About OMICS Group

OMICS Group International is an amalgamation of Open Access publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology 'Open Access', OMICS Group publishes 400 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 300 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

About OMICS Group Conferences

OMICS Group International is a pioneer and leading science event organizer, which publishes around 400 open access journals and conducts over 300 Medical, Clinical, Engineering, Life Sciences, Phrama scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.

Magnetic properties and magnetocaloric effect of field-induced ferromagnet $BaFeO_3$

Kenji Yoshii [1], Naoaki Hayashi [2], Masaichiro Mizumaki [3], Daiju Matsumura [1], Mikio Takano [4]

[1] Japan Atomic Energy Agency, Sayo, Hyogo 679-5148, Japan
[2] iCeMS, Kyoto Univ., Kyoto, 606-8501, Japan
[3] Japan Synchrotron Radiation Research Institute, Sayo, Hyogo 679-5148, Japan
[4] Okayama Univ., Okayama 700-853, Japan

References

N. Hayashi, T. Yamamoto, H. Kageyama, M. Nishi, Y. Watanabe, T. Kawakami, Y. Matsushita, A. Fujimori, and M. Takano, *Angew. Chem. Int. Ed.* **50**, 12547 (2011).

M. Mizumaki, K. Yoshii*, N. Hayashi, T. Saito, Y. Shimakawa, and M. Takano, *J. Appl. Phys.* **114**, 073901 (2013). (*Corresponding author)

K. Yoshii, N. Hayashi *et al.*, *Physical Society of Japan 2014 Annual Meeting*, March 27, (2014).

Outline

1. Introduction
   Cubic ferromagnetic $BaFeO_3$

2. Magnetic properties of $BaFeO_3$
   Magnetic measurements
   Synchrotron X-ray spectroscopic measurements

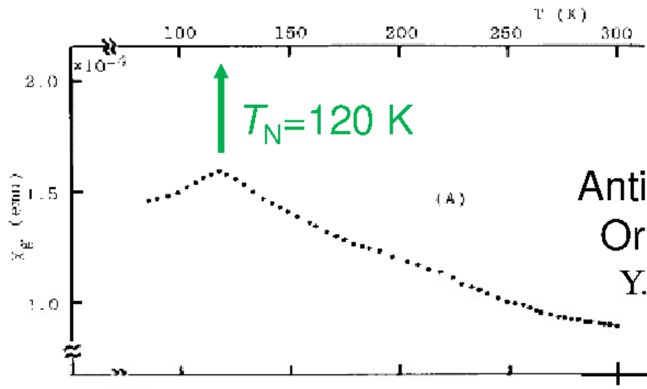
3. Magnetocaloric effect
   Possible magnetic refrigerant
   Small hysteresis, rare-earth-free

1. Cubic $BaFeO_3$ (N. Hayashi *et al.*, 2011)

Perovskite *A*FeO_3 (*A*=Ca, Sr, Ba): Fe^{4+} ($3d^4$)

Synthesized under high pressure (~GPa) with oxidizer (e.g. CaO_2)

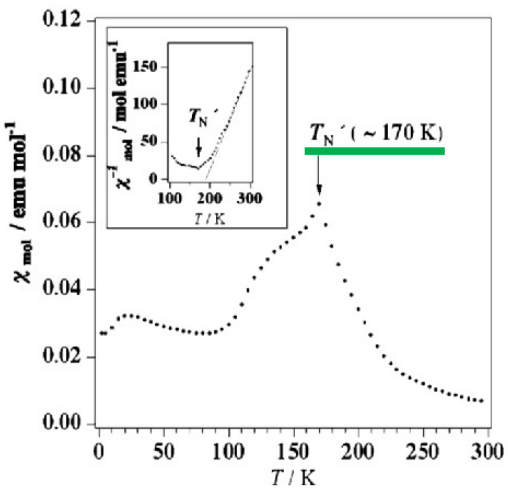
M. Takano *et al.*, *Mater. Res. Bull.* **12**, 923 (1977).



Antiferromagnetism of $CaFeO_3$

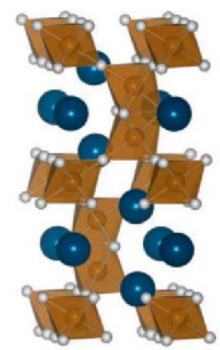
Orthorhombic structure

Y. Takeda *et al.*, *Mater. Res. Bull.* **13**, 61 (1978).



Antiferromagnetism of $BaFeO_3$

Hexagonal structure



6H-type $BaFeO_3$

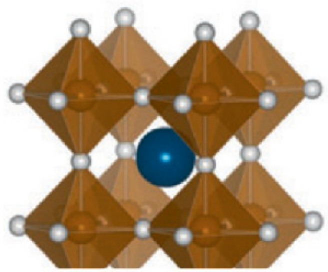
K. Mori *et al.*, *J. Appl. Cryst.* **40**, s501(2007).

