

Single Crystal Structure Analysis of a Single $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ Particle

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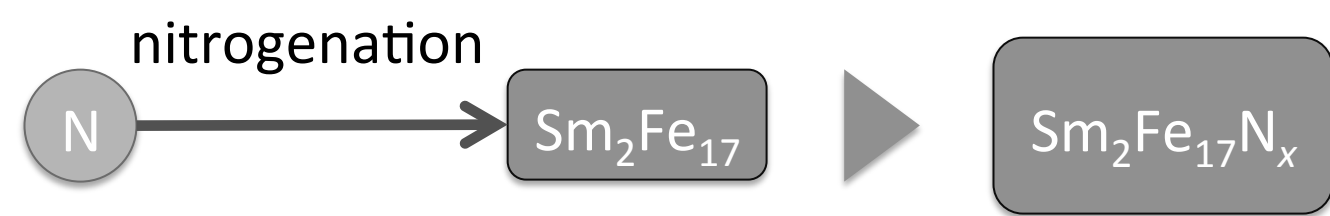
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Introduction

Magnetic properties of $\text{Sm}_2\text{Fe}_{17}\text{N}_3$

Material	$\text{Sm}_2\text{Fe}_{17}\text{N}_3$	$\text{Nd}_2\text{Fe}_{14}\text{B}$
saturation M_s (T)	1.54	1.60
anisotropy m_0H_a (T)	26	7
Curie temperature T_c (°C)	479	315

Properties are good as well as NdFeB.

