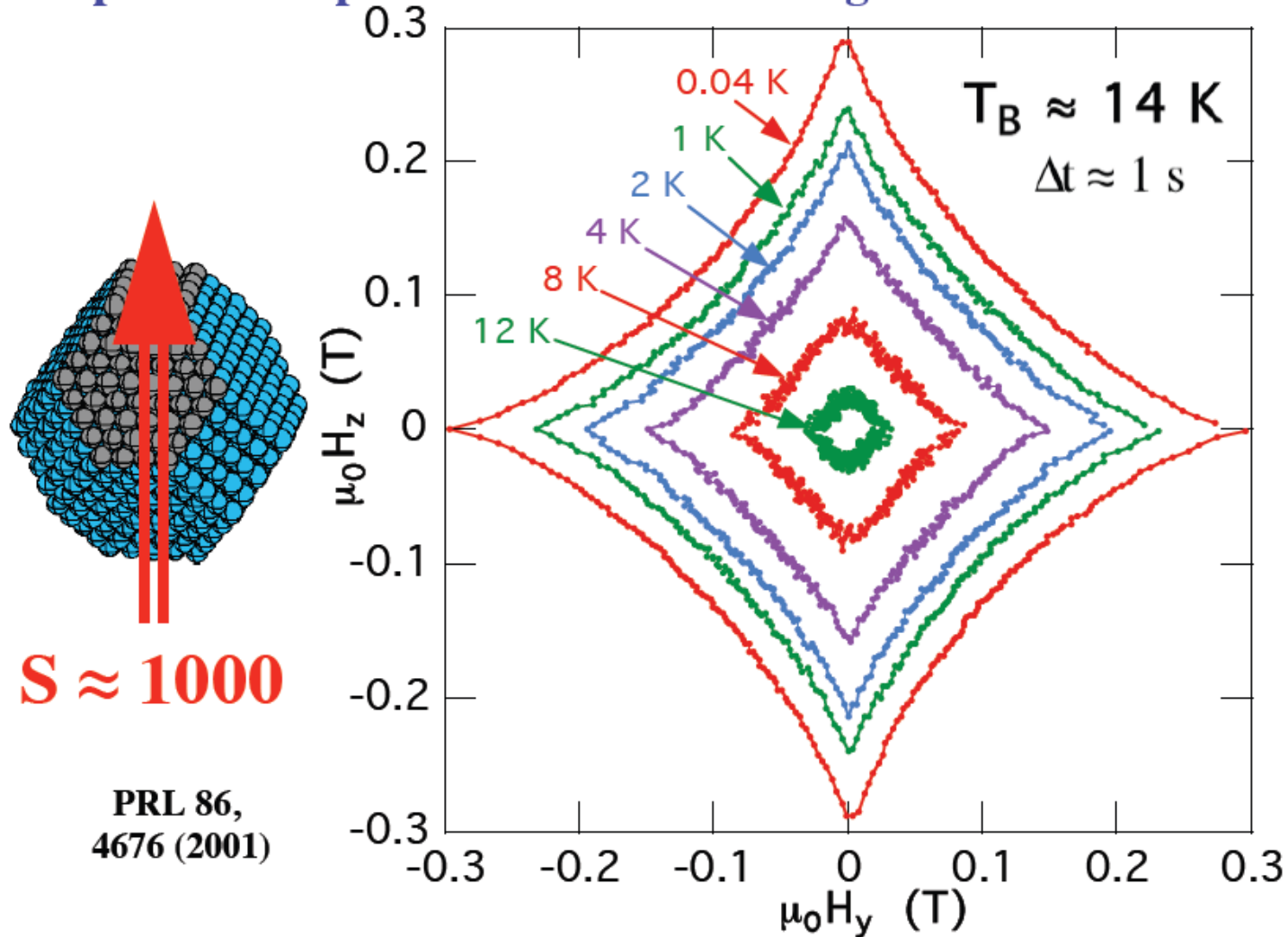
a strong **decrease of anisotropy** with increasing temperature!

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Shape anisotropy – "magnetizing" thin film

- Consider a thin magnetic film in which all magnetic moments point perpendicularly to its plane
- If the film is thin we can assume that that its thickness is negligible relative to its lateral size (no fringing field)
- The magnetic moments create "magnetic charges" on the surface of the film
- ...and the charges produce **H** field
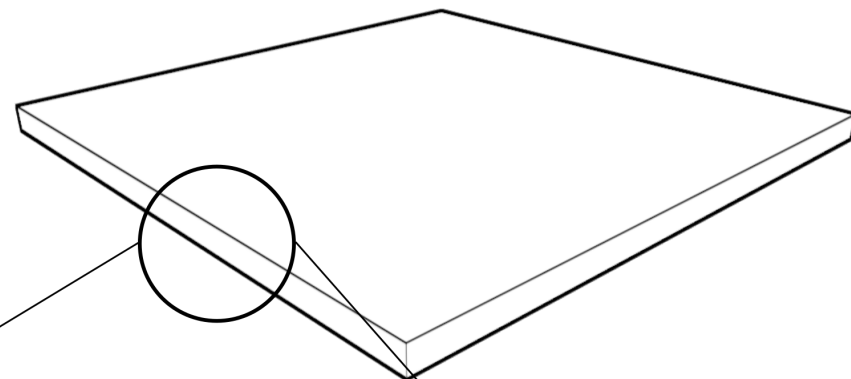
$$\nabla \cdot \vec{H} = \rho_{magn}$$
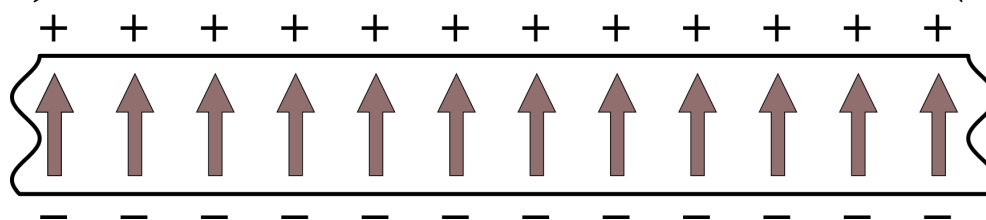
- For an infinite sheet of magnetic charge the field H is perpendicular to the sheet and can be calculated using Gauss law*:

$$\phi_m(\vec{r}) = \frac{1}{4\pi} \oint_S \frac{\vec{M} \cdot \vec{ds}}{|\vec{r}|} - \frac{1}{4\pi} \int_V \frac{\nabla' \cdot \vec{M}}{|\vec{r}|} d^3 r'$$

$$\vec{H} = -\nabla \varphi$$

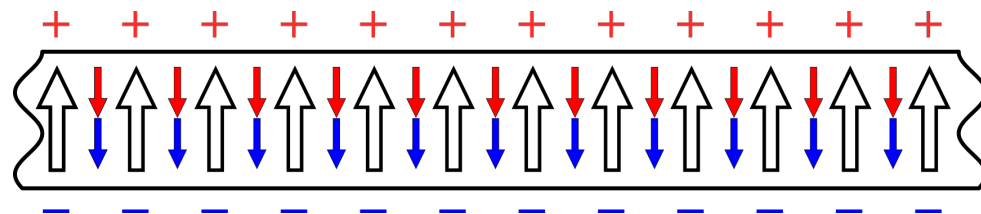$$\vec{H} \, 2\pi r^2 = \vec{M}_s \, \pi r^2$$

$$|H| = \frac{1}{2}|M_s|$$

*use Gaussian surface in form of a cylinder bisected by a sheet

Shape anisotropy – "magnetizing" thin film

- The field produced by both sides of the film (two charge sheets) is then*:

$$\vec{B} = \mu_0 \left(\vec{M}_s - 2 \cdot \frac{1}{2}\, \vec{M}_s \right) = 0$$

- If, on the other hand, the magnetization is parallel to film surface the charges are created at infinity and they produce no **H** field in the film. The induction produced by magnetization is

$$\vec{B} = \mu_0 \left(\vec{M}_s - 0 \right) = \mu_0 \vec{M}_s$$

- The energy, per unit volume, of the magnetic material in the external field is given by:

$$E = -\vec{M} \cdot \vec{B}$$

- If the field is produced by the magnetization itself the increment of energy associated with a small increase in magnetization M is given by

$$dE = -dM \cdot B$$

we drop vector signs because the vectors **M** and **B** are parallel

… and the magnetostatic energy associated with magnetization is:

$$E = - \int_0^{M_{\text{in-plane}}} \mu_0\, M\, dM = -\frac{1}{2} \mu_0\, M_{\text{in-plane}}^2$$

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*you can arrive at the same result arguing that the field is produced by a equivalent current loop of infinite radius
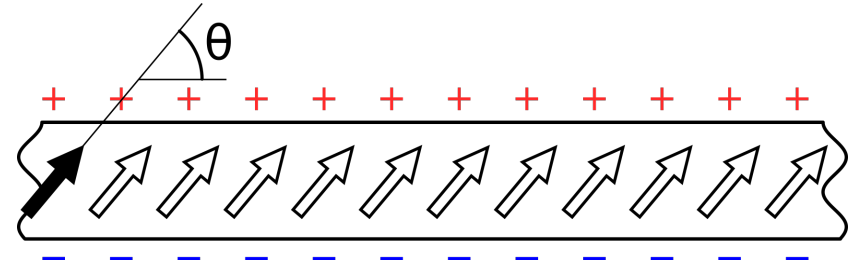
Shape anisotropy – "magnetizing" thin film

- If we now apply the external magnetic field perpendicularly (along *z* axis) to the plane of the film which has no intrinsic anisotropy (magnetocrystalline etc.) the expression for its magnetostatic energy is:

$$E = -B_z M_z - \frac{1}{2}\mu_0 M_{\text{in-plane}}^2$$

or:

shape anisotropy

$$E = -B_z M_s \sin(\theta) - \boxed{\frac{1}{2}\mu_0 M_s^2} \cos^2(\theta)$$

- The equilibrium orientation of magnetization is given by:

$$\frac{\partial}{\partial \theta} E = -B_z M_s \cos(\theta) + \frac{1}{2}\mu_0 M_s^2 \, 2\cos(\theta)\sin(\theta) = 0$$

$$\sin(\theta) = \frac{B_z}{\mu_0 M_s} \qquad M_z = \frac{B_z}{\mu_0}$$

Shape anisotropy in thin film:

- up to saturation the magnetization component along the external field direction is proportional to it

- saturation field is then equal to magnetic polarization ($\mu_0 M_s$)

- Polycrystalline spherical samples without a preferred orientation of the grains do not show, in macroscopic experiments, any magneto crystalline anisotropy [9].
- If the sample is not spherical the magnetostatic energy of the system depends on the orientation of magnetic moments within the sample (or macrospin in a simplified picture).
- The effect is of purely magnetostatic origin and is closely related to demagnetizing fields (see my **lecture 2** from 2019):

If and only if the surface of uniformly magnetized body is of second order the magnetic induction inside is uniform and can be written as:

$$\vec{B} = \mu_0 (-N \cdot \vec{M} + \vec{M})$$

N is called the demagnetizing tensor [5]. If magnetization is parallel to one of principle axes of the ellipsoid *N* contracts to **three numbers** called demagnetizing (or demagnetization) factors sum of which is one:

$$N_x + N_y + N_z = 1$$

For a general ellipsoid magnetization and induction are not necessarily parallel.

Demagnetization decreases the field inside ferromagnetic body.

