1. Magnetic anisotropy energy = f(T)
2. Anisotropic magnetic moment ≠ f(T)

Characteristic energies of metallic ferromagnets

- binding energy: 1 - 10 eV/atom
- exchange energy: 10 - 10³ meV/atom
- cubic MAE (Ni): 0.2 µeV/atom
- uniaxial MAE (Co): 70 µeV/atom

\[
\text{MAE} \approx 2 \cdot 10^4 \text{erg/cm}^3 \approx 0.2 \mu\text{eV/atom}
\]

\[
\Delta \mu_L \approx 0.1 \text{ G}
\]

Lecture 2: Magnetic Anisotropy Energy (MAE)
There are only 2 origins for MAE: 1) dipol-dipol interaction $\sim (\mu_1 \cdot \vec{r})(\mu_2 \cdot \vec{r})$ and 2) spin-orbit coupling $\mathbf{LS}$ (intrinsic $K$ or $\Delta E_{\text{band}}$).

O. Hjortstam, K. B. et al. PRB 55, 15026 (’97)

R. Wu et al. JMMM 170, 103 (’97)

Structural changes by $\approx 0.05$ Å increase MAE by 2-3 orders of magnitude ($\sim 0.2 \rightarrow 100 \mu eV/\text{atom}$)

K. Baberschke  FU Berlin  „Lectures on magnetism“ #2, Fudan Univ. Shanghai, Oct. 2005
Body-Centered-Cubic Ni and Its Magnetic Properties

C. S. Tian, D. Qian, D. Wu, R. H. He, Y. Z. Wu, W. X. Tang, L. F. Yin, Y. S. Shi, G. S. Dong, and X. F. Jin

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The body-centered-cubic (bcc) phase of Ni, which does not exist in nature, has been achieved as a thin film on GaAs(001) at 170 K via molecular beam epitaxy. The bcc Ni is ferromagnetic with a Curie temperature of 456 K and possesses a magnetic moment of $0.52 \pm 0.08 \mu_B$/atom. The cubic magneto-crystalline anisotropy of bcc Ni is determined to be $+4.0 \times 10^6$ ergs $\cdot$ cm$^{-3}$, as opposed to $-5.7 \times 10^4$ ergs $\cdot$ cm$^{-3}$ for the naturally occurring face-centered-cubic (fcc) Ni. This sharp contrast in the magnetic anisotropy is attributed to the different electronic band structures between bcc Ni and fcc Ni, which are determined using angle-resolved photoemission with synchrotron radiation.
Free energy density of MAE, $K$

(intrinsic, after subtraction of $2\pi M^2$)

tetragonal [e.g. Ni, Co, Fe (001) / Cu (001) ]:

\[
E_{tet} = -K_2 \alpha_z^2 - \frac{1}{2} K_4 \alpha_z^4 - \frac{1}{2} K_4 \alpha_x^4 + \alpha_y^4 + ... \quad (B. Heinrich et al.)
\]

\[
= - K_2 \cos^2 \theta - \frac{1}{2} K_4 \cos^4 \theta - \frac{1}{2} K_4 \frac{3}{4} \cos^4 \phi \sin^4 \theta + ... \quad (Bab et al.)
\]

\[
= (K_2 + K_4) \sin^2 \theta - \frac{1}{2} (K_4 + \frac{3}{4} K_4) \sin^4 \theta - \frac{1}{8} K_4 \cos^4 \phi \sin^4 \theta + ... \quad (traditional)
\]

hexagonal [e.g. Ni (111), Gd (0001) / W (110) ]:

\[
E_{hex} = k_2 \sin^2 \theta + \frac{1}{2} k_2 \cos^2 \phi \sin^2 \theta + k_4 \sin^4 \theta + k_6 \sin^6 \theta + k_6 \cos^4 \phi \sin^4 \theta + ... 
\]

\[
K = k_2 Y_2^0 + k_4 m Y_4^m + ... \quad \text{Legendre polyn.} \quad (B. Coqblin)
\]

each $K_i$ has a „volume“ and „surface“ contribution

\[
K_i = K_i^v + 2K_i^s/d 
\]

K. Baberschke  FU Berlin  „Lectures on magnetism“ #2, Fudan Univ. Shanghai, Oct. 2005
Spin reorientation in bulk Gd

Gd is not isotropic, it has $K_2, K_4, K_6 \neq 0$

Note also finite MAE above $T_C$
Spin reorientation in bulk Ni und Co

At the extremal value of $K_2$ a reorientation and second maximum in $\chi$ appears.