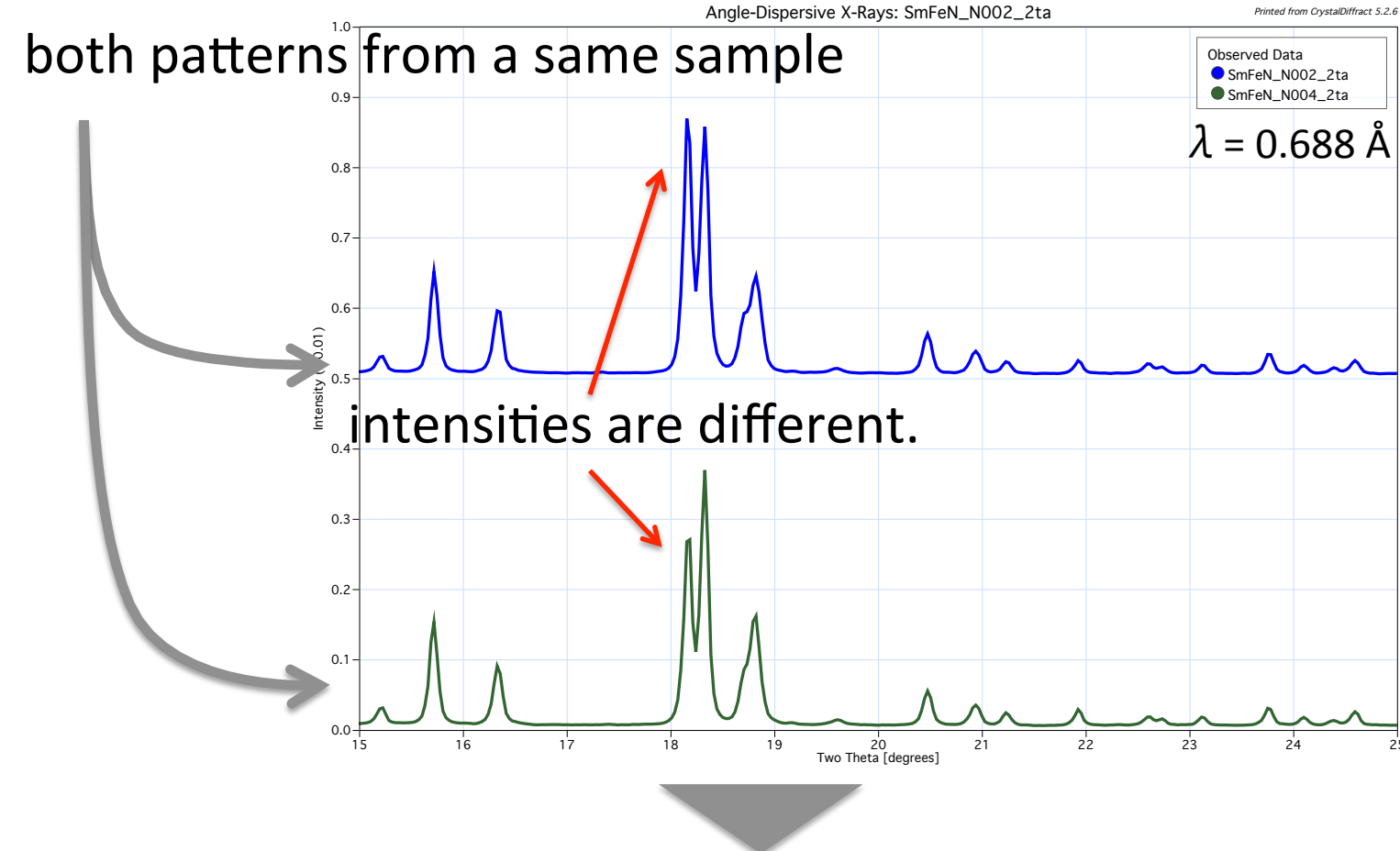


Lattice constants are changed by an amount of inserted nitrogen.

Investigation of the crystal structure is necessary to study magnetic properties.

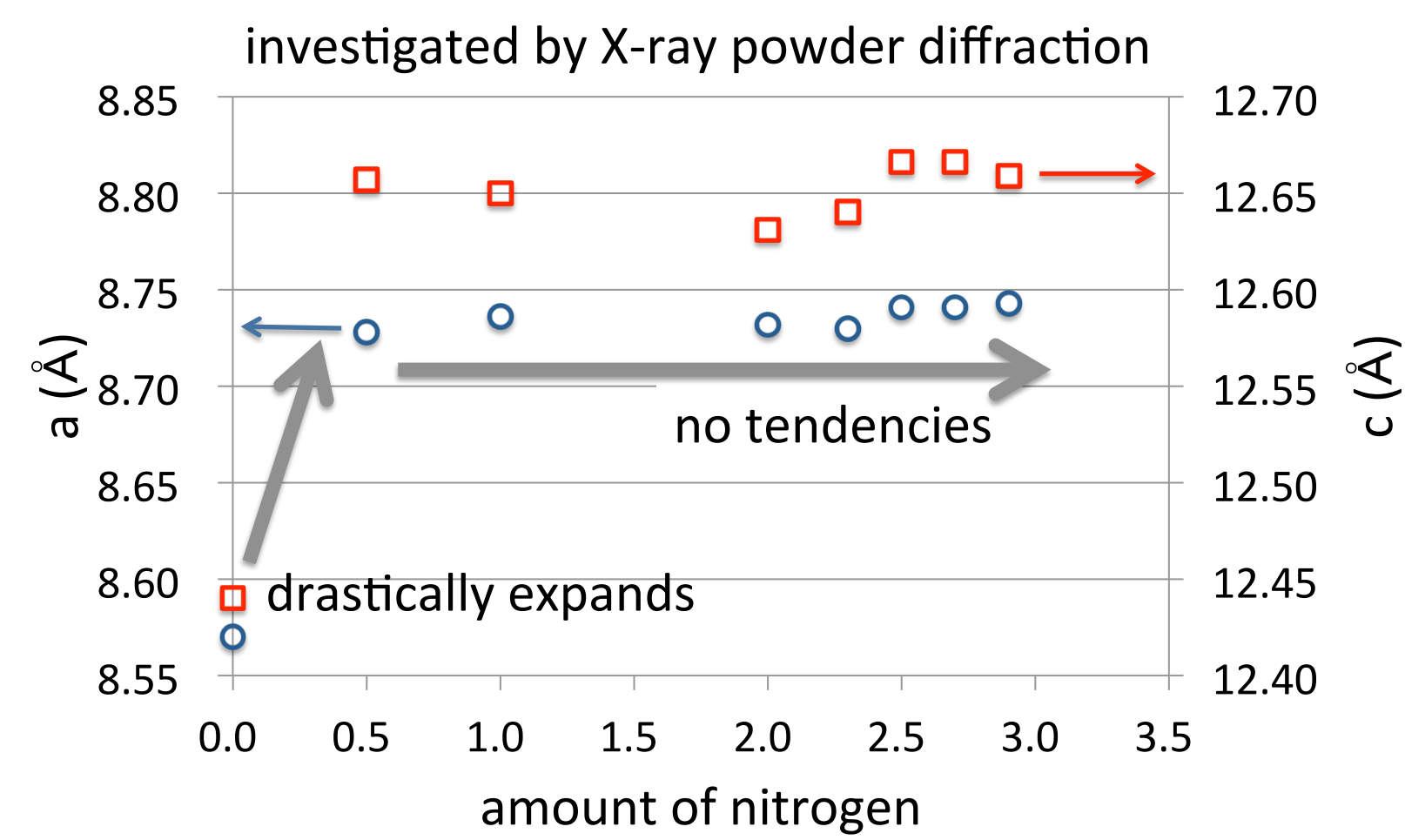
Powder diffraction patterns of a $\text{Sm}_2\text{Fe}_{17}\text{N}_x$ sample