1. Cubic $BaFeO_3$ (N. Hayashi *et al.*, 2011)

New simple synthesis route to $BaFeO_3$

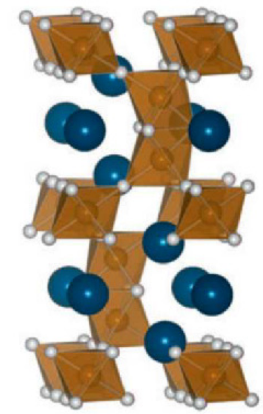
Ozone flow under ambient pressure at 200ºC

N. Hayashi *et al.*, *Angew. Chem. Int. Ed.*, **50**, 12547 (2011).

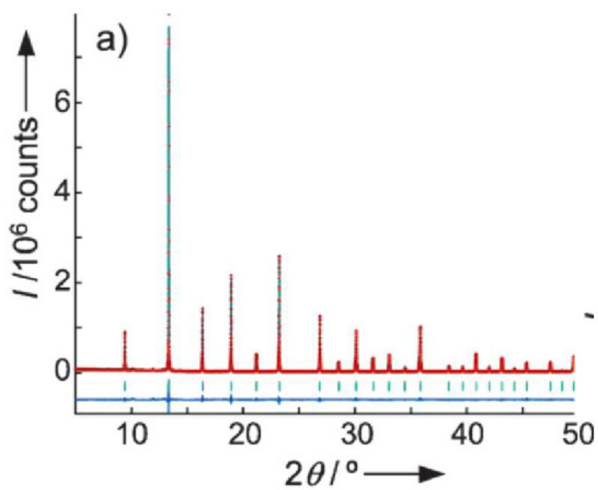


Cubic perovskite: Metastable

cf. Hexagonal: Stable



6H-type $BaFeO_3$



X-ray diffraction

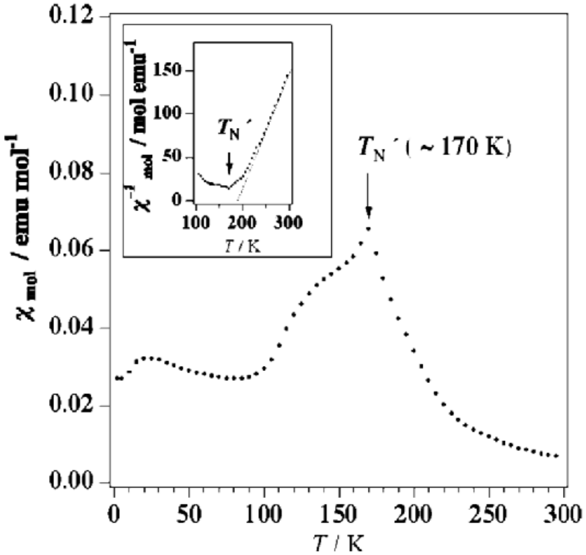
Space group *P*m3m

a = 3.97 Å

How about physical properties ?

2. Magnetic properties of $BaFeO_3$

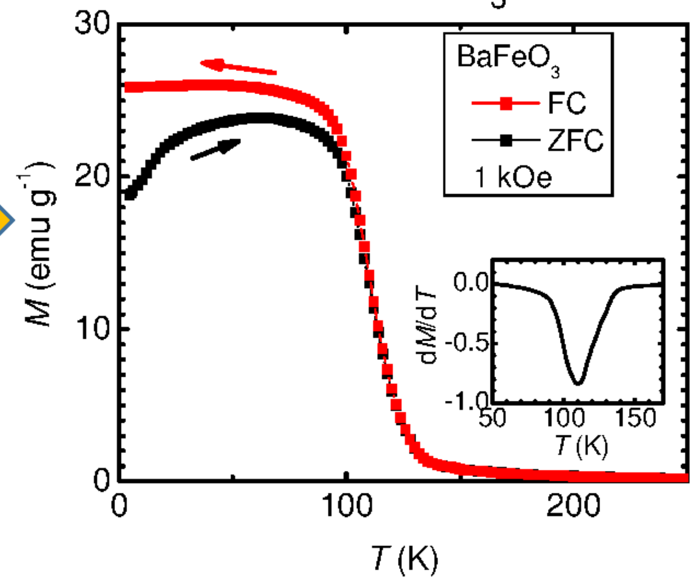
Hexagonal $BaFeO_3$



Antiferromagnetic

K. Mori *et al.*, *J. Appl. Cryst.* **40**, s501(2007).

Cubic $BaFeO_3$

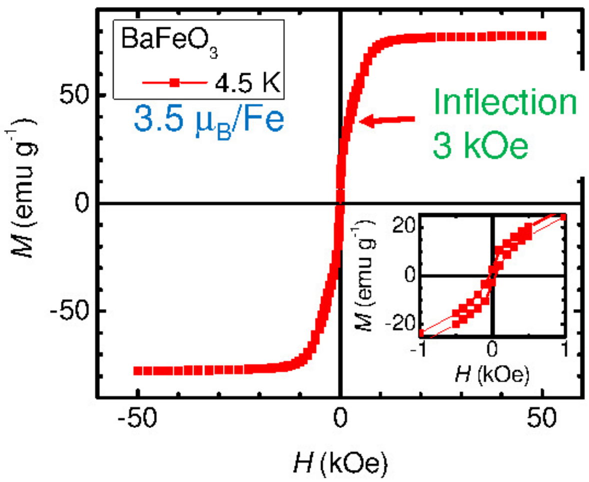


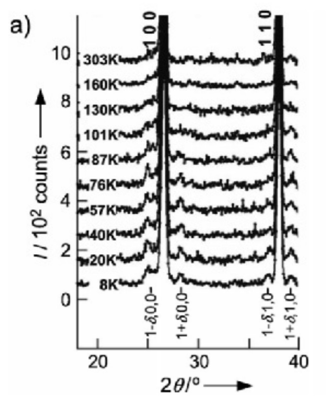
Ferromagnetic at T_C = 111 K
First FM among Fe oxides