- **Demagnetizing field is just the name of the field produced by the body itself**
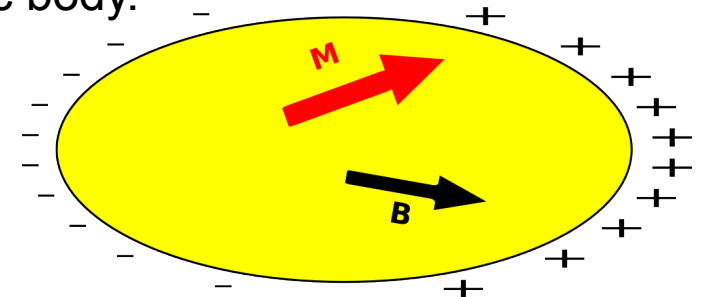
Shape anisotropy

- Polycrystalline spherical samples without a preferred orientation of the grains do not show, in macroscopic experiments, any magneto crystalline anisotropy [9].
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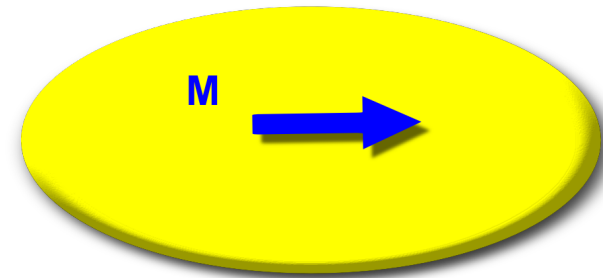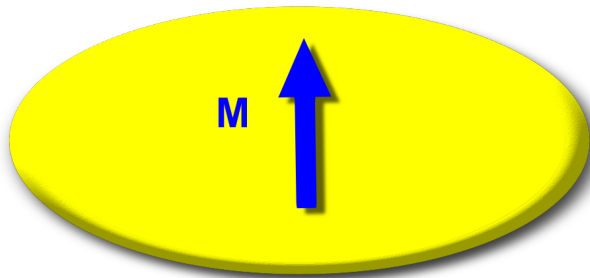
- The energy of the sample in its own stray field is given by the integral [9]:

$$E_{demag} = -\frac{1}{2} \int \vec{B}_{demag} \cdot \vec{M} \, dV = \frac{1}{2} \int \mu_0 (N \cdot \vec{M}) \cdot \vec{M} \, dV \qquad \vec{B}_{demag} = -\mu_0 N \cdot \vec{M}$$

- If the sample is an ellipsoid the demagnetizing field is uniform throughout the sample:

$$E_{demag} = \frac{1}{2} V \mu_0 (N \cdot \vec{M}) \cdot \vec{M}, \qquad V - volume \quad of \quad the \quad sample$$

- *N* is a diagonal tensor if the semiaxes of the ellipsoid coincide with the axes of the coordination system.

Shape anisotropy

- For the general ellipsoid sample we have [9]:

$$E_{demag} = \frac{1}{2} V \mu_0 (N \cdot \vec{M}) \cdot \vec{M} = \frac{1}{2} \mu_0 M^2 (N_a \alpha_1^2 + N_b \alpha_2^2 + N_c \alpha_3^2)$$

$$\vec{M} = M(\alpha_1, \alpha_2, \alpha_3)$$

- For a spherical sample we have:

$$N = \begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{bmatrix} \Rightarrow E_{demag} = \frac{1}{2} \mu_0 M^2 \frac{1}{3} (\alpha_1^2 + \alpha_2^2 + \alpha_3^2) = \frac{1}{6} \mu_0 M^2$$

no dependence on the magnetic moment orientation

- For an infinitely long cylinder* N_c is null:

$$(\alpha_1, \alpha_2, \alpha_3) = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$$

$$N = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \Rightarrow E_{demag} = \frac{1}{2} \mu_0 M^2 \frac{1}{2} (\alpha_1^2 + \alpha_2^2) = \frac{1}{2} \mu_0 M^2 \frac{1}{2} (\sin^2(\theta)\cos^2(\phi) + \sin^2(\theta)\sin^2(\phi)^2) =$$

$$E_{demag} = \frac{1}{4} \mu_0 M^2 \sin^2(\theta)$$

Uniaxial anisotropy- characteristic for elongated particles (see Stoner-Wohlfarth model)

$$N_{ellipsoid} = \begin{bmatrix} N_a & 0 & 0 \\ 0 & N_b & 0 \\ 0 & 0 & N_c \end{bmatrix}$$

*polar axis is a symmetry axis

Shape anisotropy

- For infinitely expanded and/or very thin ellipsoid we have [9] (θ=90° – moments in-plane):

$$N=\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \Rightarrow E_{demag}=\frac{1}{2}\mu_0 M^2 \alpha_3^2=\frac{1}{2}\mu_0 M^2 \cos^2(\theta)$$

> The in-plane orientation of magnetic moment of thin plate is energetically favorable*

- The equation can be rewritten to often used form:

$$E_{demag}=\frac{1}{2}\mu_0 M^2(1-\sin^2(\theta))=\frac{1}{2}\mu_0 M^2-\frac{1}{2}\mu_0 M^2 \sin^2(\theta)=K_0+K_{shape}^V \sin^2(\theta),$$

$$with \quad K_{shape}^V=-\frac{1}{2}\mu_0 M^2$$

- Magnetocrystalline and thin films shape anisotropy constants for thin films of elements at 4 K**:

	Fe (bcc)	Co (hcp)	Ni (fcc)
K_1 [J/m³]	54 800	760 000	-126 300
K^V [J/m³]	1 910 000	1 290 000	171 000

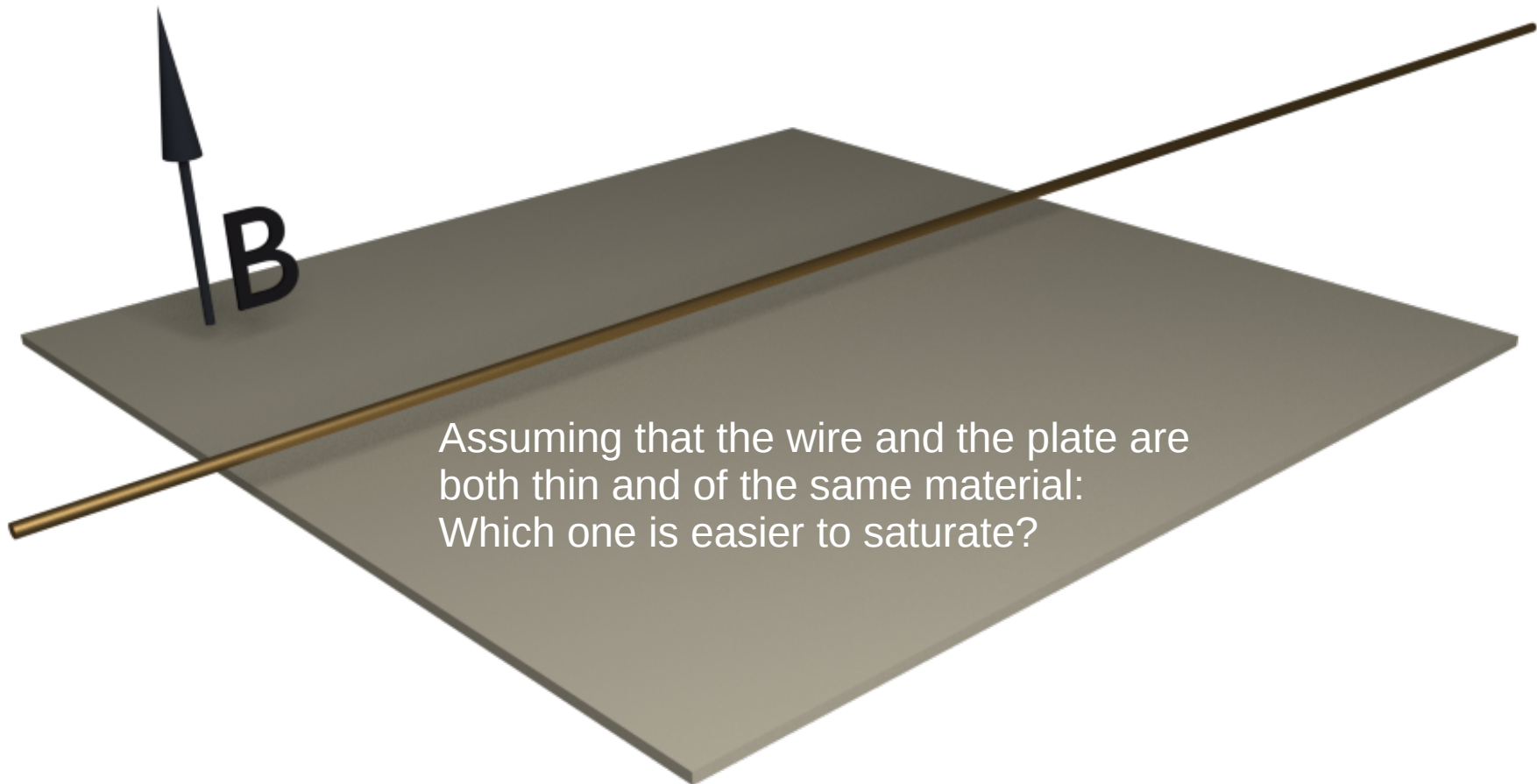> Shape anisotropy in thin films usually dominates over magnetocrystalline anisotropy

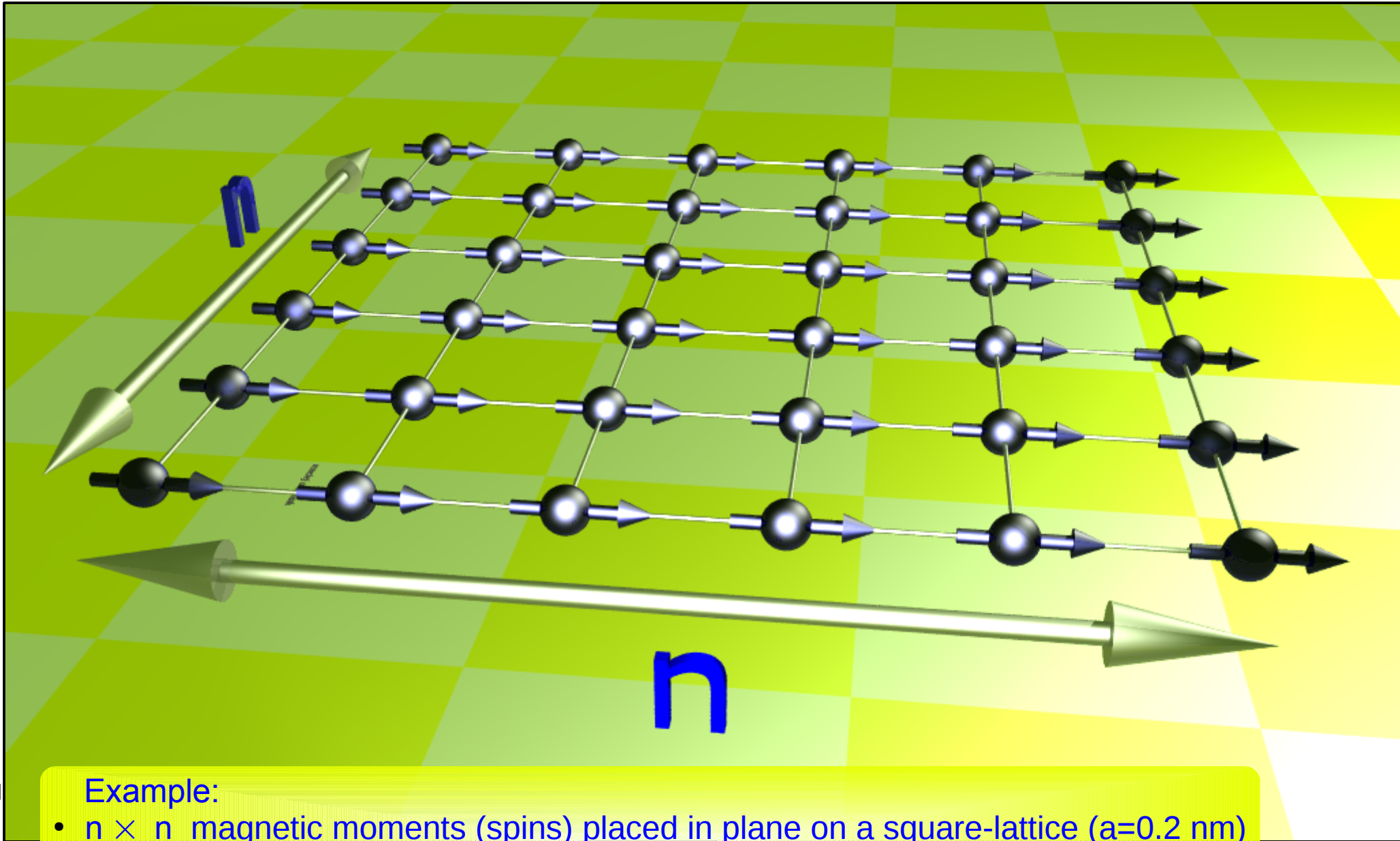*in case magnetocrystalline and other anisotropies favoring perpendicular orientation are absent

**magnetization data from: Francois Cardelli Materials Handbook, Springer 2008 (p.502), http://books.google.pl

Shape anisotropy

- From Stoner-Wohlfarth model we have: $B_S = \dfrac{2K_1}{M}$

- Substituting the expression for shape anisotropy of thin films $K^V_{shape} = -\dfrac{1}{2}\mu_0 M^2$ we get:

$$B_S = \mu_0 M_S \qquad \text{or} \qquad H_S = M_S$$

> In macrospin approximation the perpendicular saturation field of thin film is equal to its magnetization.