both patterns from a same sample



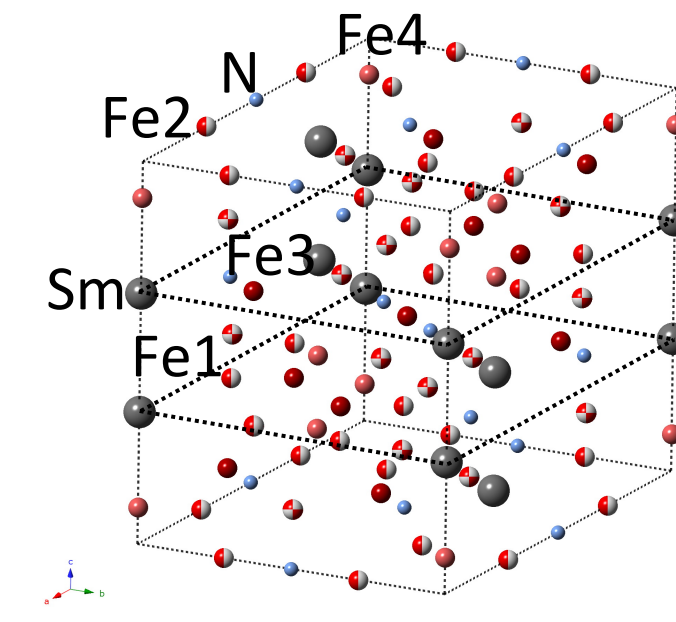
Crystal structure was not converged by Rietveld analysis.

Lattice constants of $\text{Sm}_2\text{Fe}_{17}\text{N}_x$ ($x = 0.0 - 2.9$)



Crystal structure of $\text{Sm}_2\text{Fe}_{17}\text{N}_x$ ($x = 0.5 - 2.9$)

Atomic site positions of each $\text{Sm}_2\text{Fe}_{17}\text{N}_x$ are same.



Fe1	18h	x	0.50536
		y	0.49464
		z	0.15126
Fe2	18f	x	0.2807
Fe3	9d	x	0.5
		z	0.5
Fe4	6c	z	0.0954
Sm	6c	z	0.34548
N	9e	x	0.5

