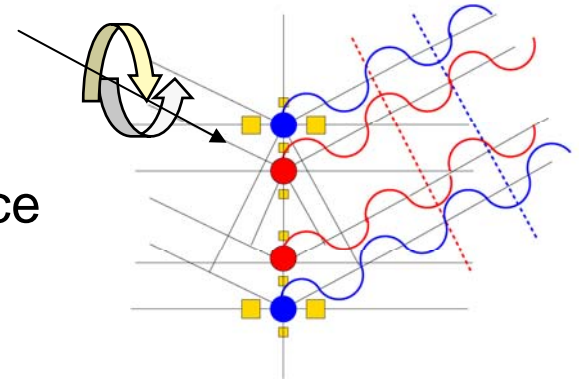


# Insights into Permanent Magnets

Daniel Haskel  
Advanced Photon Source



D. Haskel, J.C. Lang, Z. Islam, A. Cady, G. Srajer, M. van Veenendaal, P. C. Canfield, *Phys. Rev. Lett.* **95**, 217207 (2005).

Funding: LDRD 2004-041-R1

*Presented at APS monthly meeting, December 14, 2005.*

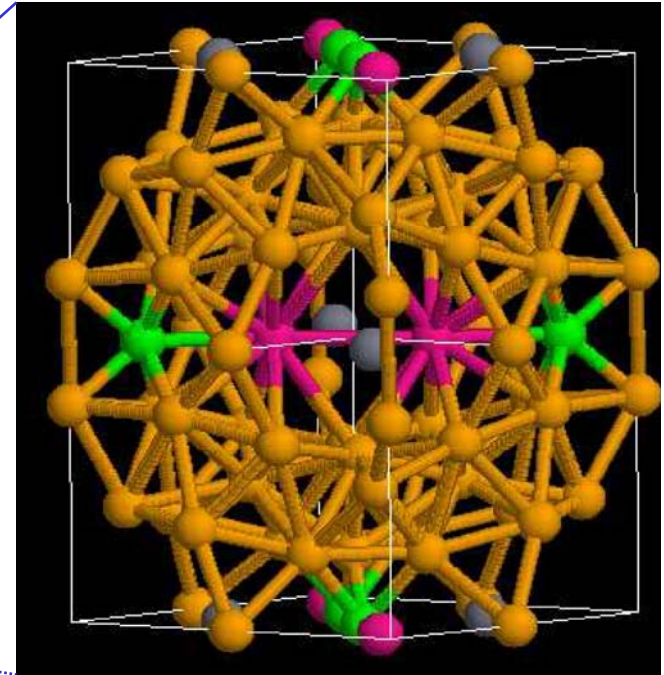
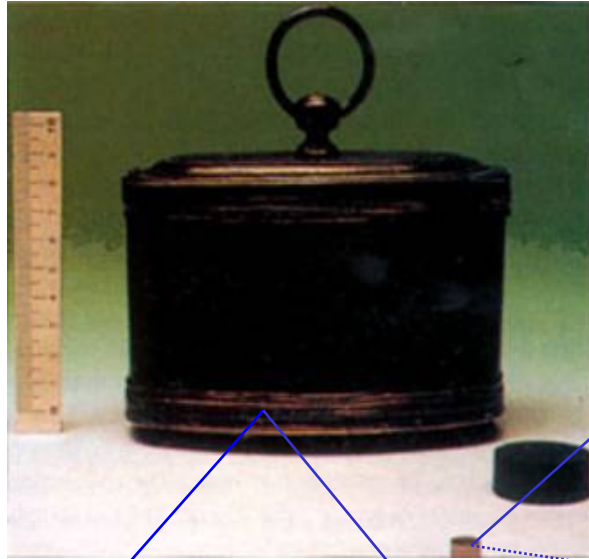
## Argonne National Laboratory



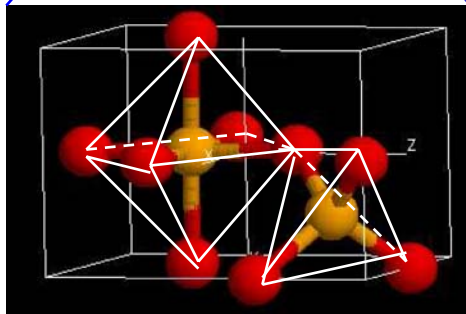
A U.S. Department of Energy  
Office of Science Laboratory  
Operated by The University of Chicago



# Permanent Magnets: Evolution brings complexity



$\text{Nd}_2\text{Fe}_{14}\text{B}$   
(artificial)



Magnetite

● O

● Fe

24 Fe atoms



● Fe ● Nd1 ● B

● Nd2

64 magnetic atoms

2 magnetic elements (Fe, Nd)

6 Fe, 2 Nd crystal sites

# Improved magnetic materials enable new technologies

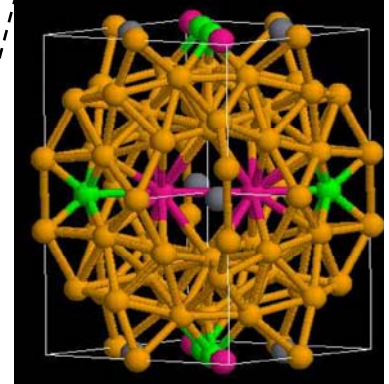
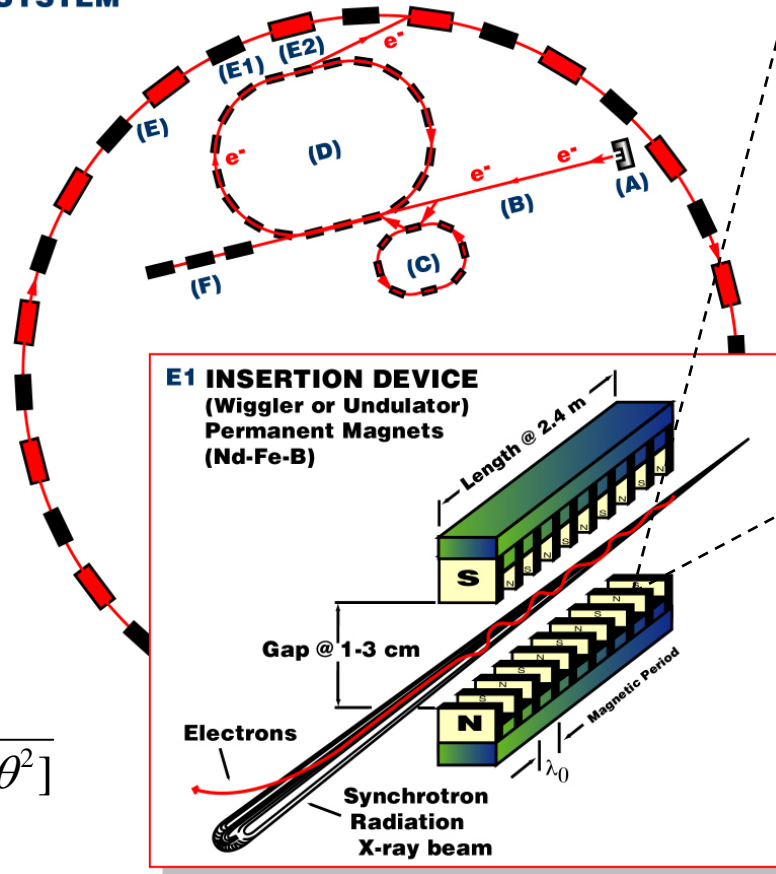
## ADVANCED PHOTON SOURCE BEAM ACCELERATION & STORAGE SYSTEM