B

Assuming that the wire and the plate are both thin and of the same material:
Which one is easier to saturate?
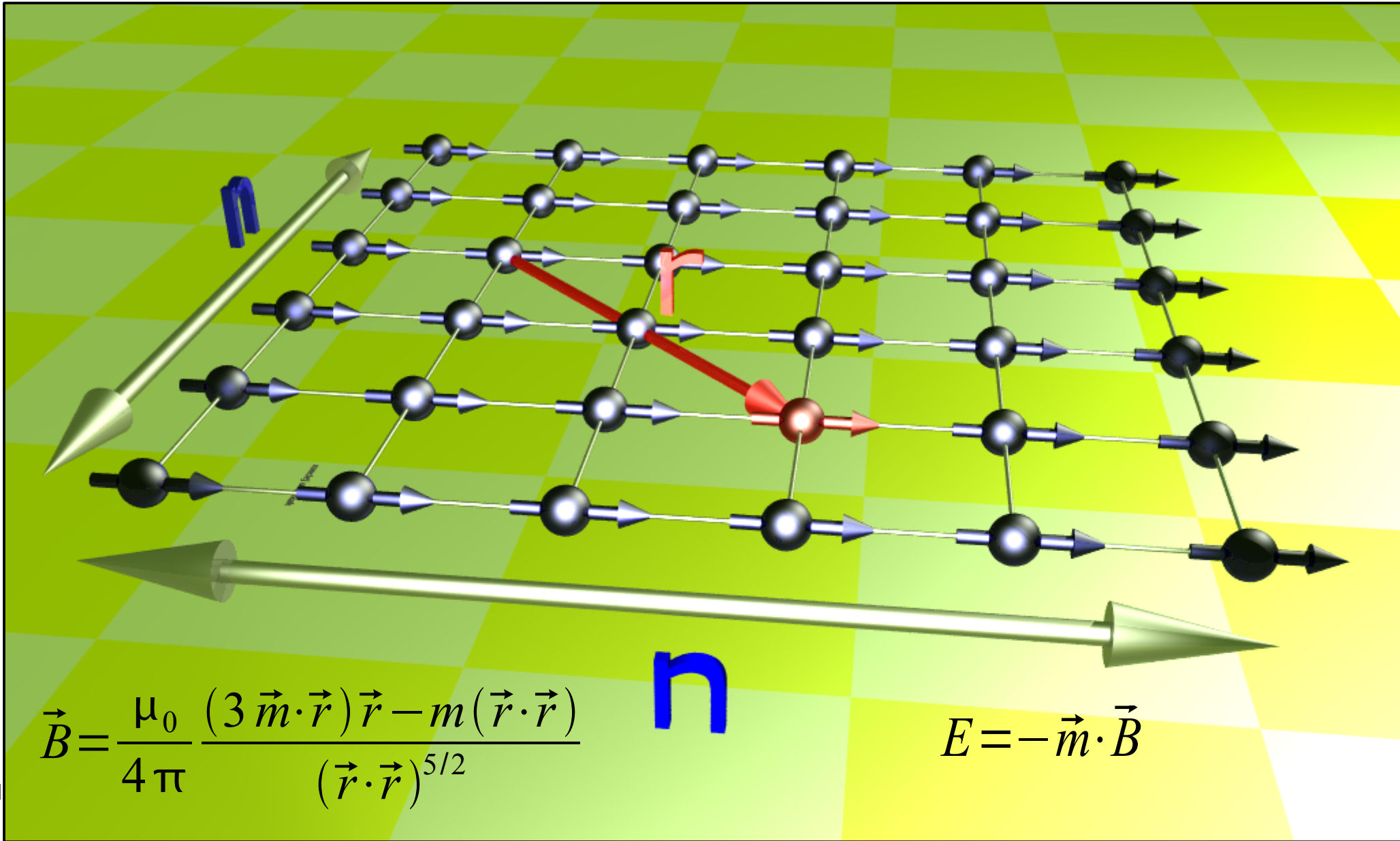
Shape anisotropy – purely magnetostatic interactions

Example:
- $n \times n$ magnetic moments (spins) placed in plane on a square-lattice (a=0.2 nm)
- magnetic moments interact purely magnetostatically
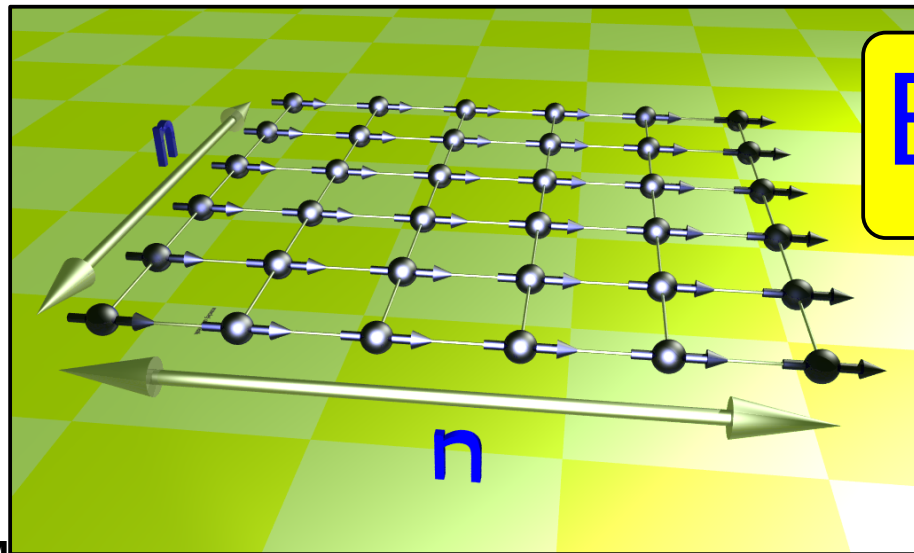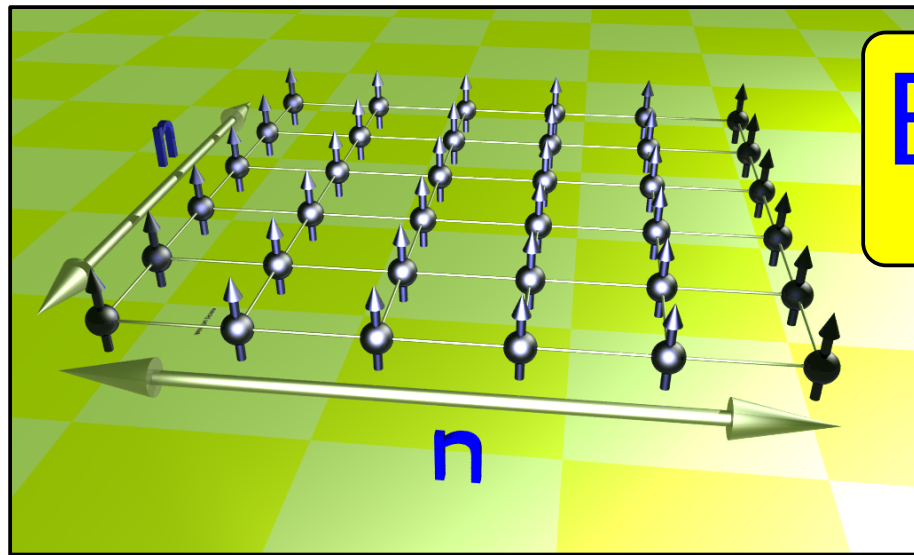- each moment is a 1 Bohr magneton ($\approx 1\times 10^{-24}$ Am^2)

$$\vec{B} = \frac{\mu_0}{4\pi} \frac{(3\,\vec{m}\cdot\vec{r})\,\vec{r} - m\,(\vec{r}\cdot\vec{r})}{(\vec{r}\cdot\vec{r})^{5/2}}$$

$$E = -\vec{m}\cdot\vec{B}$$
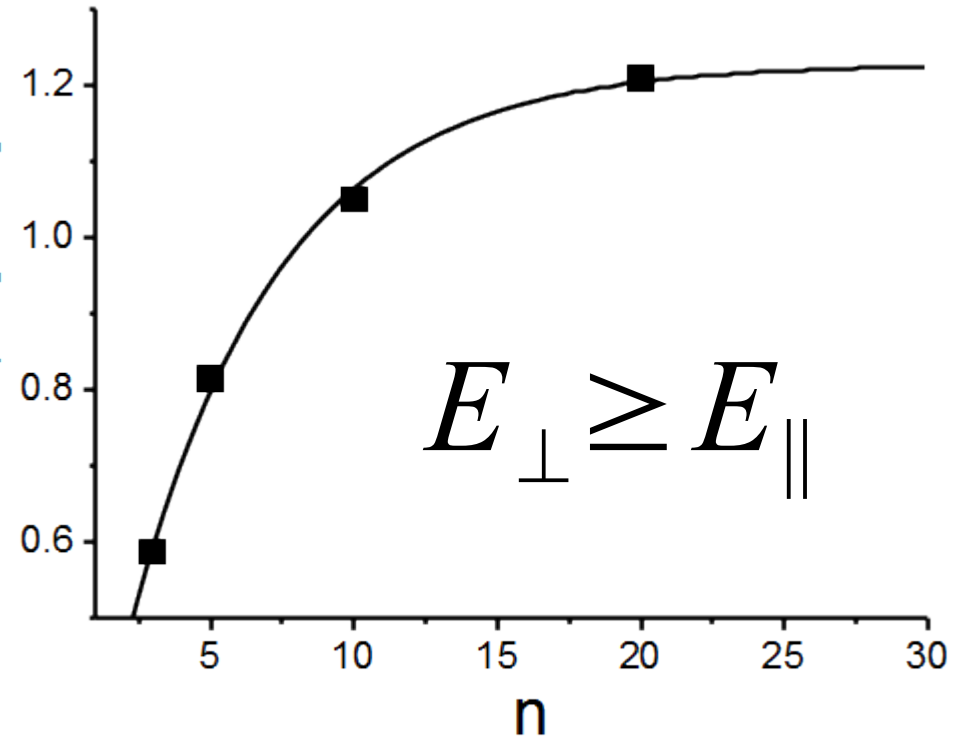
Shape anisotropy – purely magnetostatic interactions

$$E_\perp$$

$$E_{\parallel}$$

$$E_\perp \geq E_{\parallel}$$

$E_\perp$ is less negative than $E_{\parallel}$*

Magnetostatic interactions favor in-plane orientation of magnetic moments (spins) in thin magnetic films

* $E = -\vec{m} \cdot \vec{B}$

Surface anisotropy – reorientation phase transition

presence of an interface:
- **orbital motion of electrons is affected by the introduced symmetry breaking**
- **the asymmetry of the averaged orbital moments defines the interface contribution to the magnetic anisotropy**
- **in ultrathin magnetic films the interface part becomes even dominating in some cases**

outer layer of atoms
(or interface)