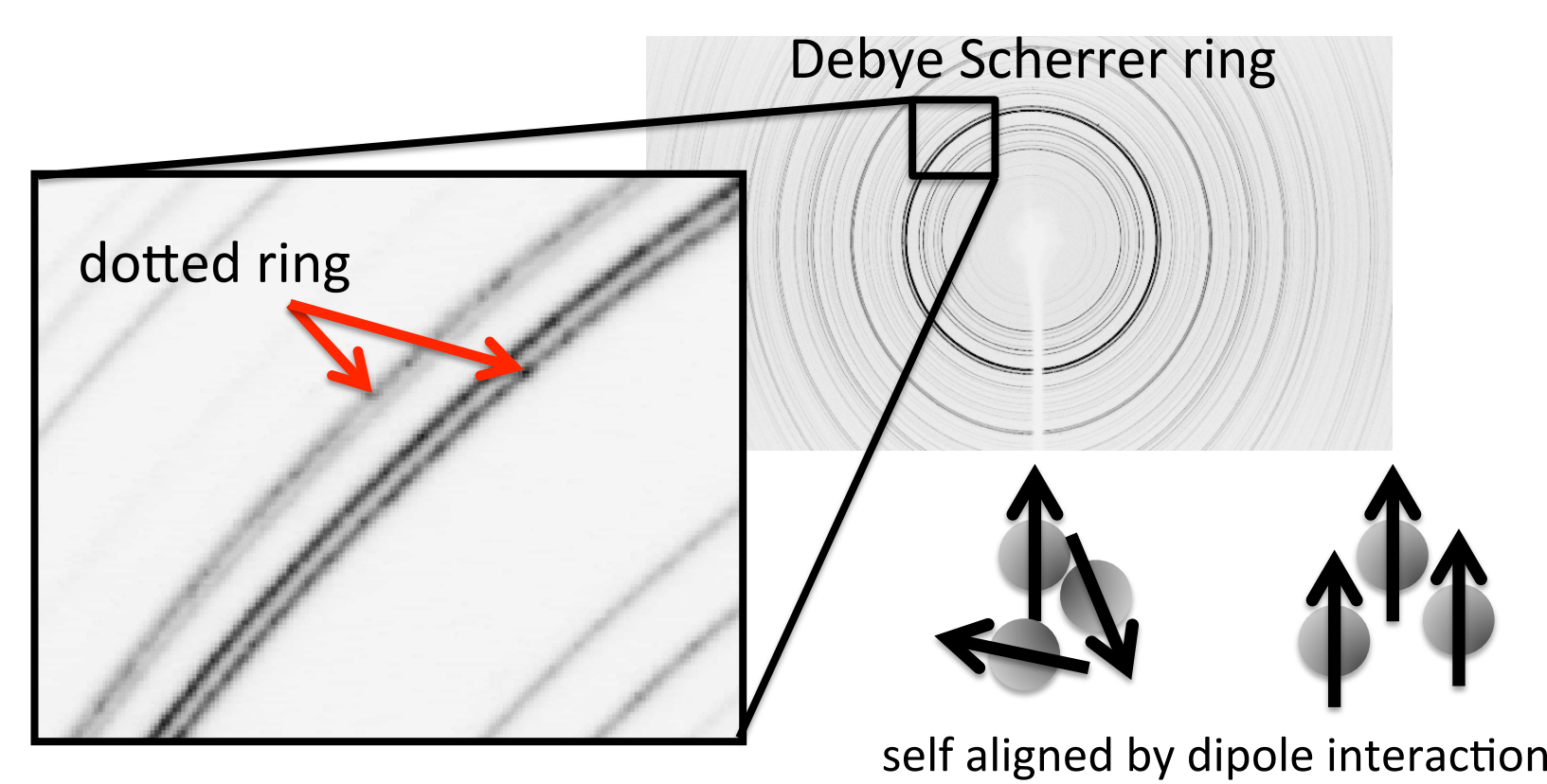
No refinements are performed in almost any previous reports. The reason is difficulty of crystal structure analysis with ferromagnetic powder samples.

purpose

We conduct to

- 1) develop a micromanipulation system for picking a single crystal particle,
- 2) analyze a single crystal structure of $\text{Sm}_2\text{Fe}_{17}\text{N}_x$ fine particles.