- A. ELECTRON GUN**
- B. ELECTRON LINEAR ACCELERATOR**  
200 MeV-650 MeV
- C. ACCUMULATOR RING**
- D. BOOSTER SYNCHROTRON**  
7 GeV
- E. STORAGE RING**  
7 GeV nominal energy
- E1 INSERTION DEVICE**
- E2 BENDING MAGNET**
- F. LOW-ENERGY UNDULATOR TEST LINE**  
400-650 MeV

NOTE: Diagrams not to scale

$$E_n [keV] = \frac{0.95 E^2 [GeV] n}{\lambda_u [cm] [1 + K^2 / 2 + \gamma^2 \theta^2]}$$

$$K = 0.934 \lambda_u [cm] B_{eff} [T]$$



Period = 3.3 cm  
N=72  
2.4 m long  
Minimum gap: 8mm  
Bmax=0.9 T  
2.9-100 keV

Also: Starter motors, brake systems, generators, seat adjusters, latches, etc.



# Modern magnets and the Rare-Earth role

Recipe for a good magnet:

- Large magnetization (pack high density of magnetic ions).
- Large coercivity (“magnetic hardness”, add rare-earth ions).

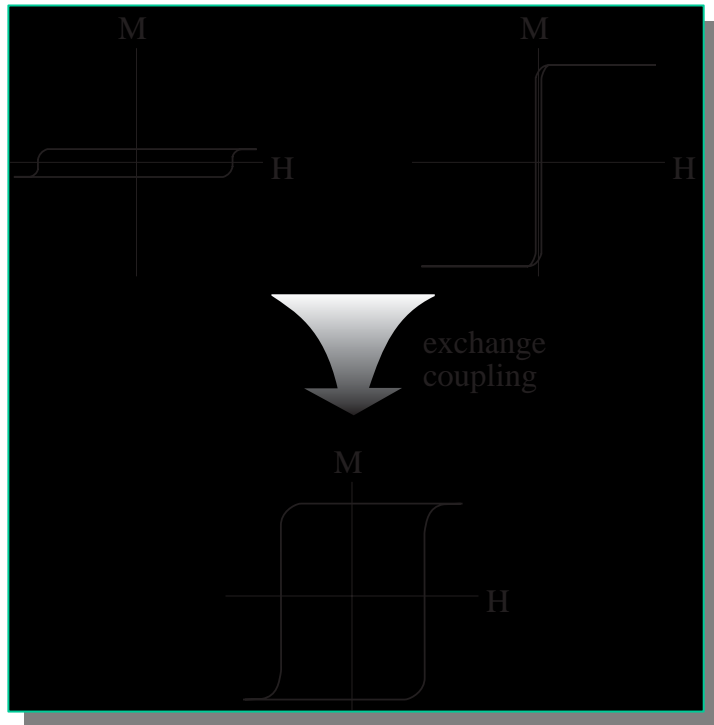
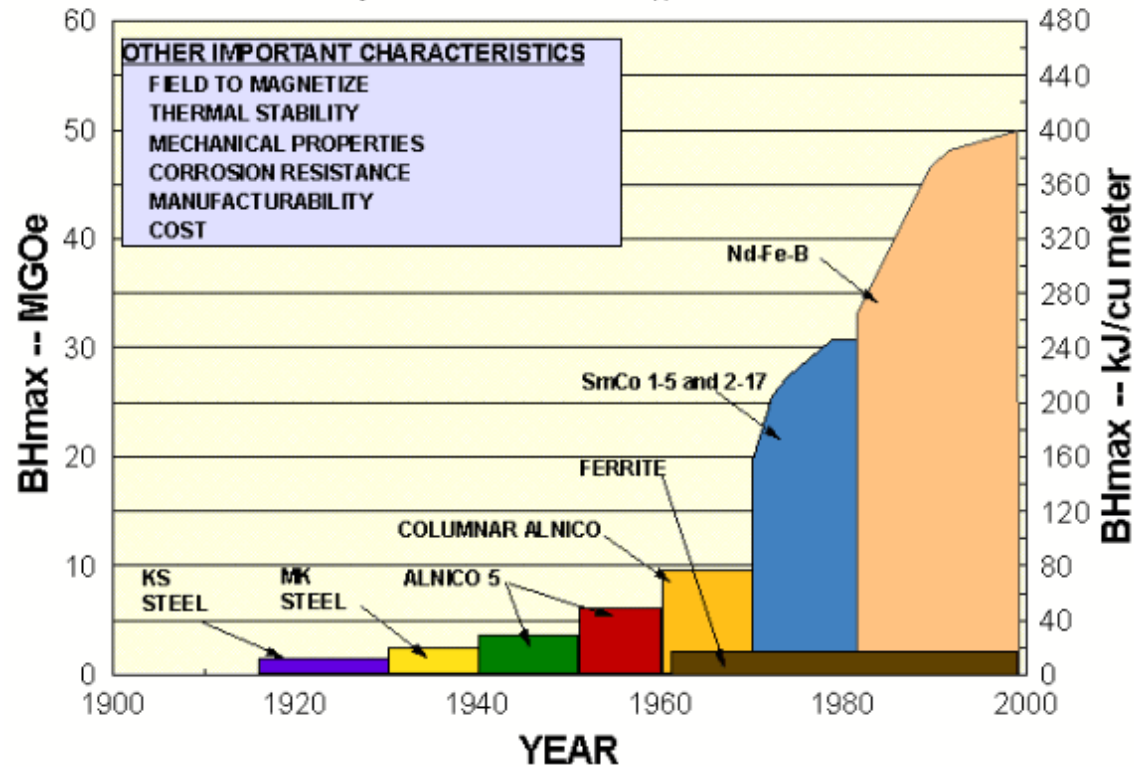