N. Hayashi *et al.*, *Angew. Chem. Int. Ed.* **50**, 12547 (2011).

M. Mizumaki *et al.*, *J. Appl. Phys.* **114**, 073901 (2013).

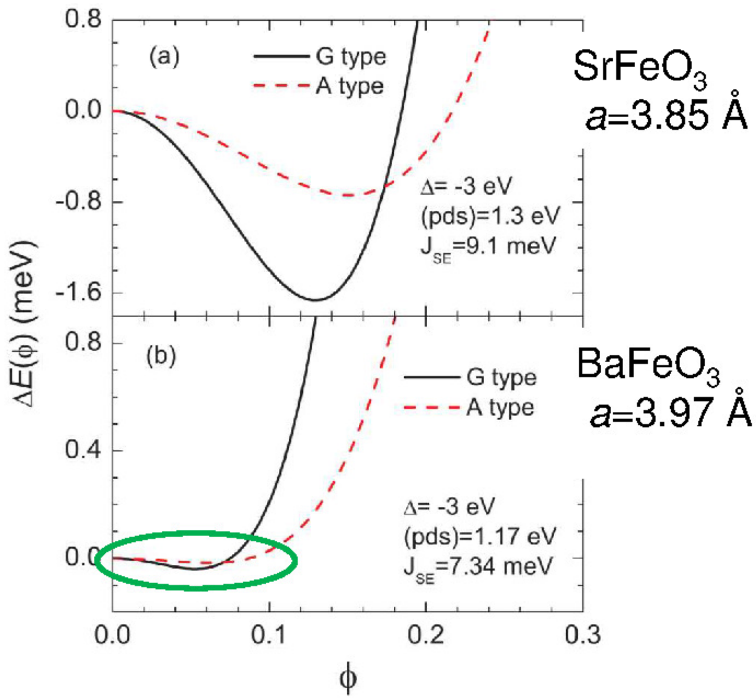
2. Magnetic properties of $BaFeO_3$: Not simple





Ground state
Spiral AFM

N. Hayashi *et al.*, *Angew. Chem. Int. Ed.* **50**, 12547 (2011).

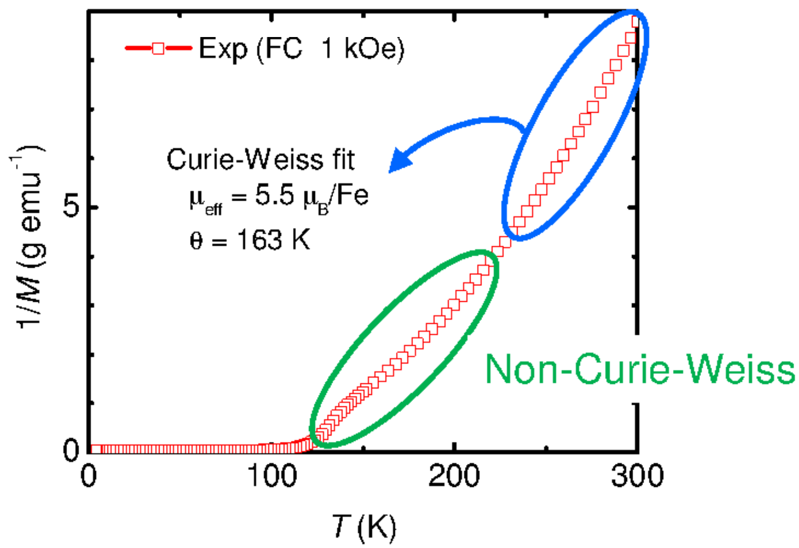


ϕ=0: FM, ϕ>0: AFM

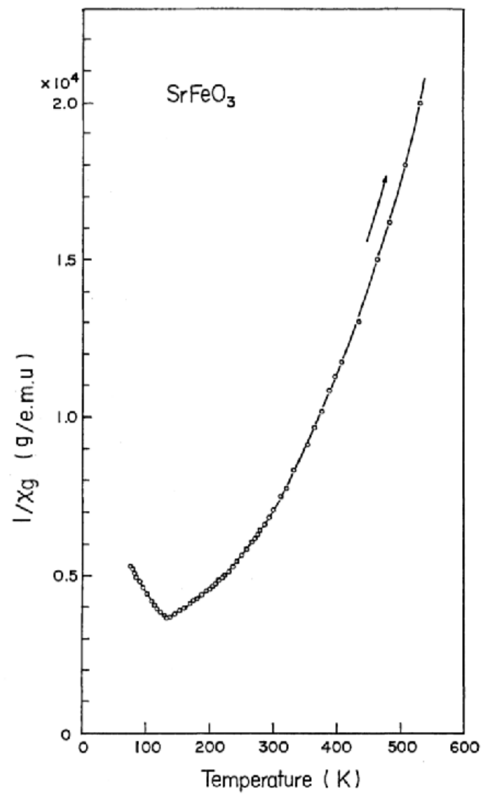
Z.Li *et al.*, *Phys. Rev. B* **85**, 134419 (2012)