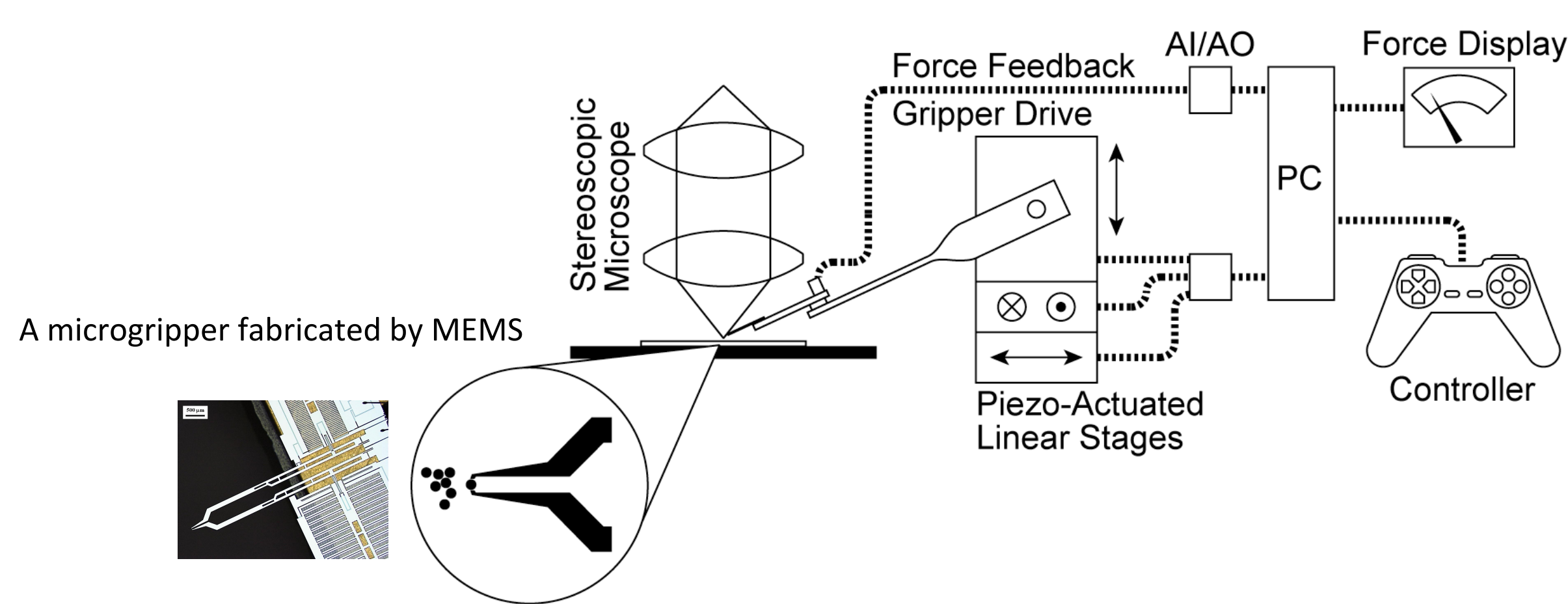
Why difference powder diffraction in same samples?



It is necessary to measure X-ray diffraction with a **single crystal**.