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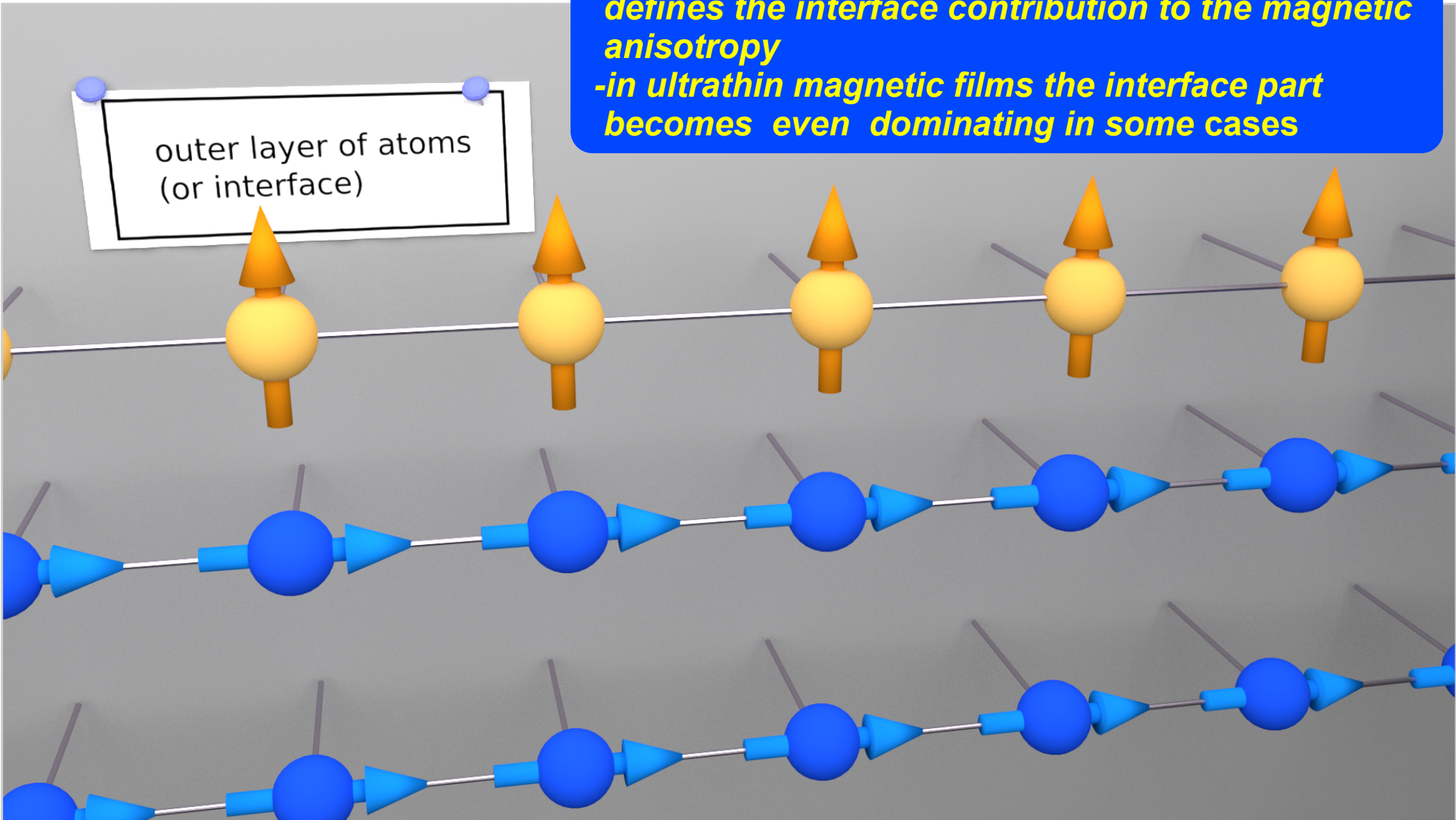
Surface anisotropy – reorientation phase transition

- Due to broken symmetry at interfaces the anisotropy energy contains terms with lower order in direction cosines than in the infinite crystal.

surface/interface
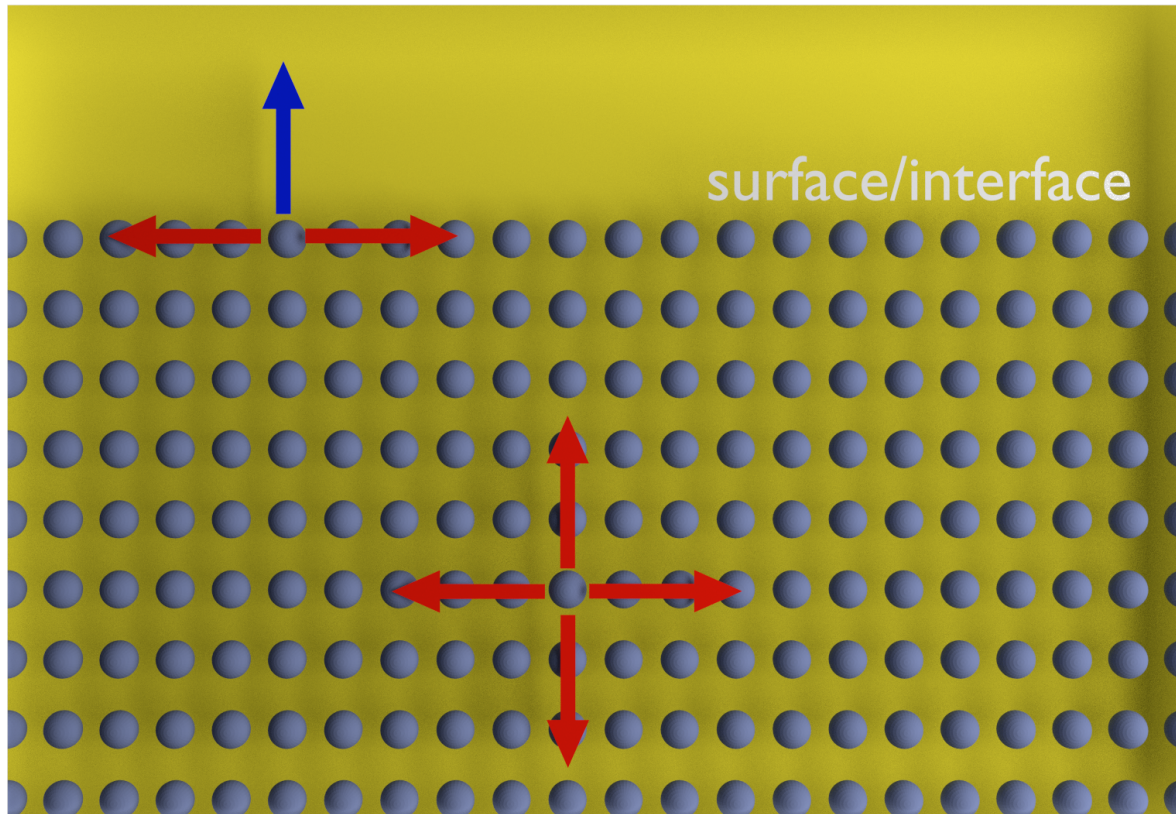
- Energy of magnetic moments of atoms occupying lattice sites in the vicinity of the surface is different for two shown orientations
- Each of the magnetocrystalline anisotropy constants can be phenomenologically divided into two parts, one related to volume contribution and the one to surface contribution [9]:

$$K^{eff} = K^v + K^s/t$$

where t is the crystal thickness.

- Energy of magnetic moments of atoms occupying lattice sites far from the outer boundary of the crystal depends on the intrinsic symmetry of the crystal
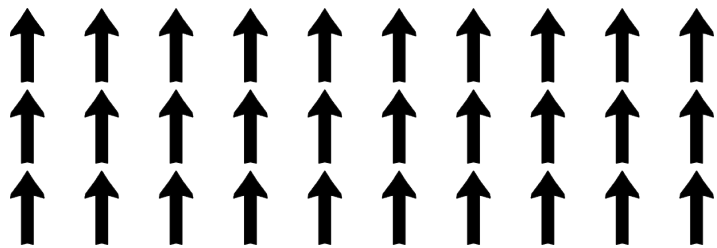
Surface anisotropy – reorientation phase transition

- Let us assume that volume contribution to the anisotropy favors in-plane alignment of magnetic moments (it could be magnetocrystalline, shape, stress etc. anisotropy).
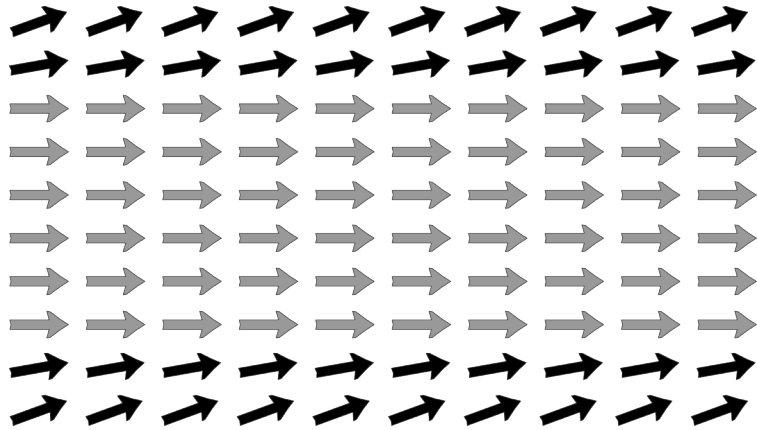
- Due to perpendicular surface anisotropy the moments close to the surface (black arrows) are deflected out of plane

- If the thickness of the sample/film is high the exchange coupling of the surface moments with the bulk ones keeps the overall moment of the sample nearly in plane

---

- If the thickness of the film is low, and the surface anisotropy is strong enough all moments point perpendicular to plane.
- Using macrospin approximation the total energy of the sample dependent on the orientation of magnetic moment can be written as [10] (we assume that the energy does not depend on azimuthal angle):

$$E_a = K_0 - K_2 \cos^2(\theta) - K_4 \cos^4(\theta) + ... \qquad *$$

-positive K_i favor perpendicular orientation

M
.
U
R
B
A
N
I
A
K 2019   *different notations of anisotropy constants can be encountered: R. Skomski et. al, Phys. Rev. B 58, 11138 (1998)

Surface anisotropy – reorientation phase transition

- Minimizing E_a with respect to θ yields the equilibrium angle:

$$\partial^2 E_a / \partial \theta^2 = 2 K_2 \cos(\theta) \sin(\theta) + 4 K_4 \cos^3(\theta) \sin(\theta) = 0 \quad \Rightarrow \quad \cos(\theta) \sin(\theta)(2 K_2 + 4 K_4 \cos^2(\theta)) = 0$$

- We have extrema for:

$$\theta = 0, \ \pi/2, \quad \cos^2(\theta) = \frac{-K_2}{2 K_4}$$

- It can be shown that [10]:

-for $K_2 > 0$ and $K_4 > 0$ the magnetization is perpendicular to the plane

-for $K_2 > 0$ and $2K_4 < -K_2$ the canted magnetization is a ground state

-the region for $K_2 < 0$ and $2K_4 > -K_2$ is called a *coexistence region* – both perpendicular and in-plane orientations of magnetization correspond to local minimum; they are separated by energy barrier
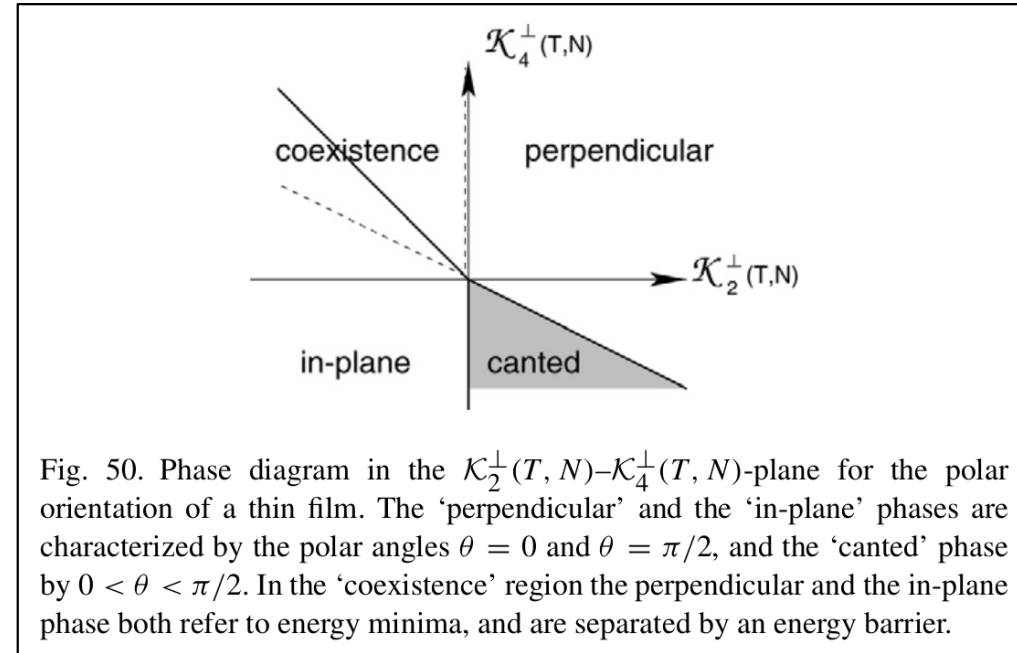

Fig. 50. Phase diagram in the $\mathcal{K}_2^\perp(T, N)$–$\mathcal{K}_4^\perp(T, N)$-plane for the polar orientation of a thin film. The 'perpendicular' and the 'in-plane' phases are characterized by the polar angles $\theta = 0$ and $\theta = \pi/2$, and the 'canted' phase by $0 < \theta < \pi/2$. In the 'coexistence' region the perpendicular and the in-plane phase both refer to energy minima, and are separated by an energy barrier.

image source: P.J. Jensen, K.H. Bennemann, Surface Science Reports **61**, 129 (2006)