AFM-FM transition at 3kOe: Consistent with calculation

2. Magnetic properties of $BaFeO_3$: Not simple



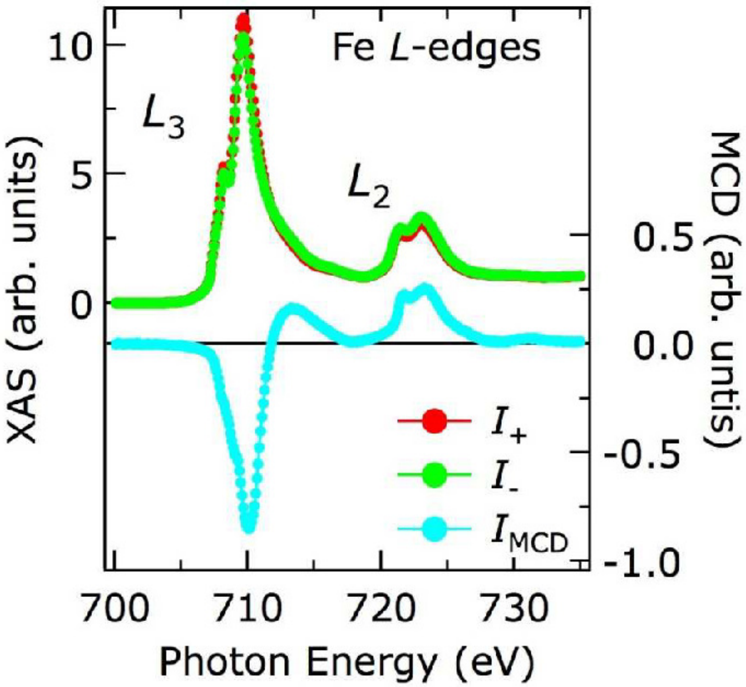
N. Hayashi *et al.*, *Angew. Chem. Int. Ed.* **50**, 12547 (2011).
M. Mizumaki *et al.*, *J. Appl. Phys.* **114**, 073901 (2013).



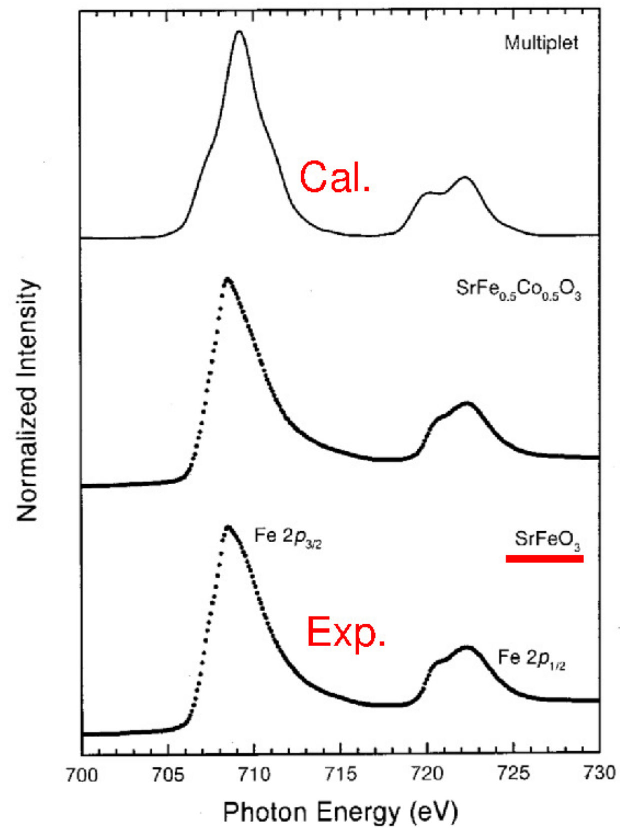
M. Takeda *et al.*, *J. Phys. Soc. Jpn.* **33**, 967 (1972).

Non Curie-Weiss behavior: Common in Fe^{4+} systems
Tendency toward magnetic order ?
Further investigation needed

2. Magnetic circular dichroisim: Fe^{3+} state



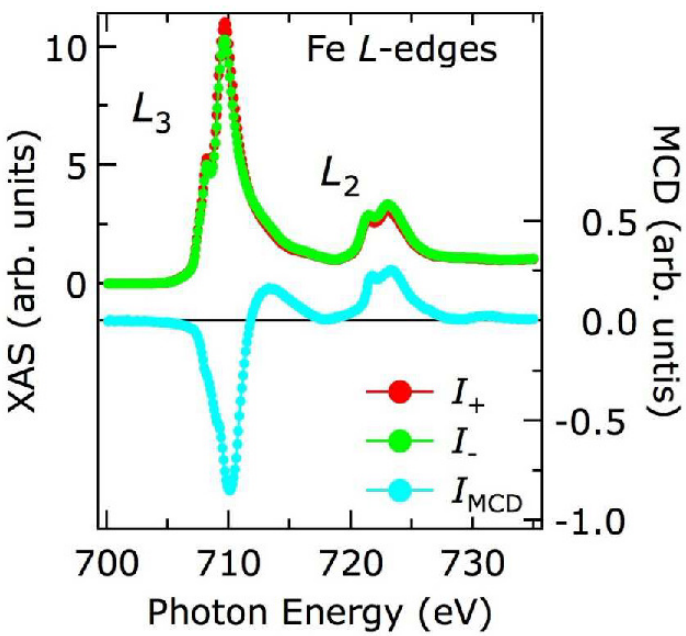
15K@BL25SU, SPring-8
19 kOe



M. Abbate *et al.*, *Phys. Rev. B* **65**, 165120 (2002).

Actual electronic state of Fe^{4+}: $Fe^{3+}\underline{L}$ ($3d^5$) instead of Fe^{4+} ($3d^4$)