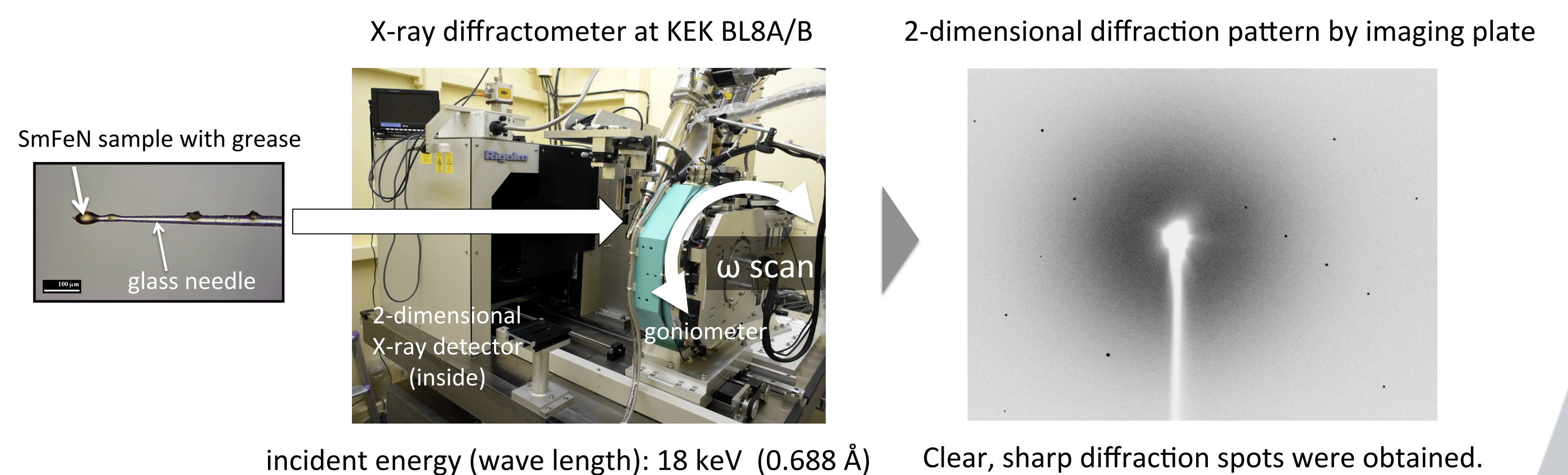
Experimental methods

micromanipulation system for picking a fine particle



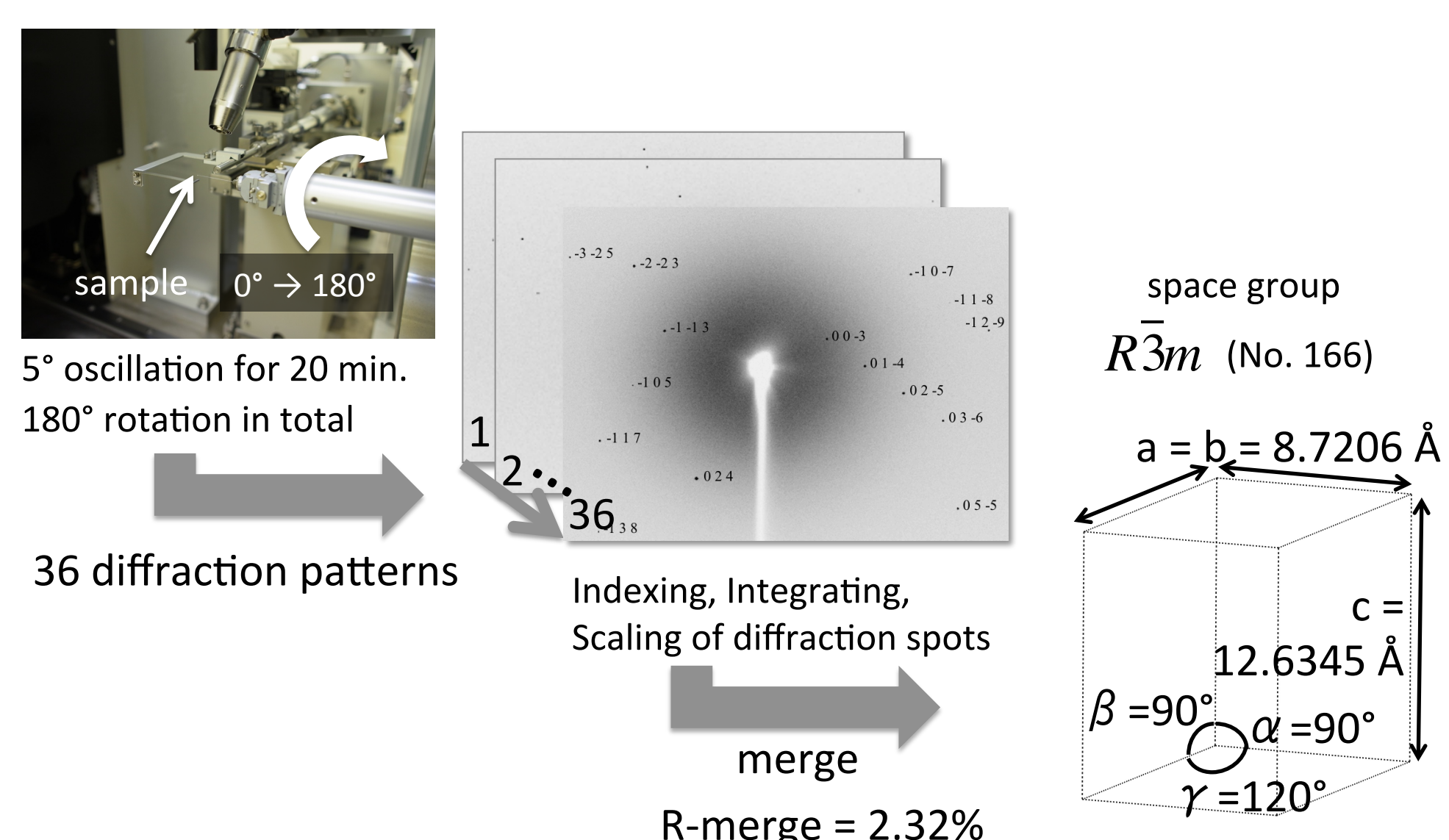
It enable us to pick a particle of approximately $10 \mu\text{m}$.