Surface anisotropy – reorientation phase transition

- Recalling the presence of surface anisotropy terms we get:

each anisotropy constant is divided into bulk (volume) and surface term

$$E_a = K_0 - (K_2^v + K_2^s/t)\cos^2(\theta) - (K_4^v + K_4^s/t)\cos^4(\theta) + \ldots$$

- Neglecting higher order terms we get the sample thickness for which the effective anisotropy is zero (neglecting constant K_0):

$$t_{RPT} = -\frac{K_2^s}{K_2^v}$$

- Usually, when considering thin films, the sample has two surfaces contributing surface anisotropy. As a consequence the multiplier 2 is added*:

RPT – reorientation phase transition
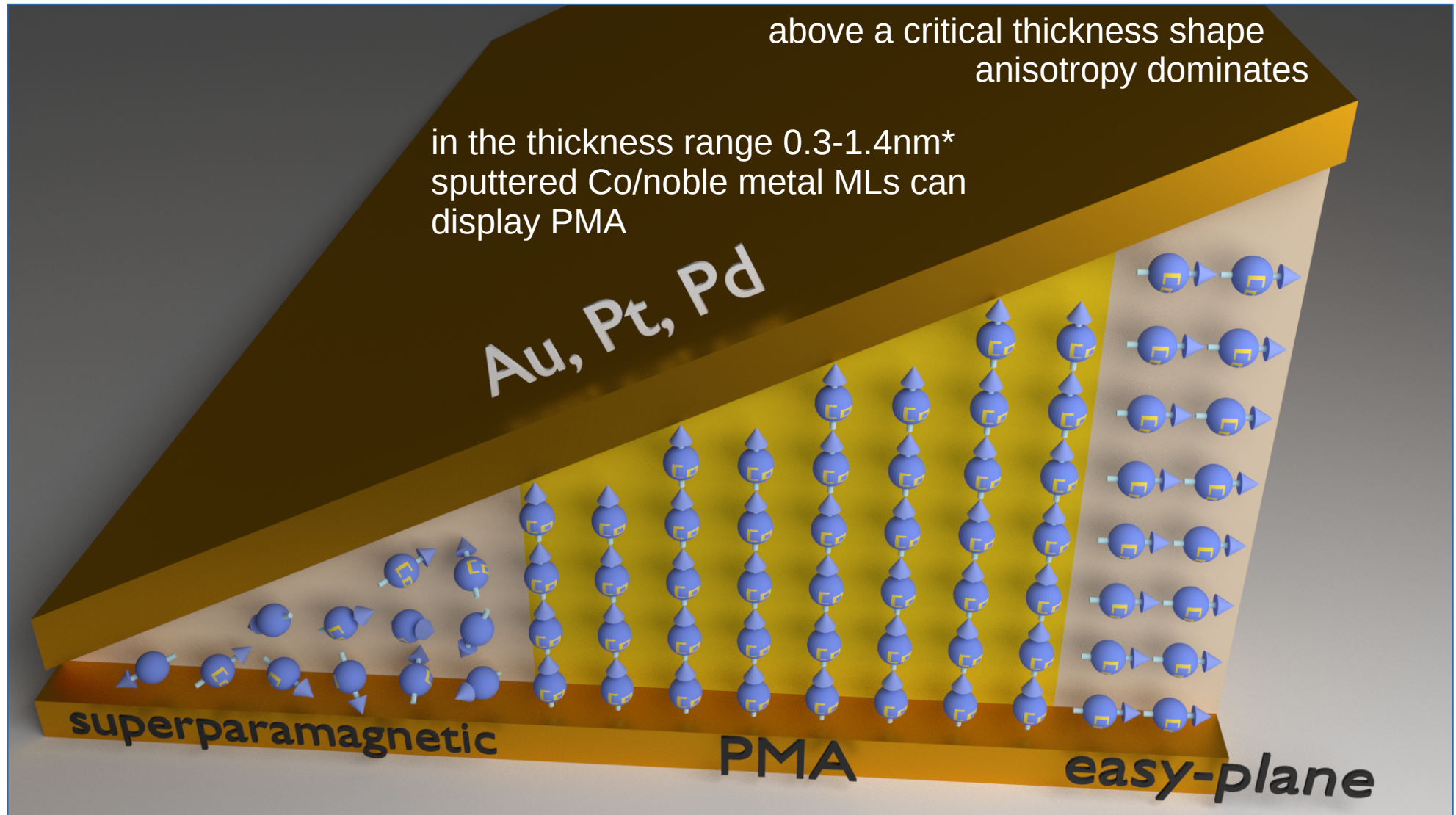SRT -spin reorientation transition

$$t_{RPT} = -\frac{2K_2^s}{K_2^v}$$

- For film thickness > t_{RPT} the magnetization of the film lies in-plane (if the external field is absent).
- RPT may be caused by:
-temperature change
-change of the thickness of magnetic layer
-change of the thickness of the overlayer

*in general both surfaces can be characterized by different surface anisotropy constants.

Perpendicular magnetic anisotropy in Co based multilayers

Co based multilayers in which magnetic layer is sandwiched between noble metal spacer possess perpendicular magnetic anisotropy (PMA) in limited thickness range – this is due to **surface anisotropy** of the interfaces

above a critical thickness shape anisotropy dominates

in the thickness range 0.3-1.4nm* sputtered Co/noble metal MLs can display PMA

Au, Pt, Pd

superparamagnetic

PMA

easy-plane

2019 *for Co/Au MLs the PMA range is approximately 0.5-1.2nm

- From the expression with surface anisotropy we have:

$$K_{eff} = K_2^v + 2 K_2^s / t$$

$$K_{eff} t = K_2^v t + 2 K_2^s$$

- Plotting $K_{eff} t \; vs \; t$ one can determine volume and surface contributions to anisotropy with a linear fit:

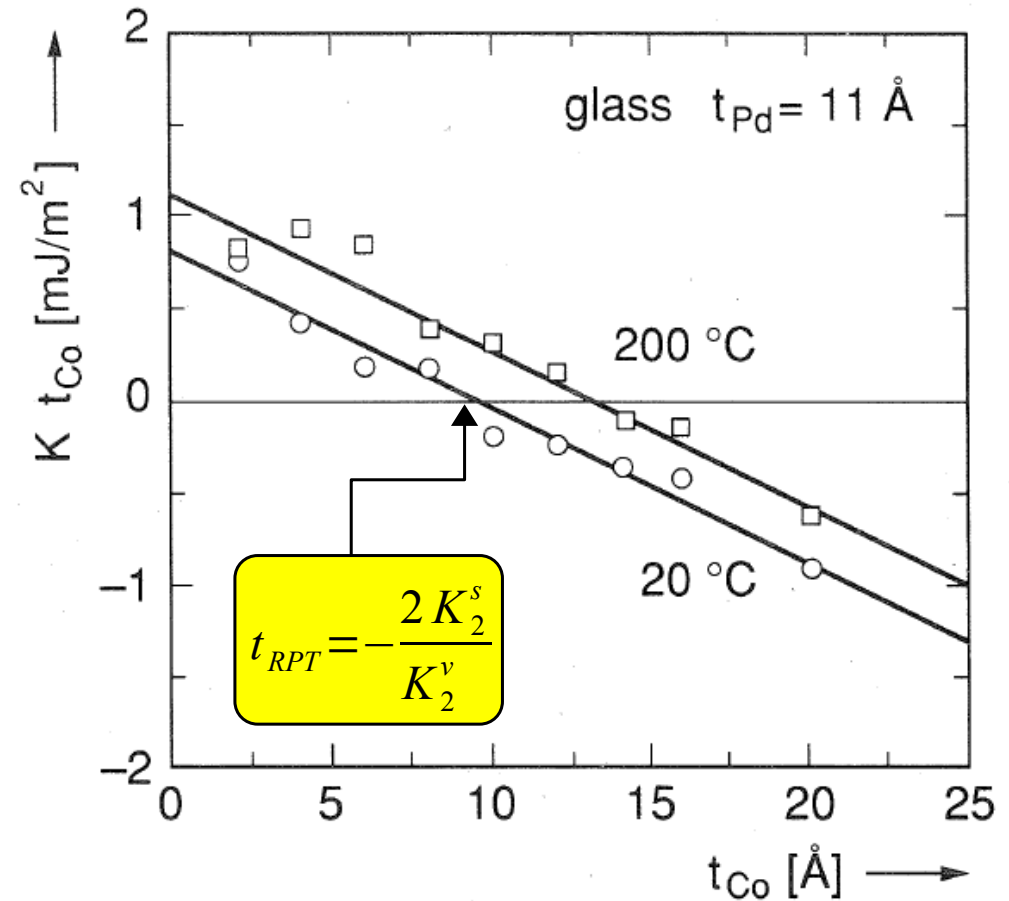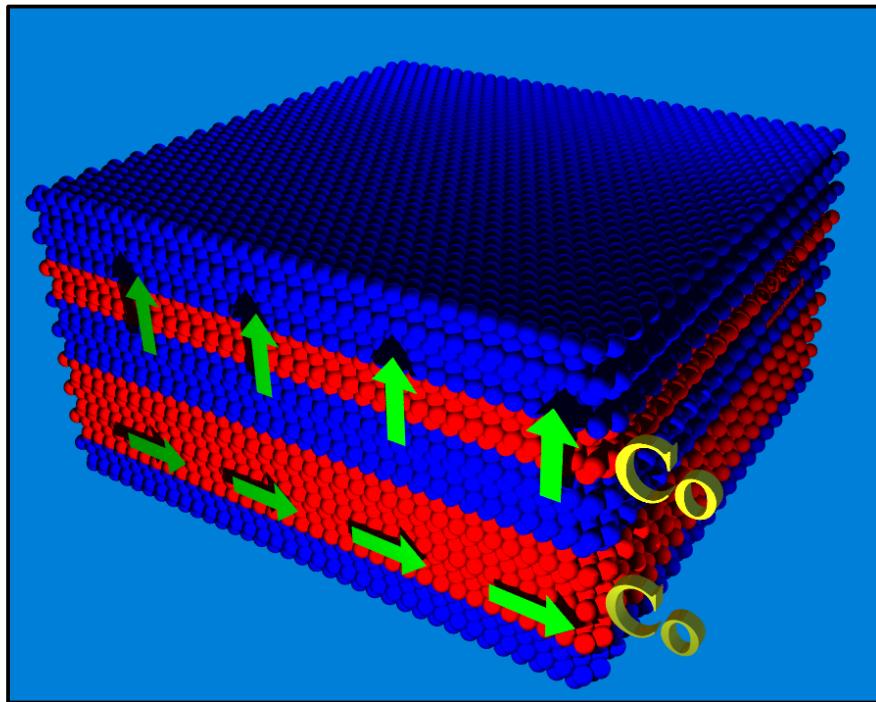- K_V - slope
- $K_S - \frac{1}{2} K_{eff}$ t for t=0

$$t_{RPT} = - \frac{2 K_2^s}{K_2^v}$$

Fig. 2. Dependence of $K t_{Co}$ on t_{Co} for polycrystalline Co/Pd multilayers, deposited at $T_s = 20$ and 200°C.

MAGNE

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- RPT may be caused by:
  -temperature change
  -change of the thickness of magnetic layer
  -change of the thickness of the overlayer

FIG. 1. Cobalt wedge remnant state image $P(i,j)$ determined for a fully saturated sample in both $H_\perp > 0$ and $H_\perp < 0$ directions. On the basis of magnetometric analysis, localization of different magnetization states is marked. Points show the coercivity wall positions registered for different $H_\perp$ field pulse ($\Delta = 900$ ms) magnitudes (measured in Oe). Solid black lines have been fitted to the coercivity wall data, registered at $H_\perp = 135$ Oe, using $H_C(x,y)$ function with $h_C^* = 0.8$ nm as the best fitting parameter. Below the horizontal dashed line in the gold region growth imperfections are clearly visible.