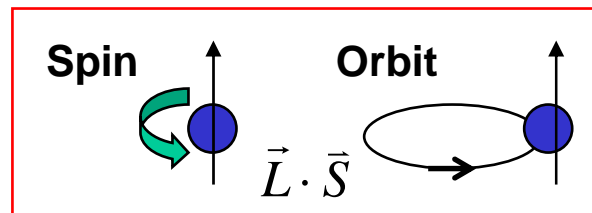
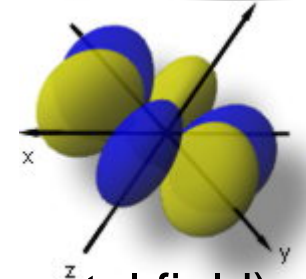
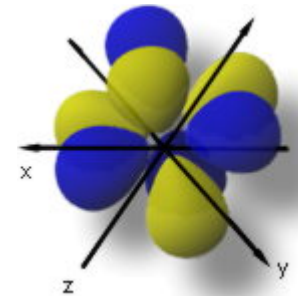
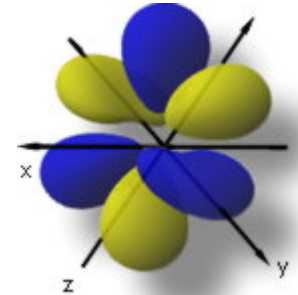
Figure I  
Development of Permanent Magnets in the 1900's



# Modern magnets and the Rare-Earth role

1																	2
H																	He
3	4											5	6	7	8	9	10
Li	Be											B	C	N	O	F	Ne
11	12											13	14	15	16	17	18
Na	Mg											Al	Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104
Fr	Ra	A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Rare-Earths:  
4f electrons



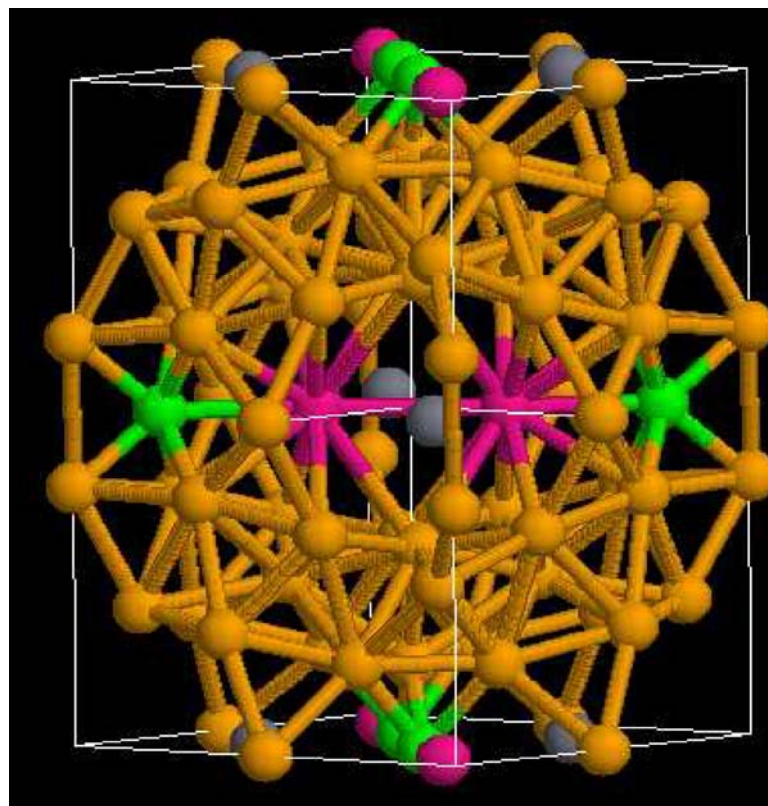
- *Aspherical* 4f orbitals interact with surrounding electrons (crystal field).
- *Spin-orbit coupling* + crystal field determine preferred spin orientation, “pinning” the magnetic moments.



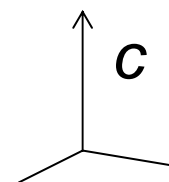
# Nd<sub>2</sub>Fe<sub>14</sub>B: Best in its class

J.F.Herbst, *Reviews of Modern Physics* 63, 819 (1991)

- Tetragonal  $P4_2/mnm$   
 $a=8.8\text{\AA}$ ,  $c=12.2\text{\AA}$
- **2 RE sites**, 6 TM sites  
68 atoms/unit cell
- Fe:  $\sim 31 \mu_B/\text{f.u.}$   
Nd:  $\sim 6 \mu_B/\text{f.u.}$
- Ferromagnet:  $T_c \sim 585\text{K}$