X-ray diffraction measurement



Results and discussion

Lattice constants of $\text{Sm}_2\text{Fe}_{17}\text{N}_x$



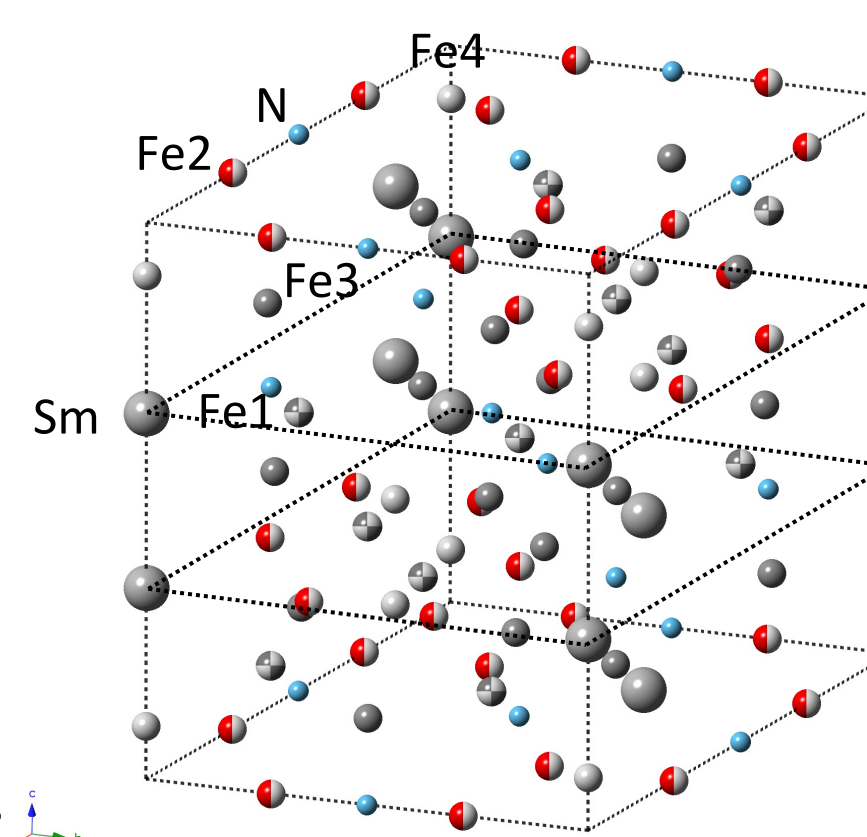
Single crystal structure analysis of $\text{Sm}_2\text{Fe}_{17}\text{N}_x$