Kisielewski et al., J. Appl. Phys. 93, 7628 (2003)

MAGNETIC MATERIALS AND HYSTERESIS

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Perpendicular magnetic anisotropy in Co based multilayers

- RPT may be caused by:
-temperature change
-change of the thickness of magnetic layer
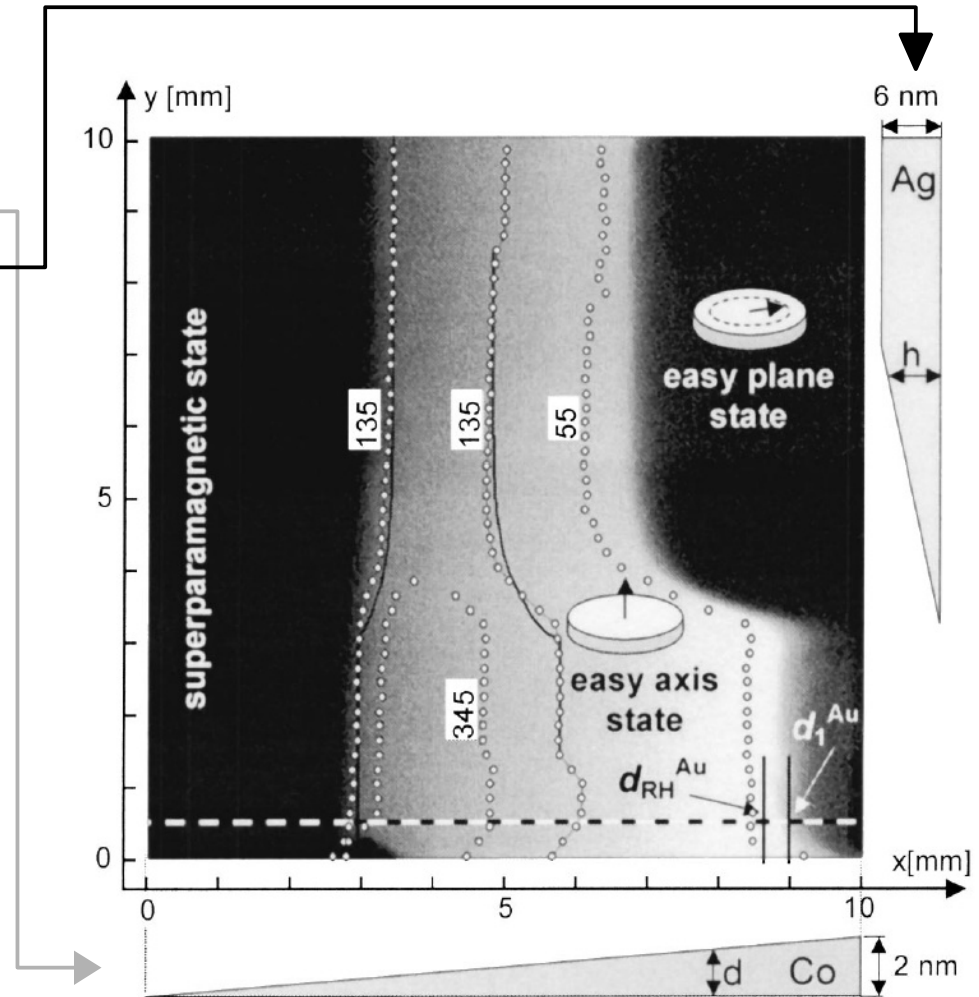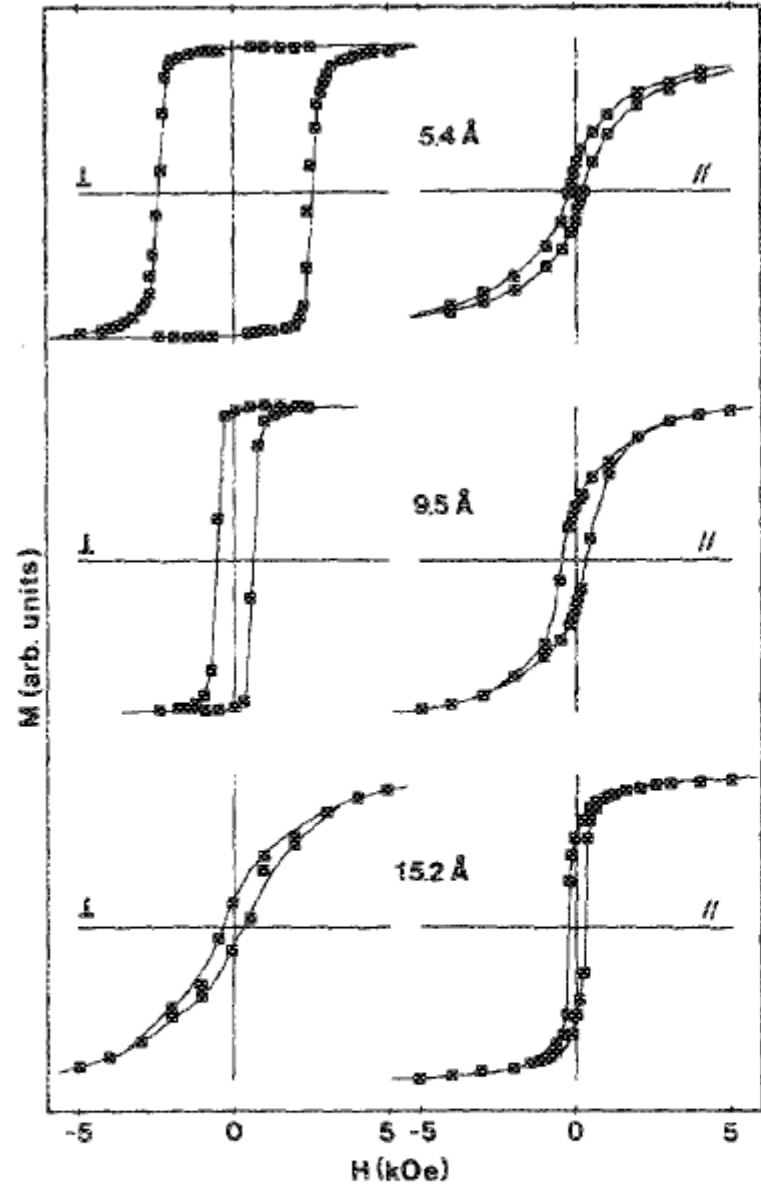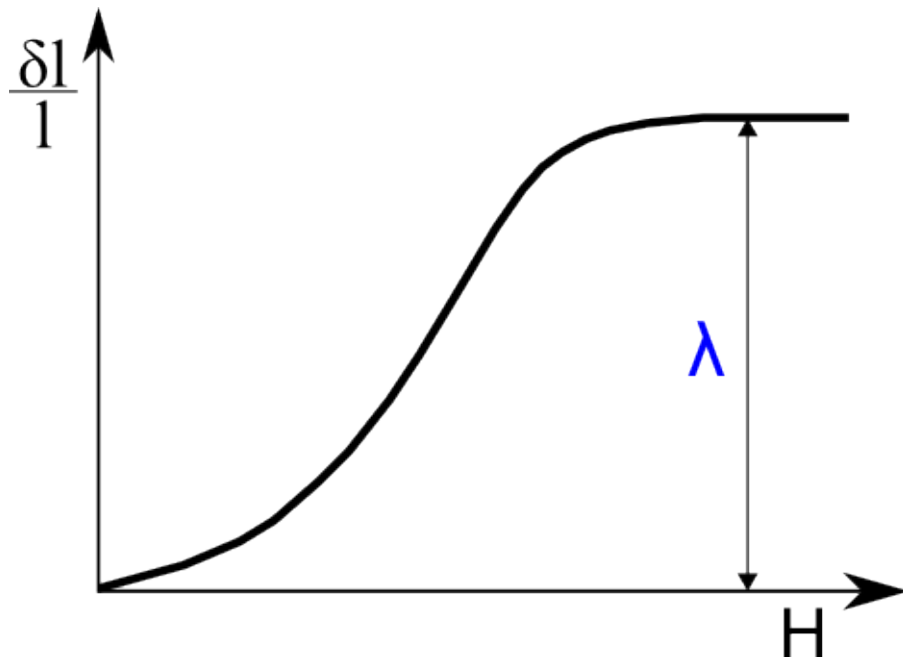-change of the thickness of the overlayer

FIG. 4. Hysteresis loop with H perpendicular ($\perp$) and parallel ($\parallel$) to the film plane, for Au/Co/Au sandwiches with $t = 5.4$, 9.5, and 15.4 Å, a $T = 10$ K.

Stress anisotropy and magnetostriction

- Magnetostriction is a change of materials physical dimensions as a result of the change of the orientation of magnetization
- The direction of magnetization changes under the influence of external field or temperature.

The relative deformation is usually small; of the order of 10^{-6} to 10^{-5} [6]; in Tb λ is approx. 0.002 at RT.

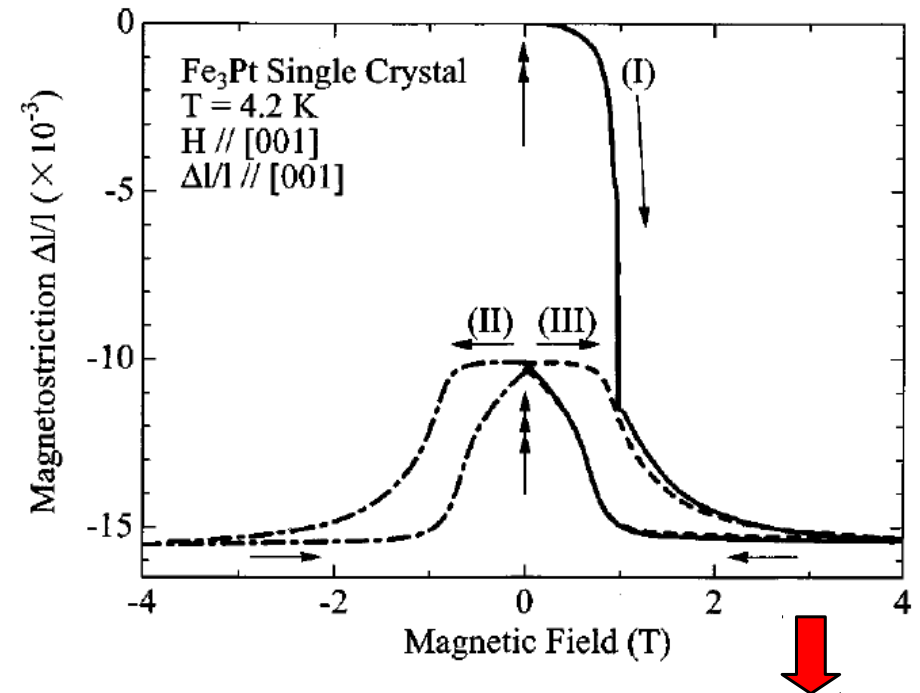- The typical strain versus field dependence shows saturation which is expressed by the value of magnetostriction constants λ:

FIG. 4. Magnetostriction of an ordered Fe₃Pt. Strain of 1.5×10^{-2} is obtained by application of a magnetic field of 4 T, which is indicated by (I). The total strain comes to about 2.0×10^{-2} including the strain due to the thermally induced martensitic transformation shown in Fig. 3. The reversible strain is 5×10^{-3} by applying and removing the magnetic field, which is indicated by (II) and (III).
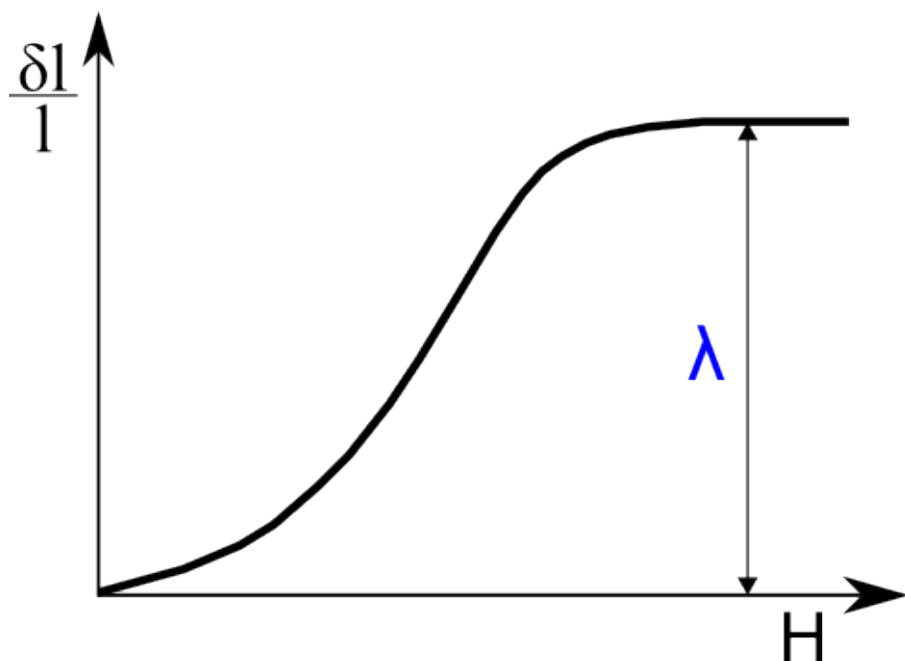
- In giant magnetostriction materials the strain exceeds 0.5%