2. Magnetic circular dichroisim: Fe^{3+} state



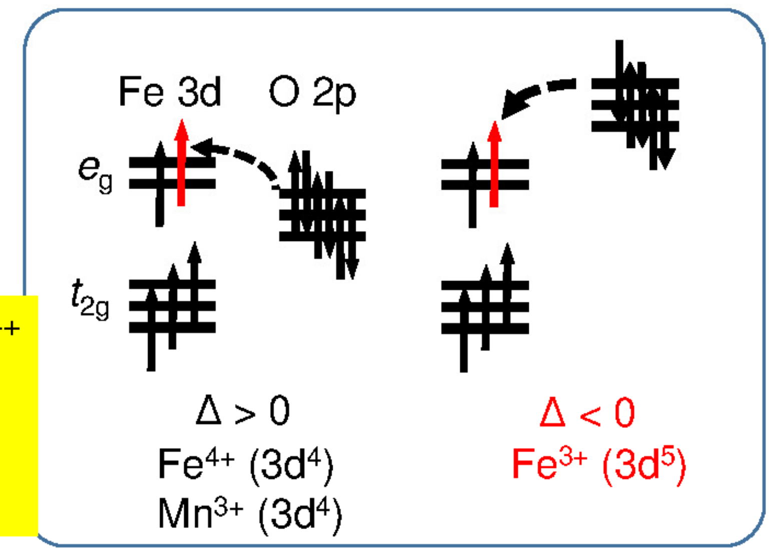
Magnetic circular dichroism (MCD) at 15 K

$$-\frac{\int_{L_3}(\mu_+-\mu_-)\,d\omega - \int_{L_2}(\mu_+-\mu_-)\,d\omega}{\int_{L_3+L_2}(\mu_++\mu_-)\,d\omega} = -\frac{1}{n_h\hbar}\left(\langle S_z\rangle - \frac{7}{2}\langle T_z\rangle\right)$$

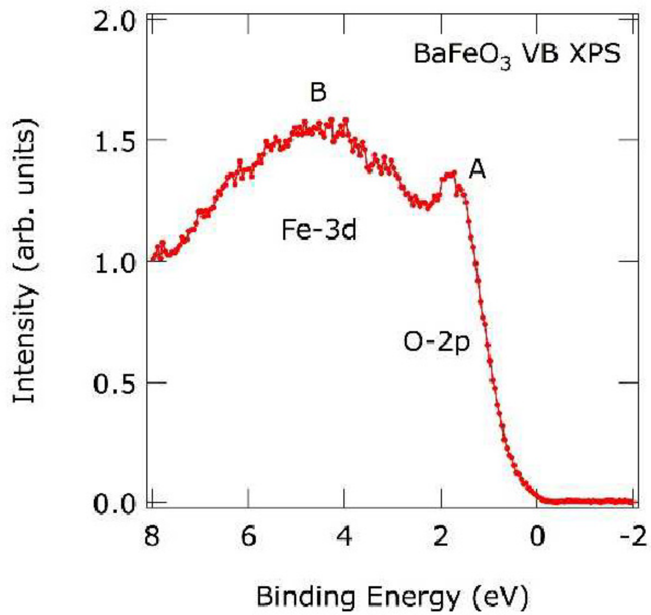
$$-\frac{\int_{L_3+L_2}(\mu_+-\mu_-)\,d\omega}{\int_{L_3+L_2}(\mu_++\mu_-)\,d\omega} = -\frac{3}{4n_h\hbar}\langle L_z\rangle$$

Spin moment 3.40 μ_B
Orbital moment 0.02 μ_B

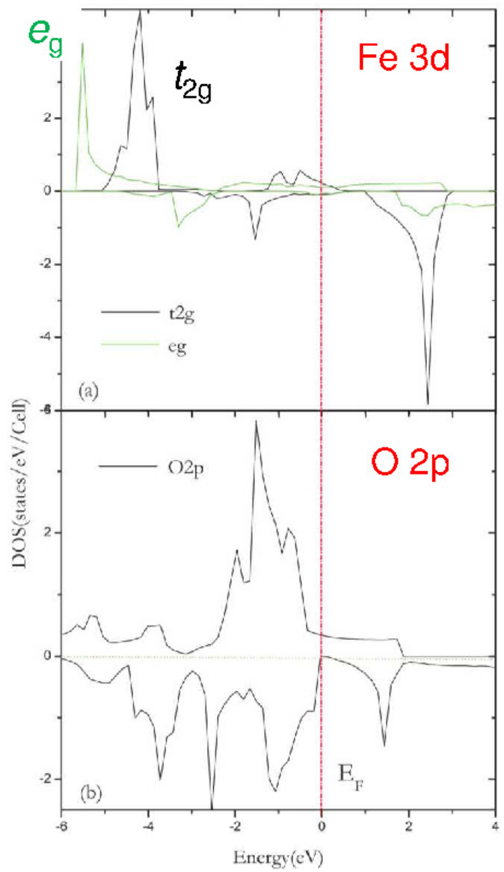
Actual electronic state of Fe^{4+}
$Fe^{3+}\underline{L}$ ($3d^5$)
Negative charge transfer
$\Delta < 0$