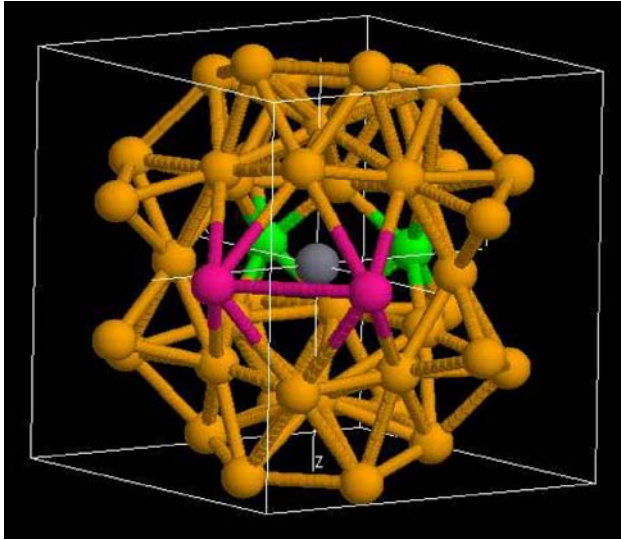
- Nd 4g
- Nd 4f
- B
- Fe



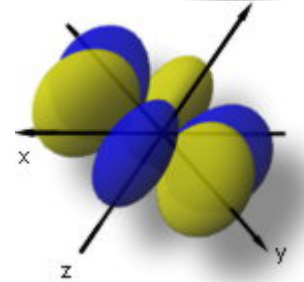
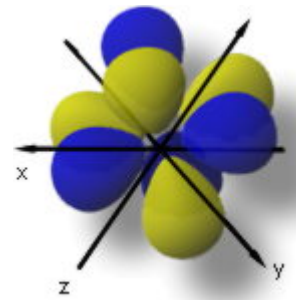
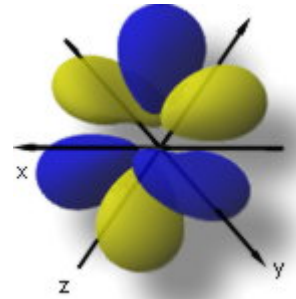
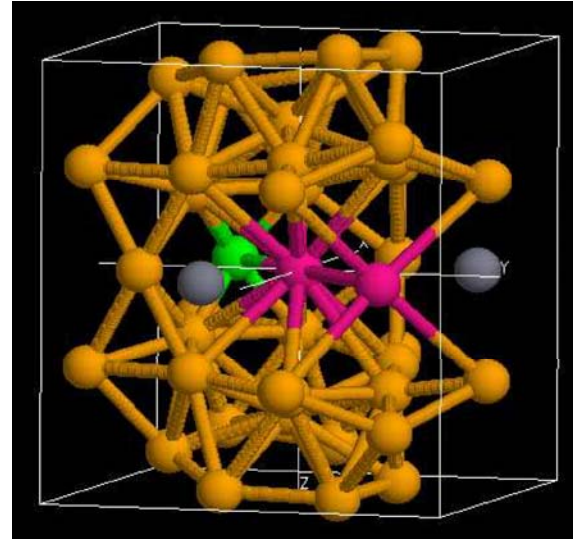
- Easy axis:  $[001]$  (c-axis) at room temperature.
- Magnetocrystalline anisotropy dominated by Nd RE ions.



# The rare-earth role: $\text{Nd}_2\text{Fe}_{14}\text{B}$



- Nd g
- Nd f
- B
- Fe



Rare-earth Nd ions are simultaneously present in two different crystalline environments.

*What are their roles?*

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Goal: To measure Nd site-specific magnetism.  
Tool: Resonant diffraction and absorption  
of CP x-rays.

**Diffraction:** site selectivity.

**Absorption:** site-averaging.

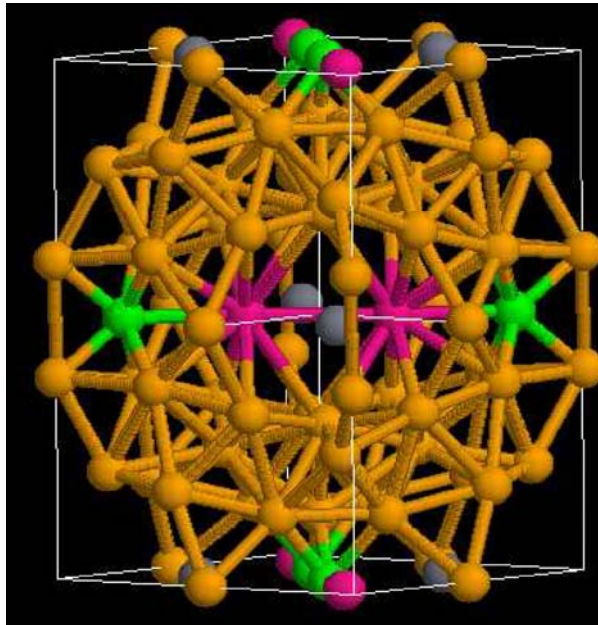
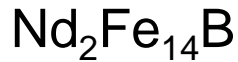
**Atomic resonance:** element specificity.

**CP x-rays:** coupling to magnetization.

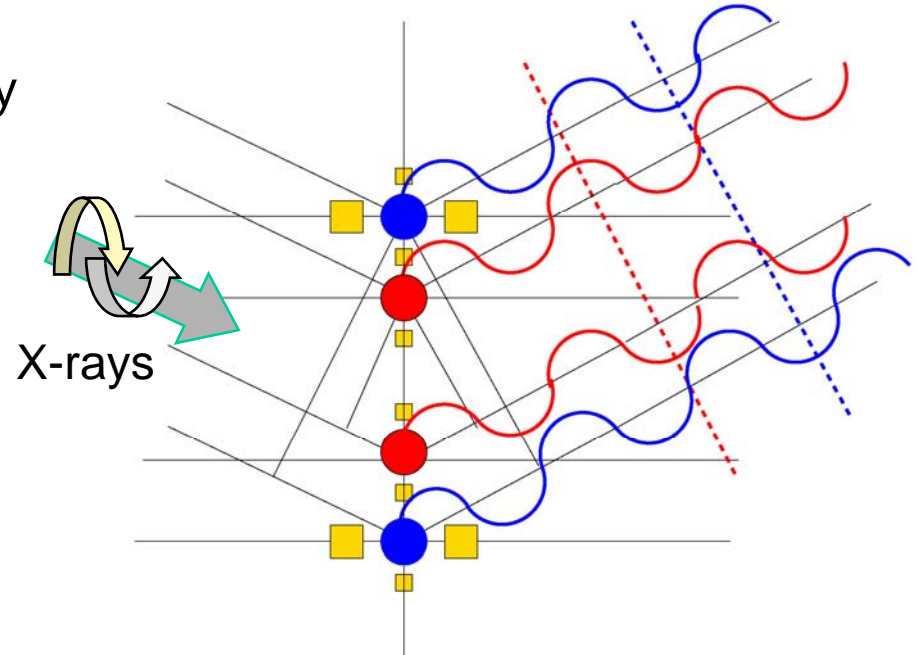


# Exploiting the crystal's symmetry for site separation

- Diffraction = site selectivity
- Atomic resonance = element specificity
- CP x-rays = couple to magnetization