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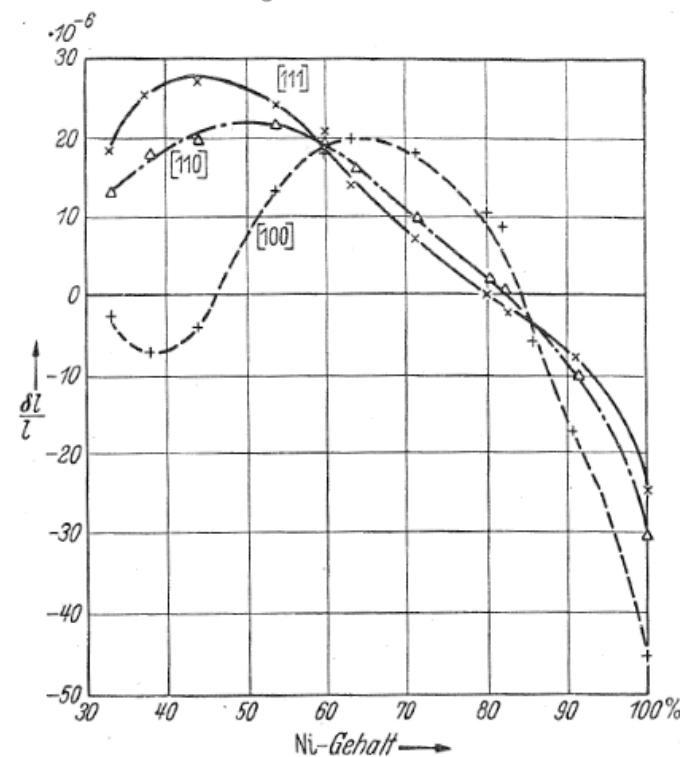

Abb. 186. Sättigungsmagnetostriktion von Einkristallen der Nickel-Eisen-Legierungen zwischen 30% und 100% Nickel für die drei kristallographischen Hauptrichtungen. [Nach F. LICHTENBERGER: Ann. Phys., Lpz. V, Bd. 10 (1932) S. 45.]

- The dependence dl/l(H) is different for different orientations of applied field relative to crystal axes

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Stress anisotropy and magnetostriction

- In most practical applications the saturation distortion can be described by expression with small number of constants [11]:

$$\lambda = \frac{3}{2}\lambda_{100}\left(\alpha_1^2\beta_1^2 + \alpha_2^2\beta_2^2 + \alpha_3^2\beta_3^2 - \frac{1}{3}\right) + 3\lambda_{111}\left(\alpha_1\alpha_2\beta_1\beta_2 + \alpha_2\alpha_3\beta_2\beta_3 + \alpha_3\alpha_1\beta_3\beta_1\right),$$

where α_1, α_2, α_3 – direction cosines of magnetic moment direction; β_1, β_2, β_3- **direction cosines of the direction along which the deformation is measured**.

- In amorphous and polycrystalline materials (without the texture) the above expression simplifies to:

$$\lambda = \frac{3}{2}\lambda_S\left(\cos^2\theta - \frac{1}{3}\right)$$

distorsion at angle θ relative to magnetization (which may be different from the external field direction)

$\lambda > 0$

- Distortion along the magnetization direction is twice that observed for plane perpendicular to the field (see the drawing→)
- Below Curie temperature the spontaneous magnetization leads to **spontaneous distortion of lattice** [9]: cubic cell deforms to tetragonal system

field directions

distorted specimen

initial shape of the sample
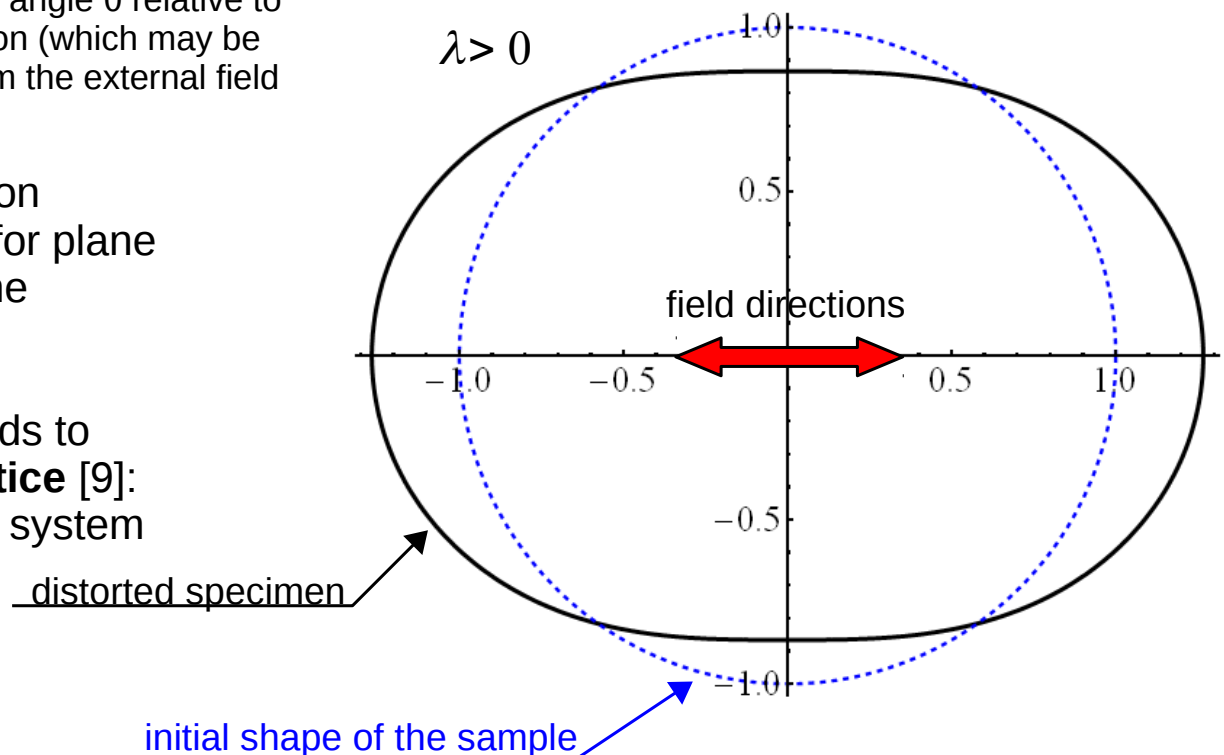
Stress anisotropy – magnetomechanical effect*

- Stress applied to a ferromagnetic body will affect the orientation of magnetization through magnetostriction [6].
- The applied stress changes the magnetization reversal characteristics:
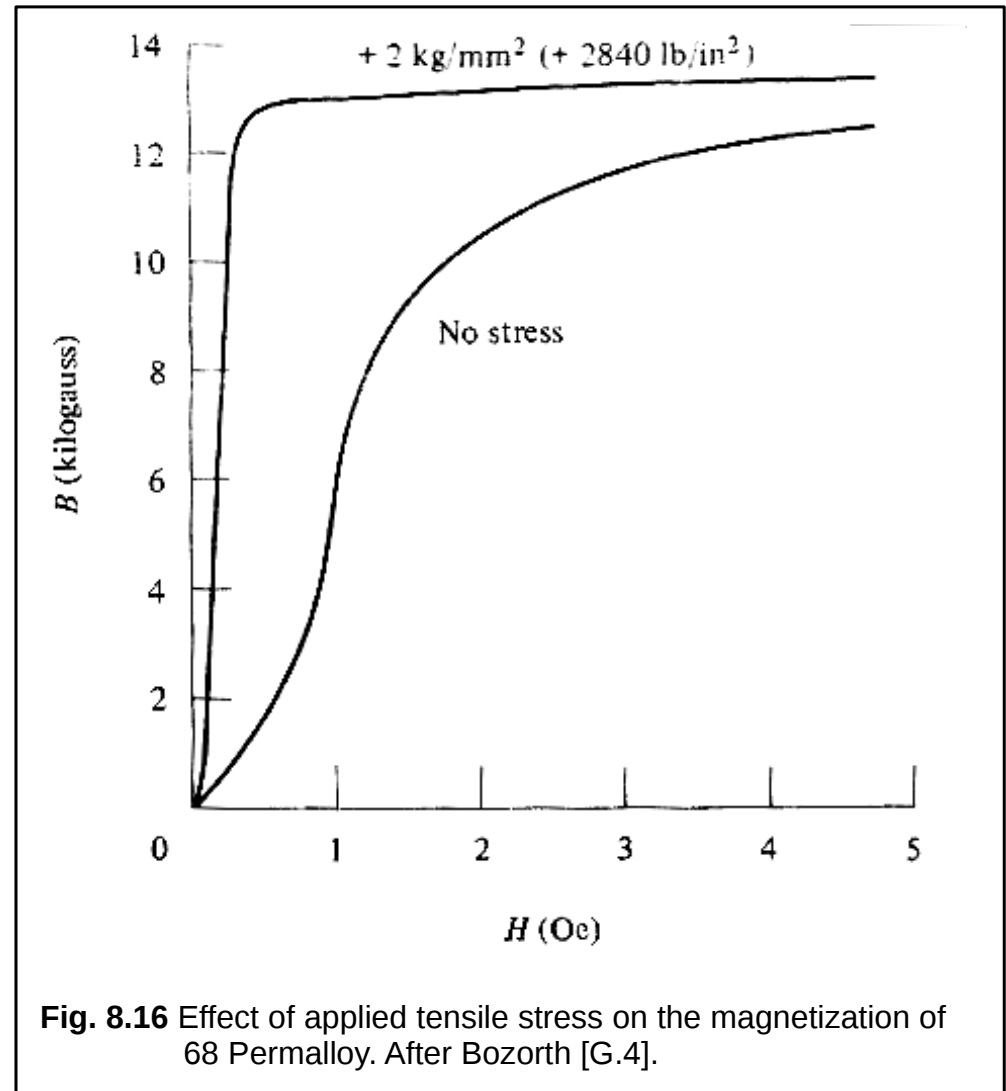

Fig. 8.16 Effect of applied tensile stress on the magnetization of 68 Permalloy. After Bozorth [G.4].

*called inverse magnetostrictive effect, too

Stress anisotropy – magnetomechanical effect

- The part of the energy of a cubic crystal depending on magnetic moment orientation and **the stress applied to crystal** can be shown to be [3]:

$$E = K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + \ldots - \frac{3}{2}\lambda_{100}\sigma(\alpha_1^2\gamma_1^2 + \alpha_2^2\gamma_2^2 + \alpha_3^2\gamma_3^2)$$

$$-3\lambda_{111}\sigma(\alpha_1\alpha_2\gamma_1\gamma_2 + \alpha_2\alpha_3\gamma_2\gamma_3 + \alpha_3\alpha_1\gamma_3\gamma_1),$$

$\gamma_1, \gamma_2, \gamma_3$ - direction cosines of the external stress σ

magnetocrystalline anisotropy

- When the magnetostriction is isotropic ($\lambda_{100} = \lambda_{111} = \lambda_{si}$) the last two terms reduce to*:

$$E_{stress} = -\frac{3}{2}\lambda_{si}\sigma\cos^2\theta$$

where θ is the angle between macrospin (magnetization) and the the stress directions

- The effect of stress on isotropic sample depends on the sign of the $\lambda_{si}\sigma$ product

- The effect of stress is to introduce additional anisotropy to the ferromagnetic system

*with $(\alpha_1, \alpha_2, \alpha_3) = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$