R-factor = 1.94%, wR2 = 2.47%, Goodness of Fit = 0.831

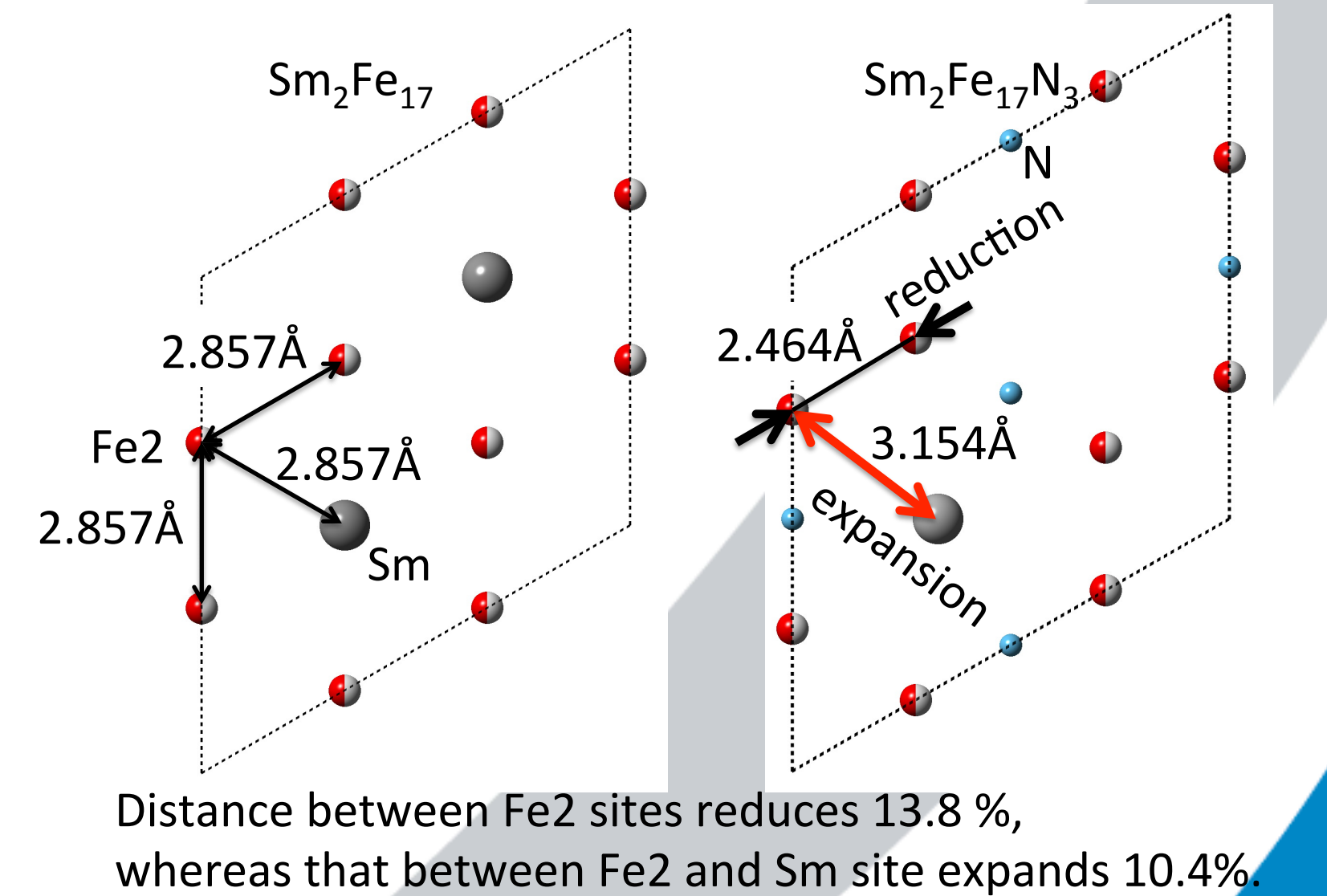
N occupancy was slightly changed, and the value converged on 1.0. \rightarrow nitrogen = 3

			$\text{Sm}_2\text{Fe}_{17}$	$\text{Sm}_2\text{Fe}_{17}\text{N}_3$
Fe1	18h	x	0.5	0.504819
		y	0.5	0.495179
		z	0.16667	0.152431
Fe2	18f	x	0.33333	0.282628
Fe3	9d	x	0.5	0.5
		z	0.5	0.5
Fe4	6c	z	0.097	0.094825
Sm	6c	z	0.33333	0.343085
N	9e	x	-	0.5

Each atomic site in $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ was determined. The Fe2 (18f) site shifts largely from $\text{Sm}_2\text{Fe}_{17}$.



Difference of distances between Fe-Fe and Fe-Sm



Summary

- We have developed a micromanipulation system for picking a fine particle. We succeeded to pick a single crystal $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ particle.
- We conducted X-ray diffraction of a single $\text{Sm}_2\text{Fe}_{17}\text{N}_x$ particle. We also succeeded to determine a single crystal structure of a single $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ particle.
- In the future, this method enable us to analyze relation between crystal structure and magnetic properties with difference amount of nitrogen.