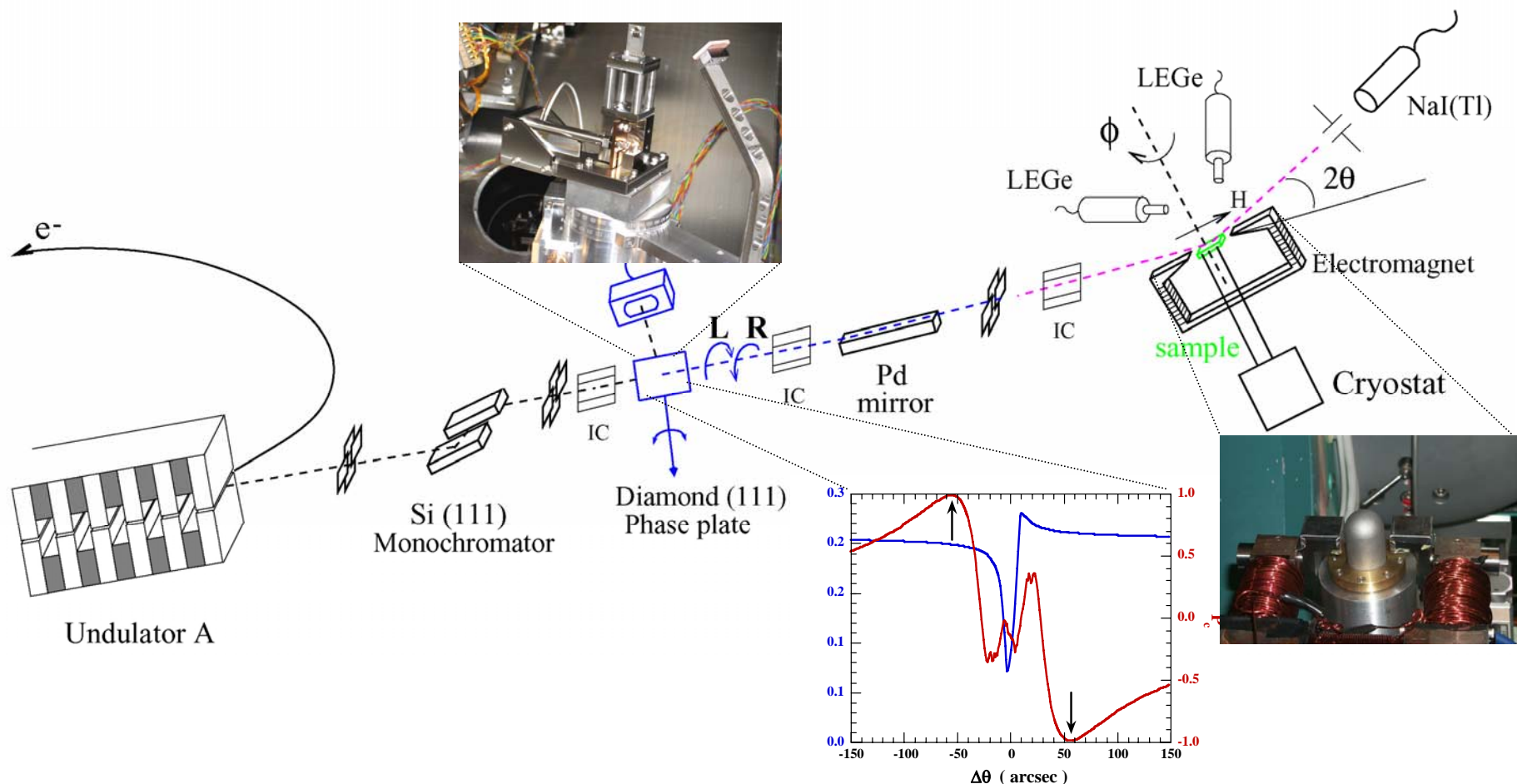
- Nd (1)
- Nd (2)
- B
- Fe



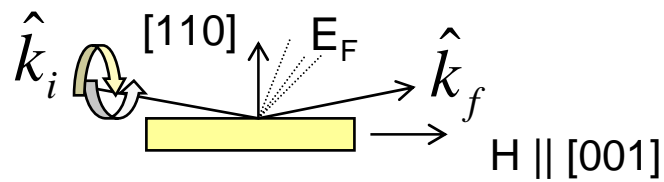
Site	(110)	(220)	(440)
Nd2 (f)	3%	96.4%	48.5%
Nd1 (g)	97%	3.6%	51.5%