SRT for hcp Co

$$\sin \theta = \left( \frac{K_2}{2K_4} \right)^{1/2}$$

Fig. 6. The variation of the initial susceptibility with temperature in nickel.

Fig. 7. Temperature dependence of magnetocrystalline anisotropy constants of Ni. (a) $K_1$, (b) $K_2$, $K_3$, $K_4$, and $K_5$. Accuracy of data is considerably reduced near $T_c$: dashed lines in the insert (68 A1) and (76 A1). Solid line is to guide the eye through confidence limits (76 A1).

Fig. 5. Temperature dependence of the angle $\theta$ between the direction of spontaneous magnetization and the $c$ axis of a single crystal of hcp Co [61 B5]. Points: data. Curve: calculated from $\sin \theta = \left( -K_2/2K_1 \right)^{1/2}$.

LB III, 19a, p.45

K. Baberschke  FU Berlin

„Lectures on magnetism“ #2, Fudan Univ. Shanghai, Oct. 2005
Ferromagnetic resonance on Fe$_n$/V$_m$(001) superlattices

A.N. Anisimov et al.

\[
\mu_L / \mu_S = \frac{g-2}{2} \quad \text{(Kittel'49)}
\]

in solids $g$ and $\mu$ are tensors

<table>
<thead>
<tr>
<th>bcc (001) Fe$_n$/V$_m$ superlattice</th>
<th>bcc Fe-bulk</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{</td>
<td></td>
</tr>
<tr>
<td>2.264</td>
<td>2.268</td>
</tr>
<tr>
<td>2.09</td>
<td>2.09</td>
</tr>
</tbody>
</table>
For thin films the Curie temperature can be manipulated

\[ K_i = K_i^v + 2 \frac{K_i^s}{d} \]

\[ t = \frac{T}{T_C(d)} \]

P. Poulopoulos and K. B.
Free energy density of MAE, $K$

(intrinsic, after substraction of $2\pi M^2$)

tetragonal [e.g. Ni, Co, Fe (001) / Cu (001)]:

$$E_{tet} = - K_2 \alpha_z^2 - \frac{1}{2} K_{4\perp} \alpha_z^4 - \frac{1}{2} K_4 || (\alpha_x^4 + \alpha_y^4) + ... \quad (B. Heinrich et al.)$$

$$= - K_2 \cos^2 \theta - \frac{1}{2} K_{4\perp} \cos^4 \theta - \frac{1}{2} K_4 || \frac{1}{4} (3 + \cos 4\varphi) \sin^4 \theta + ... \quad (Bab et al.)$$

$$= (K_2 + K_{4\perp}) \sin^2 \theta - \frac{1}{2} (K_{4\perp} + \frac{3}{4} K_4 ||) \sin^4 \theta - \frac{1}{8} K_4 || \cos 4\varphi \sin^4 \theta + ...$$

$$= K_2 \sin^2 \theta + K_{4\perp} \sin^4 \theta + K_4 || \cos 4\varphi \sin^4 \theta + ... \quad (traditional)$$

hexagonal [e.g. Ni (111), Gd (0001) / W (110)]:

$$E_{hex} = k_2 \sin^2 \theta + \frac{1}{2} k_2 || \cos 2\varphi \sin^2 \theta + k_4 \sin^4 \theta + k_{6\perp} \sin^6 \theta + k_6 || \cos 6\varphi \sin^6 \theta + ...$$

$$K = k_2 Y_2^0 + k_{4m} Y_4^m + ... \quad Legendre polyn. \quad (B. Coqblin)$$

*each K$_i$ has a „volume“ and „surface“ contribution*

$$K_i = K_i^V + 2K_i^s/d$$
2b *ab initio* calculations

\[ g_{II} - g_{II} = g_{e} \lambda (\Delta_{II} - \Delta_{II}) \]

anisotropic \( \mu_{L} \) $\leftrightarrow$ MAE

\[ \text{MAE} \propto \frac{\zeta_{LS}}{4\mu_{B}} \Delta \mu_{L} \]

O. Hjortstam, K. B. et al. PRB 55, 15026 ('97)
The surface and interface MAE are certainly large (L. Néel, 1954) but count only for one layer each. The inner part (volume) of a nanostructure will overcome this, because they count for n-2 layers.