Stress anisotropy – magnetomechanical effect

- The effect of the stress on magnetization reversal for positive $\lambda_{si}\sigma$ product [3]:
1) the magnetic moments within the specimen point in one of four easy directions
2) the application of tensile stress causes domains with magnetic moment perpendicular to the stress to dwindle
3) still higher stress leaves only magnetic moments parallel to the stress
4) Application of the weak magnetic field is sufficient to move 180 Deg domain wall and saturate the specimen

$$E_{stress} = -\frac{3}{2}\lambda_{si}\sigma\cos^2\theta$$

lower energy under stress
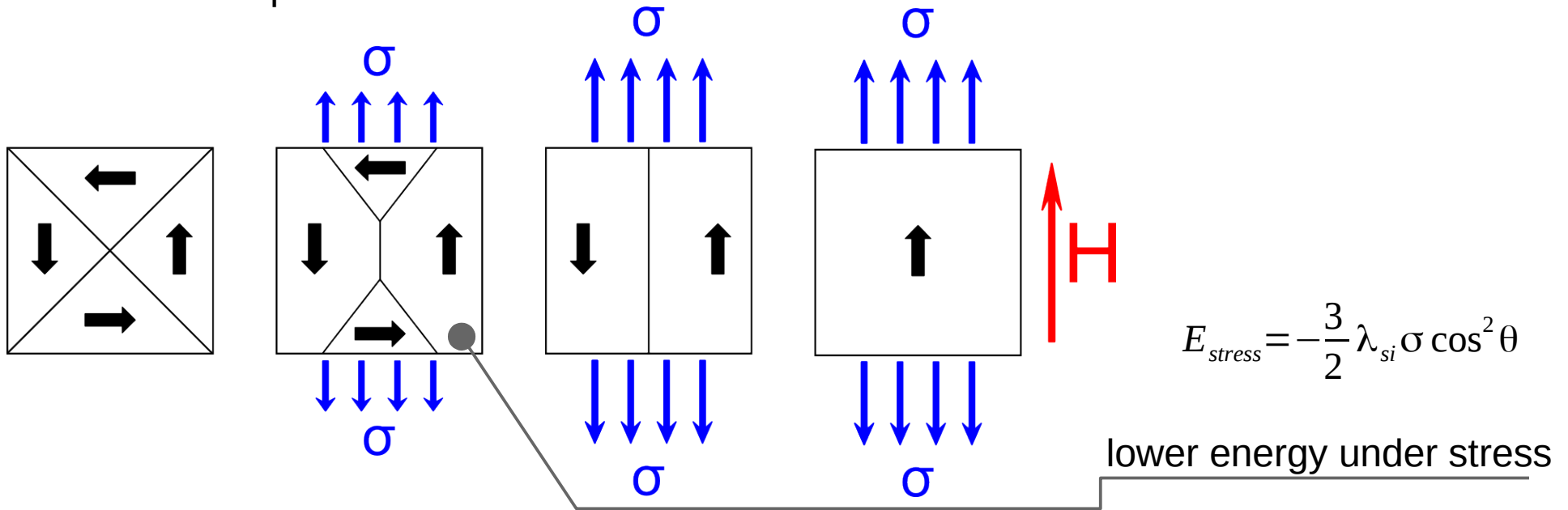
- If compressive stress was applied instead "vertical domains" would disappear and the field would initially (for small H) be perpendicular to magnetic moments.
- In Ni samples the stress of 6.4×10^6 Pa [3] causes stress anisotropy to be roughly equal to magnetocrystalline anisotropy.

Array (or configurational) anisotropy

- In present days many applications (sensors, recording, magnonic devices etc.) make use of patterned magnetic samples
- If the elements of the pattern form a more or less regular array and if the distances between the individual elements are comparable with their sizes the magnetostatic interactions between the elements can lead to additional, separable, contribution to anisotropy apart from that characterizing the elements alone (magnetoscrystalline, shape etc.) [19,20]
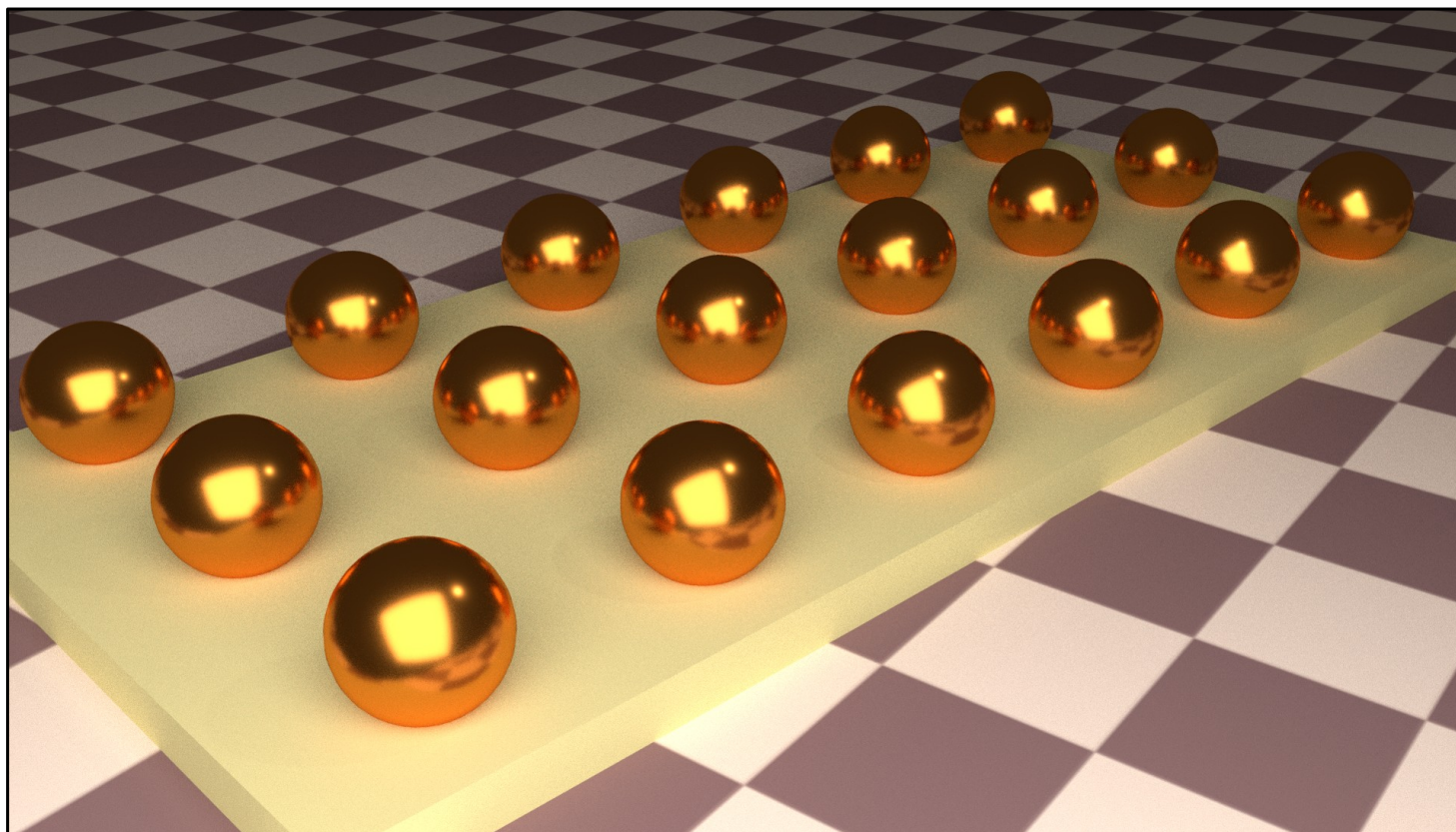
The individual elements of the array (spheres) have no shape anisotropy (they may show other anisotropies) but the array as a whole favors orientation of the moments along its longer edge.

Array (or configurational) anisotropy

- For an array of iron ellipses with 1:3 aspect ratio there is a significant dependence of the hysteresis on the repetition period of the array [20]

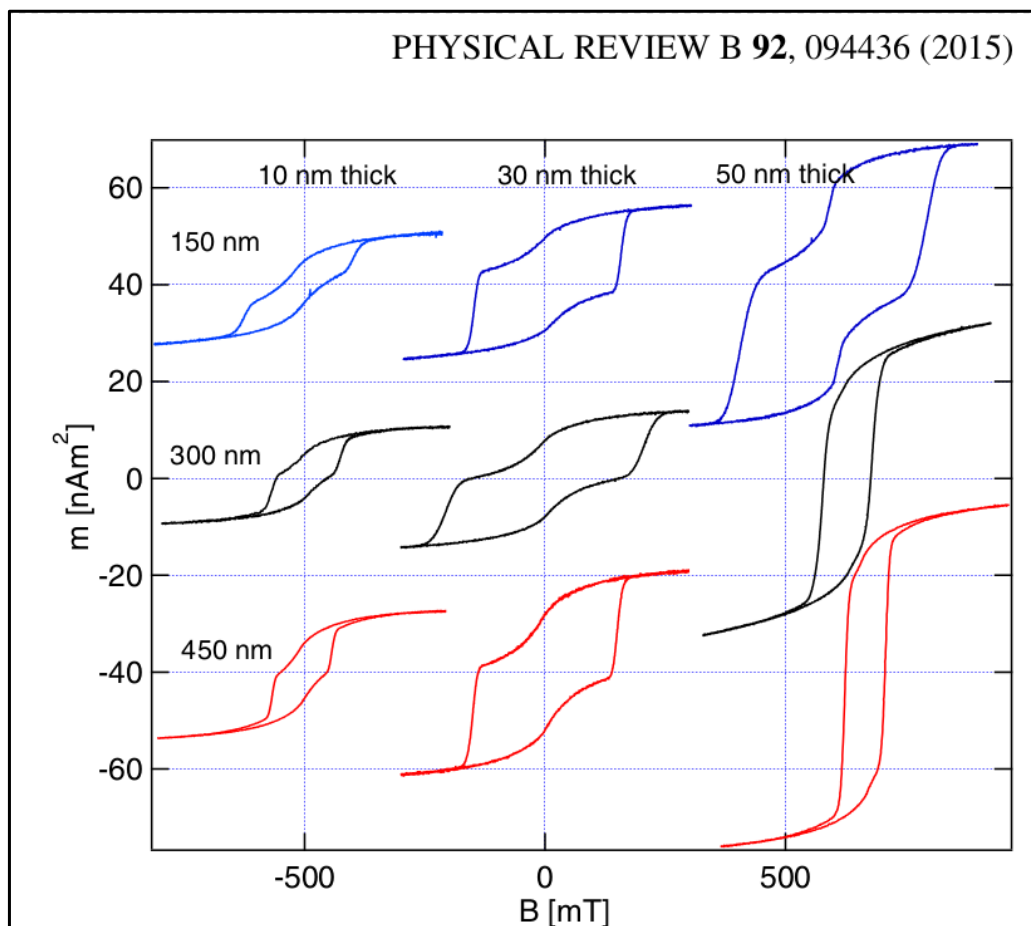PHYSICAL REVIEW B **92**, 094436 (2015)

FIG. 2. (Color online) Size and thickness dependence of hysteresis curves of Fe ellipses with the field applied along the long axes. The interparticle separation is twice the lateral size of corresponding ellipses. The film thicknesses and the long axes are noted in the figure. All curves are drawn to scale with an ofset for all except the central one.
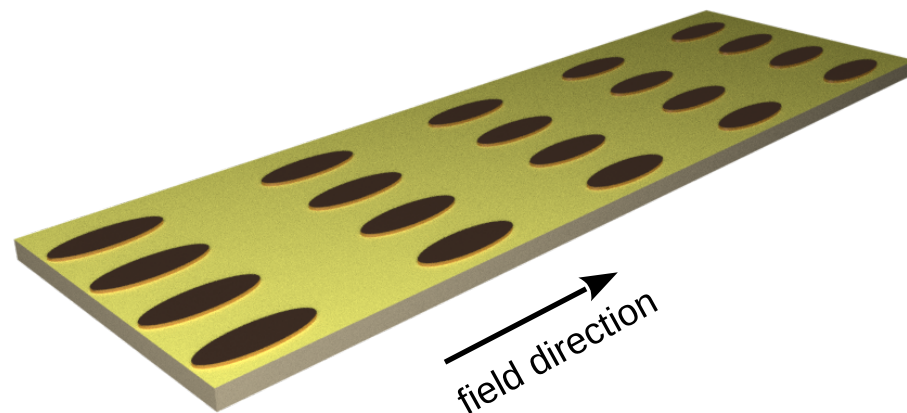
- The in-plane proportions of the array (the ratio of the ellipsoid size to the period) are constant here
- The slimness of iron islands changes along rows of hysteresis loops
- The array can be 1D, 2D or 3D [19]

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Solution to the warm-up problem:

- the divergence of magnetization is zero – no volume magnetic charges

- the surface is always parallel to magnetization vector or magnetic moments [in spherical coordinates (r, φ, θ) the surface normal has no φ components; magnetic moments have only φ components] – no surface magnetic charges

- with no magnetic charges and no free currents the magnetic field strength *H* is zero everywhere

- and because of

$$\vec{B} = \mu_0 (\vec{M} + \vec{H})$$

the magnetic induction is $\vec{B} = \mu_0 \vec{M}$ inside the torus and **zero outside**.