# Experiment: Beamline 4-ID-D, Advanced Photon Source



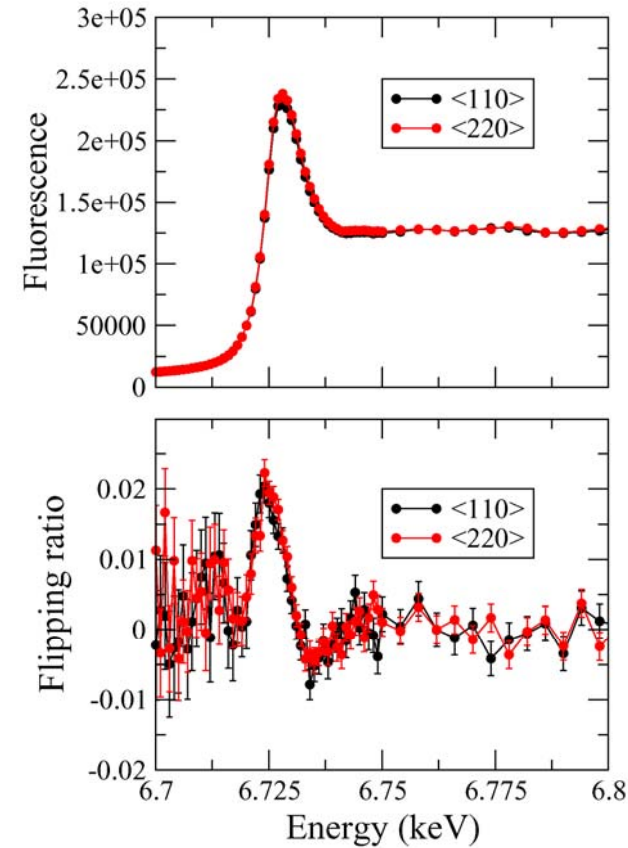
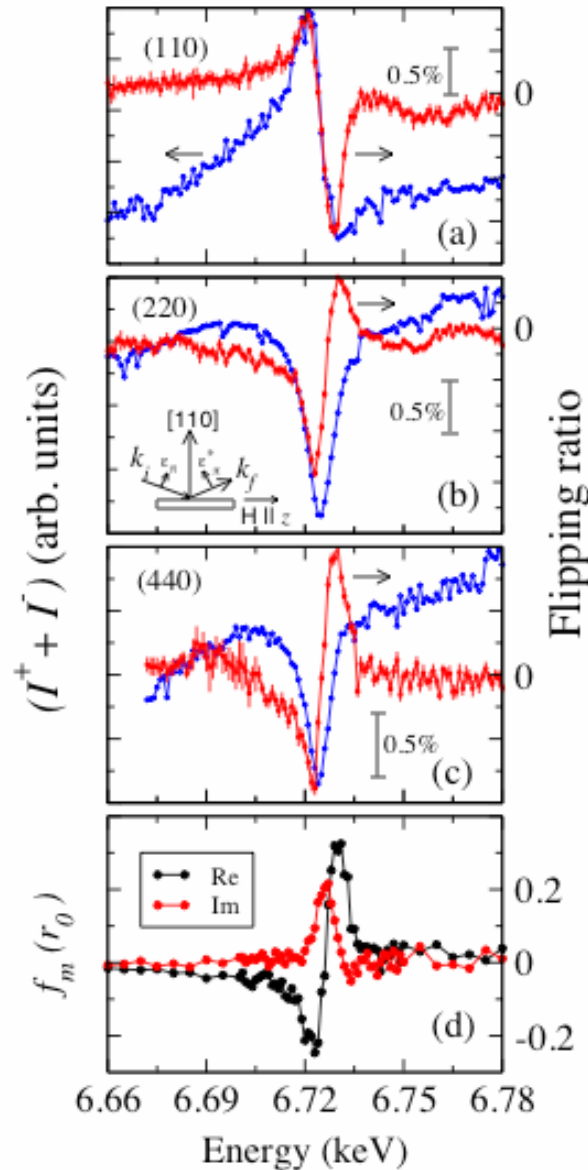
- Resonant diffraction (and absorption) at fix Q (scan ID gap; Monochromator, Phase plate, and sample angles with E. Flip helicity (many times) at each E point.



Diffraction: DANES and MDANES

Absorption: XANES and XMCD

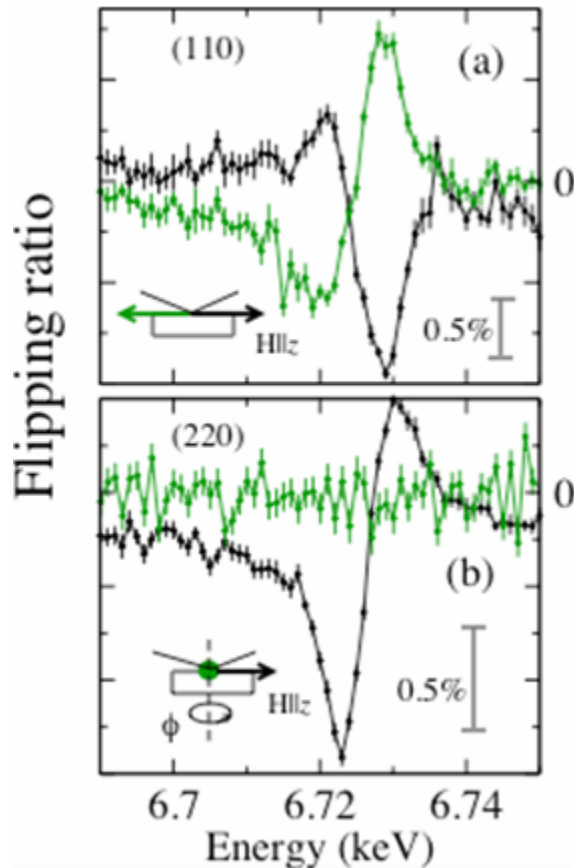
Nd  $L_2$   
( $2p_{1/2}$ )



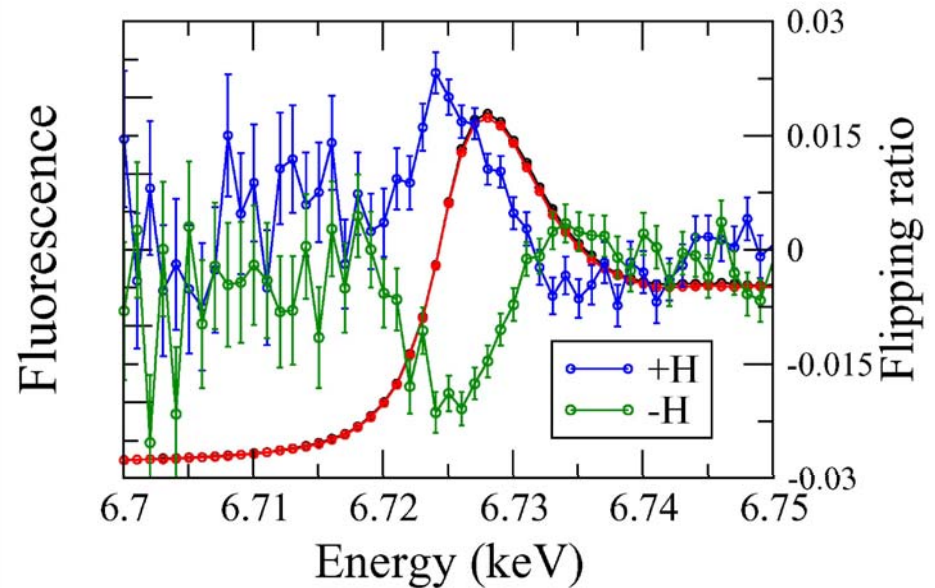
- (110) and (220) reflections probe element *and* site-specific magnetism.
- Absorption element specific but yields site-averaged magnetism.