K. Baberschke  FU Berlin „Lectures on magnetism“ #2, Fudan Univ. Shanghai, Oct. 2005
A. Berghaus, M. Farle, Yi Li, K. Baberschke

*Absolute determ. of the mag. anisotropy of ultrathin Gd and Ni/W(110).*

San Luis Potosi, Mexico, Proc. in Physics 50, 61 (1989)
M. Farle et al., PRB 55, 3708 (1997)

Only with $K_4 \neq 0$ a continues SRT is possible!

Do not use $K_{\text{eff}} = 2\pi M^2 - K_i$ … because $f(T)$ and $f'(T)$ are different.
Use the ratio $K_i / 2\pi M^2 \Rightarrow f(T) / f'(T)$
Oxygen surfactant assisted growth: a new procedure to prepare ferromagnetic ultrathin films

- Oxygen acts as surfactant for Fe, Co and Ni films on Cu(100)
- Change of magnetic anisotropy by surfactant
- Induced magnetic moment of surfactant
Improved growth by oxygen surfactant

O($\sqrt{2} \times 2\sqrt{2}$)R45°/Cu(100)  
missing row reconstruction  
c(2 × 2)O/Ni/Cu(100)

From AES ⇒ oxygen floats on top of Ni film

Local structure: Surface EXAFS Ni on O/Cu(100)

\[ R_{nn} = (1.85 \pm 0.03) \text{ Å} \]
\[ h = 0.41 \text{ Å} \]

Comparison to theory (T.S. Rahman):
\[ R_{nn} = 1.87 \text{ Å} \]
\[ h = 0.44 \text{ Å} \]

Electronic structure from X-ray absorption spectroscopy

Ni L$_{2,3}$-edge

O K-edge

NEXAFS $\Rightarrow$ no bulklike NiO is formed
\[
F \sim \left(2\pi M^2 - K_{2\perp} \right) \cos^2 \theta
\]

\[
K = K^V + \frac{K^{S1} + K^{S2}}{d}
\]

<table>
<thead>
<tr>
<th>Interface</th>
<th>(K_s) ((\mu\text{eV/atom}))</th>
<th>(d_c) (ML)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni/vacuum</td>
<td>-107</td>
<td>10.8</td>
</tr>
<tr>
<td>Ni/Cu</td>
<td>-59</td>
<td>7.6</td>
</tr>
<tr>
<td>Ni/CO</td>
<td>-81 (van Dijken et al.)</td>
<td>7.3</td>
</tr>
<tr>
<td>Ni/H(_2)</td>
<td>-70 (van Dijken et al.)</td>
<td>6.8</td>
</tr>
<tr>
<td>Ni/O (surfactant)</td>
<td>-17</td>
<td>4.9</td>
</tr>
</tbody>
</table>

**Experiment**

- Ni/Cu(001)
- 2\(\pi M^2\) vs. \(1/d\) (ML)
- Ni vacuum, Ni + Cu cap, Ni + O surfactant

**Theory**

Results of ab initio calculations

Density of states

- DOS shows that topmost Ni moment is basically unchanged
- O-induced surface state seen in the vicinity of $X$-point is responsible for change in MAE
- theory reveals induced moment in surfactant oxygen

Induced magnetism in oxygen: Ni on O/Cu(100)

Oxygen K-edge XMCD → orbital moment $\mu_L$

**BESSY: UE56/2-PGM2**

- $2p_{xy}$, $4sp$
- $2p_{3d}$

15 ML Ni on O/Cu(100) 300K

Theory: Ruqian Wu (UC Irvine):

- Induced moments in oxygen:
  - $\mu_S = 0.053 \mu_B$
  - $\mu_L = 0.0021 \mu_B$
Induced magnetism in oxygen: Co and Fe films

Co on O/Cu(100)

Fe on O/Cu(100)
Conclusion

- spin reorientation transition changes dramatically with surfactant
  → surface anisotropy is strongly reduced in magnitude
- Fe, Co and Ni induce magnetic moment in surfactant
- fair agreement with ab initio calculations