2. Hard X-ray photoemission of $BaFeO_3$



BL47XU, SPring-8, RT
hν = 8 keV
bulk sensitive

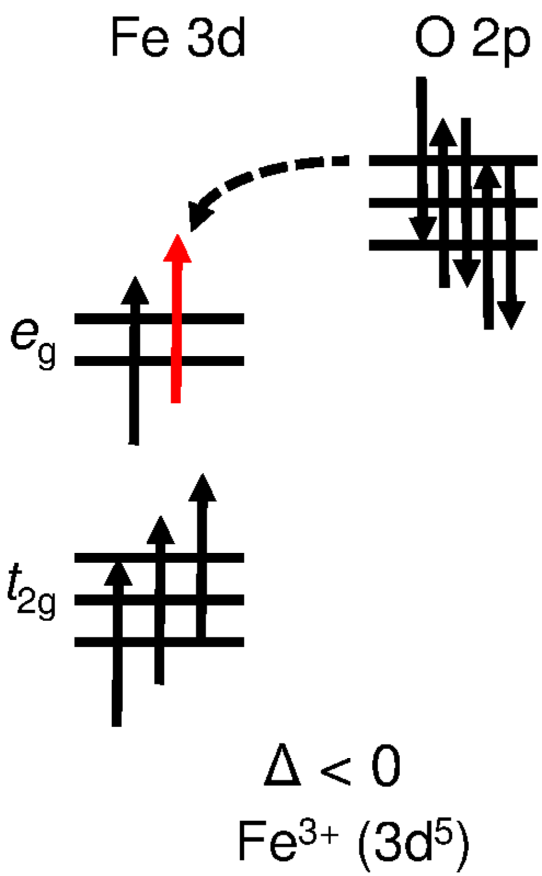


Z.Li *et al.*, *Phys. Rev. B* **85**, 134419 (2012)

Negative charge transfer: Consistent with band calculation

M. Mizumaki *et al.*, *ICTMC-19*, Niigata, Japan (2014)

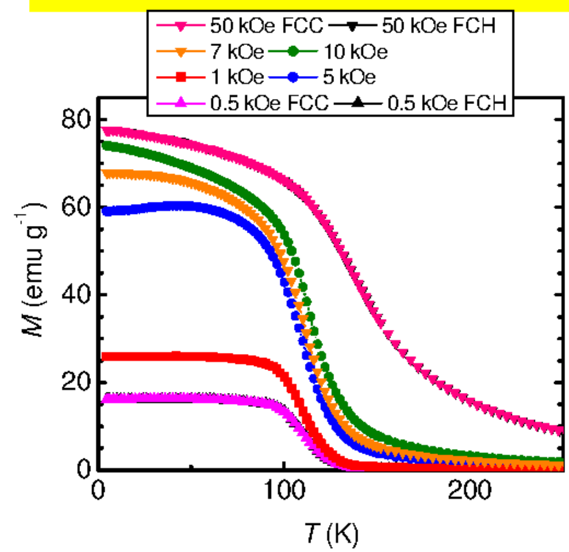
$BaFeO_3$: Negative charge transfer system



Jahn-Teller inactive
Cubic structure

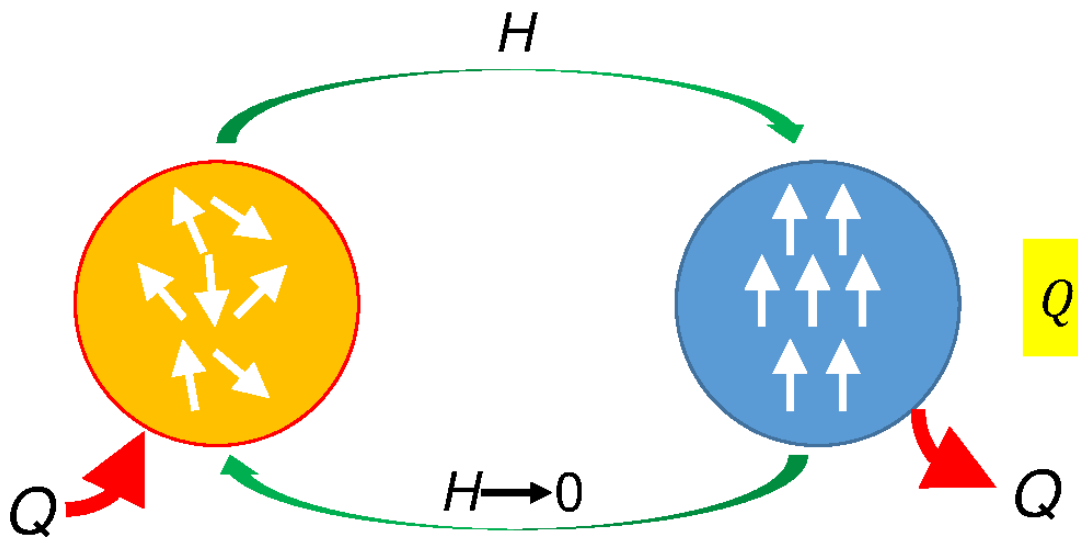
Narrow *MH* curves
Absence of orbital moment