# Orientation dependence of resonant magnetic scattering, absorption.

## Diffraction



## Absorption

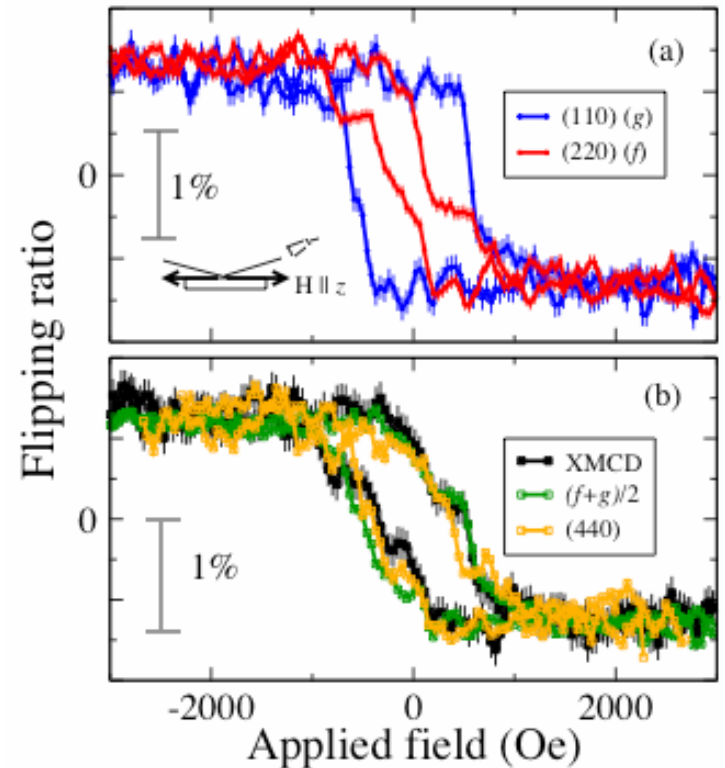
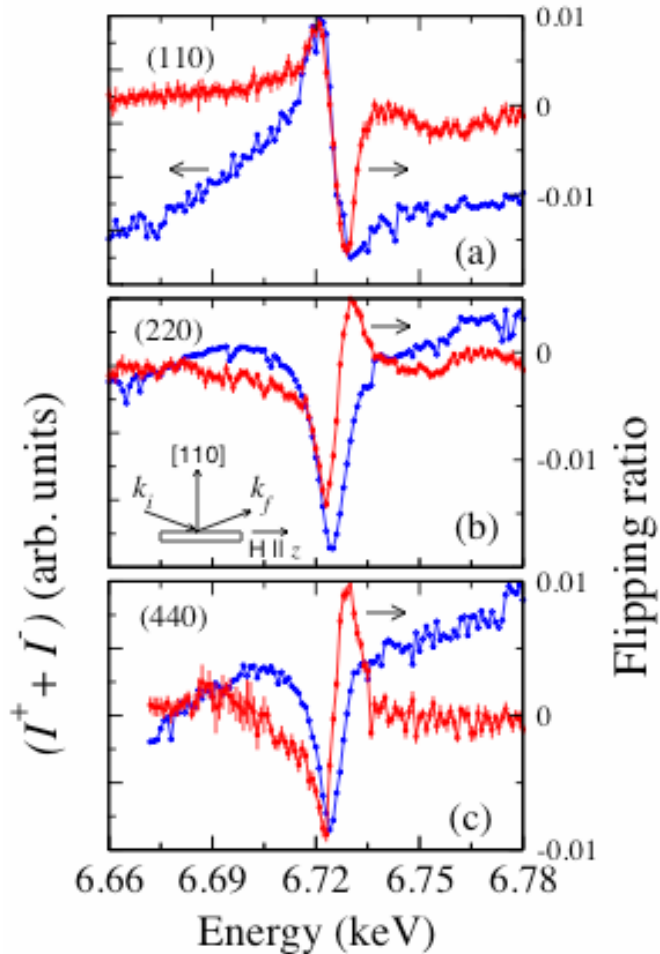


$$\mu_m \propto \hat{k} \cdot \vec{m}$$

- Exploit orientational dependence of diffraction and absorption to study magnetization reversal.