Origin of small hysteresis



→ Beneficial to magnetic refrigeration

3. Magnetocaloric effect (MCE): Magnetic refrigeration



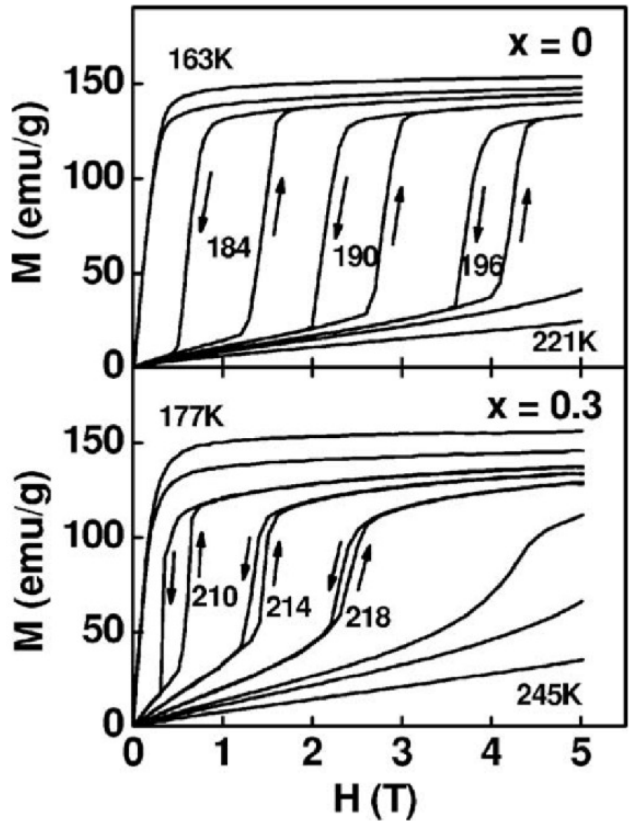
$$Q \sim \Delta S = \int_0^H \left(\frac{\partial M}{\partial T}\right)_H dH$$

Efficient refrigeration
Free from chlorofluorocarbon
Small apparatus: Free from gases