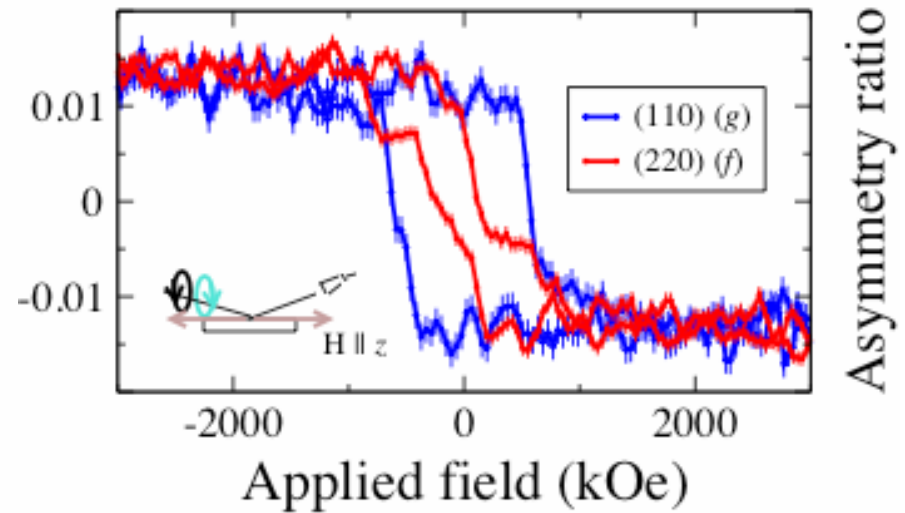
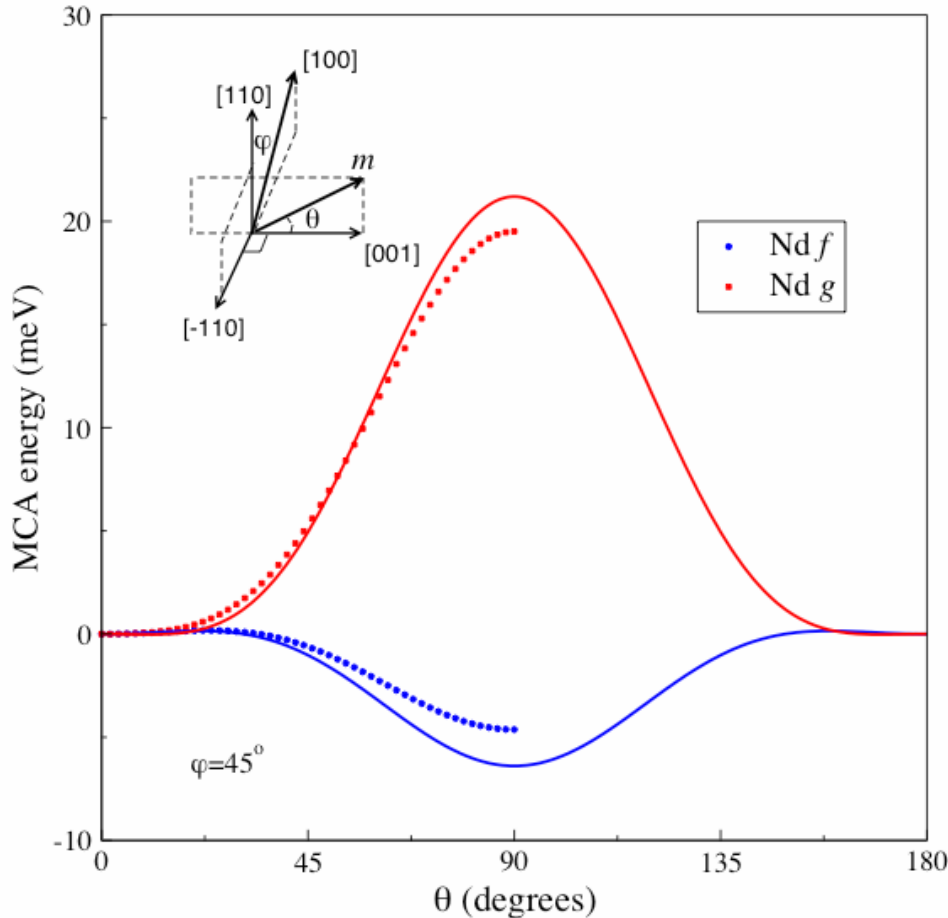
$$I_{cm} \propto [(\hat{k}_i \cdot \hat{m}) + (\hat{k}_f \cdot \hat{m}) \cos 2\Theta]$$

# Nd magnetic moment reversal, site-by-site.



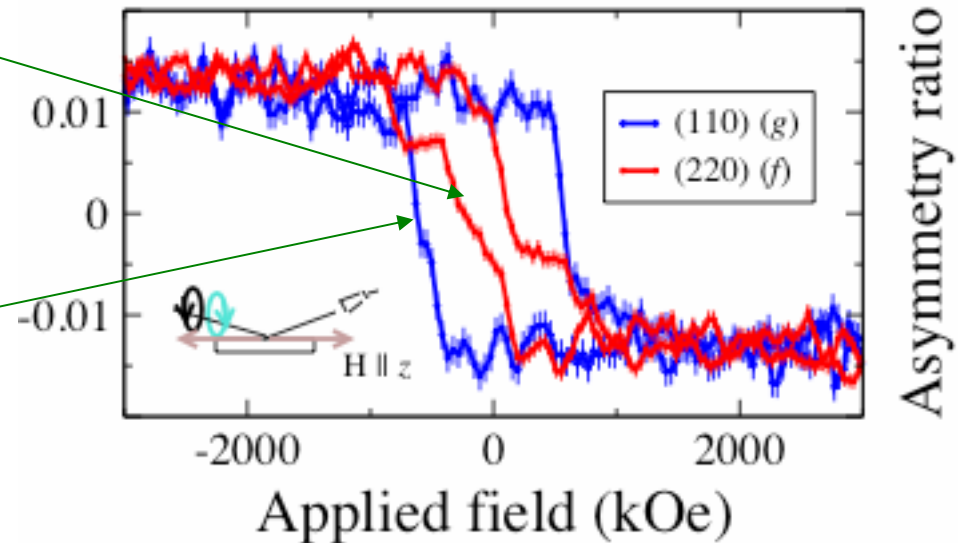
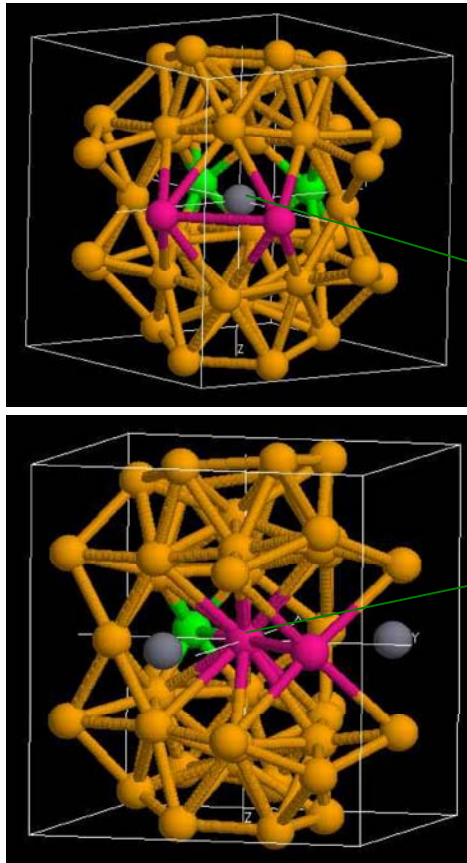
Site	(110)	(220)	(440)
Nd <i>f</i>	3%	96.4%	48.5%
Nd <i>g</i>	97%	3.6%	51.5%

# Theoretical calculations



M. Van Veenendaal (NIU, ANL), CEF parameters M. Yamada et al (1988).

# Manipulate magnetic hardness by atomic engineering



- Only one Nd site responsible for magnetic hardness.
- Replace “faulty” ions with other RE ions, or even Gd (isotropic).

# Acknowledgments

---

## Samples

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## Theory

M. Van Veenendaal (NIU, ANL)

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Z. Islam

A. Cady

G. Srajer

## Digital lock-in

Boris Deriy (ASD)

Kurt Goetze (AOD)

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