K. A. Gschneidner, Jr., V. K. Pecharsky, and A. O. Tsokol, *Rep. Prog. Phys.* **68**, 1479 (2005).

3. Hysteretic loss in MCE

$La_{0.5}Pr_{0.5}Fe_{11.5}Si_{1.5}C_x$



Hysteresis during field cycle
Energy loss

Suppression of hysteresis
Efficient refrigeration

J. Shen *et al.*, *Appl. Phys. Lett.* **91**, 142504 (2007).

3. $BaFeO_3$: Possible MCE material

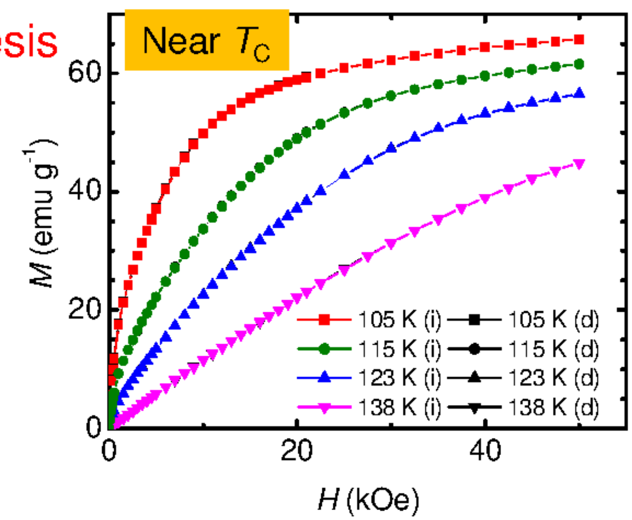
(1) Large entropy change: Ferromagnet

$$\Delta S = \int_0^H \left(\frac{\partial M}{\partial T}\right)_H dH$$

(2) Rare-metal free

(3) Stability against corrosion
Impurities removed in water

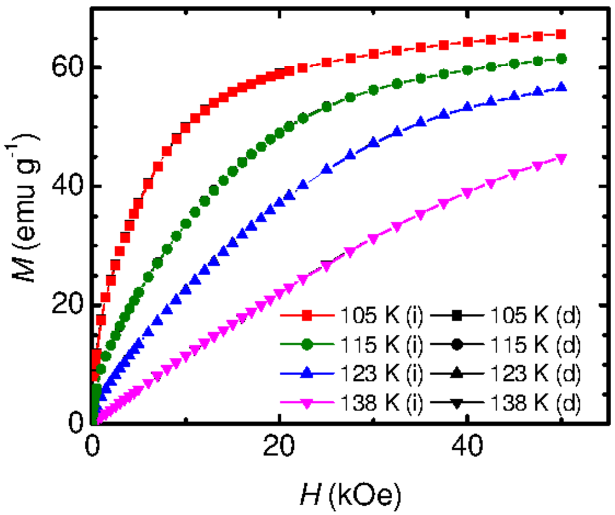
(4) Low hysteresis

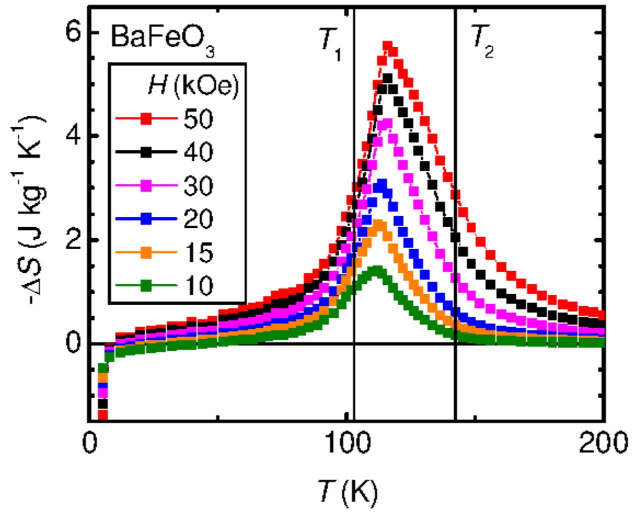


$$\Delta S = \int_0^H \left(\frac{\partial M}{\partial T}\right)_H dH$$

Enhances at T_C

3. Entropy change

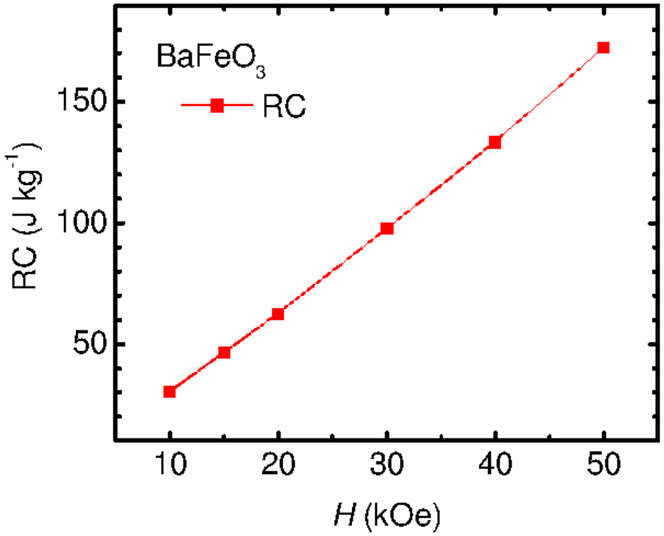




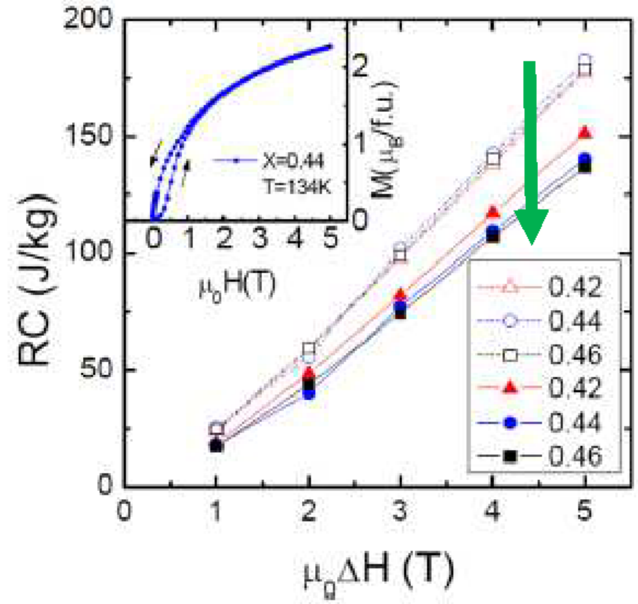
$$\Delta S = \int_0^H \left(\frac{\partial M}{\partial T}\right)_H dH = \frac{1}{\Delta T}\left(\int_0^H M(T+\Delta T)dH - \int_0^H M(T)dH\right)$$

- Entropy change 5.8 J kg^{-1} K^{-1} for H=50kOe
  Comparable to magnanites, Largest among non-rare-earth systems
- Negative -ΔS below 10 K：AFM ground state
- Integration between T_1 and T_2 = RC (Refrigerant Capacity)：170 J kg^{-1}

3. Refrigerant capacity



$Sm_{1-x}Sr_xMnO_3$



Comparable to manganites
Similar magnetic moments
(3-4 μ_B/Fe or Mn)

Hysteretic loss
Corrected by arrow

N.S.Bingham *et. al*, *J. Appl.Phys.* **111**,07D705 (2012)

Summary

We have studied the magnetic properties and MCE of $BaFeO_3$.

The characteristics are:

(1) Field-induced ferromagnet with T_C= 111 K
First FM material among Fe oxides

(2) Almost no thermal and field hysteresis

(3) Fe^{4+} ion: Actually $Fe^{3+}\underline{L}$
Negative charge transfer system: No hysteresis

(4) Large MCE for LNG (110K) and cooling of high-T_C cuprates
Rare-earth-free MCE material

Let Us Meet Again

We welcome you all to our future conferences of OMICS Group International

Please Visit:

http://materialsscience.conferenceseries.com/

Contact us at

materialsscience.conference@omicsgroup.us

materialsscience@omicsgroup.com