

Anion-excess Bixbyite $\text{Gd}_2\text{Ce}_2\text{O}_7$: Effect of Radiation on Anion Sublattice

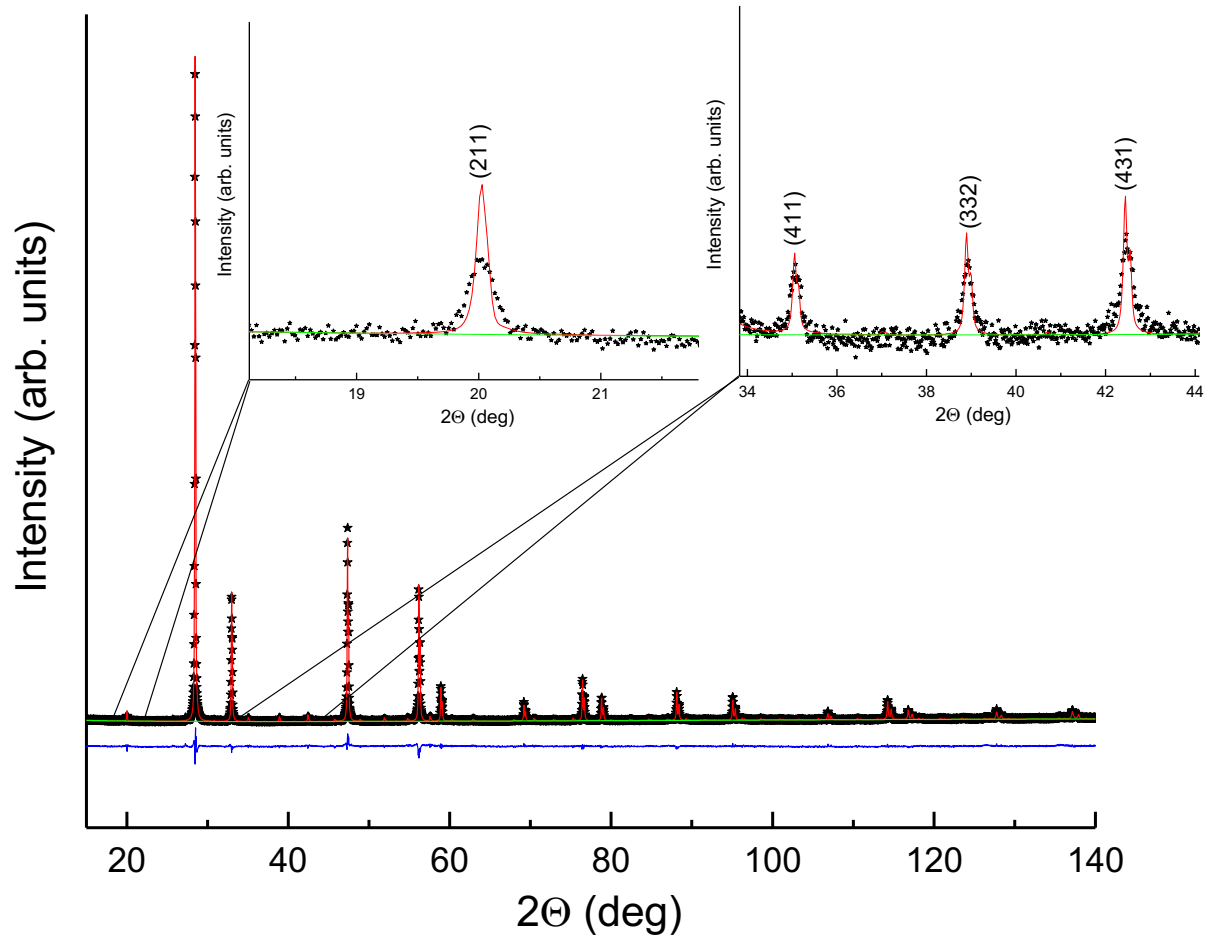
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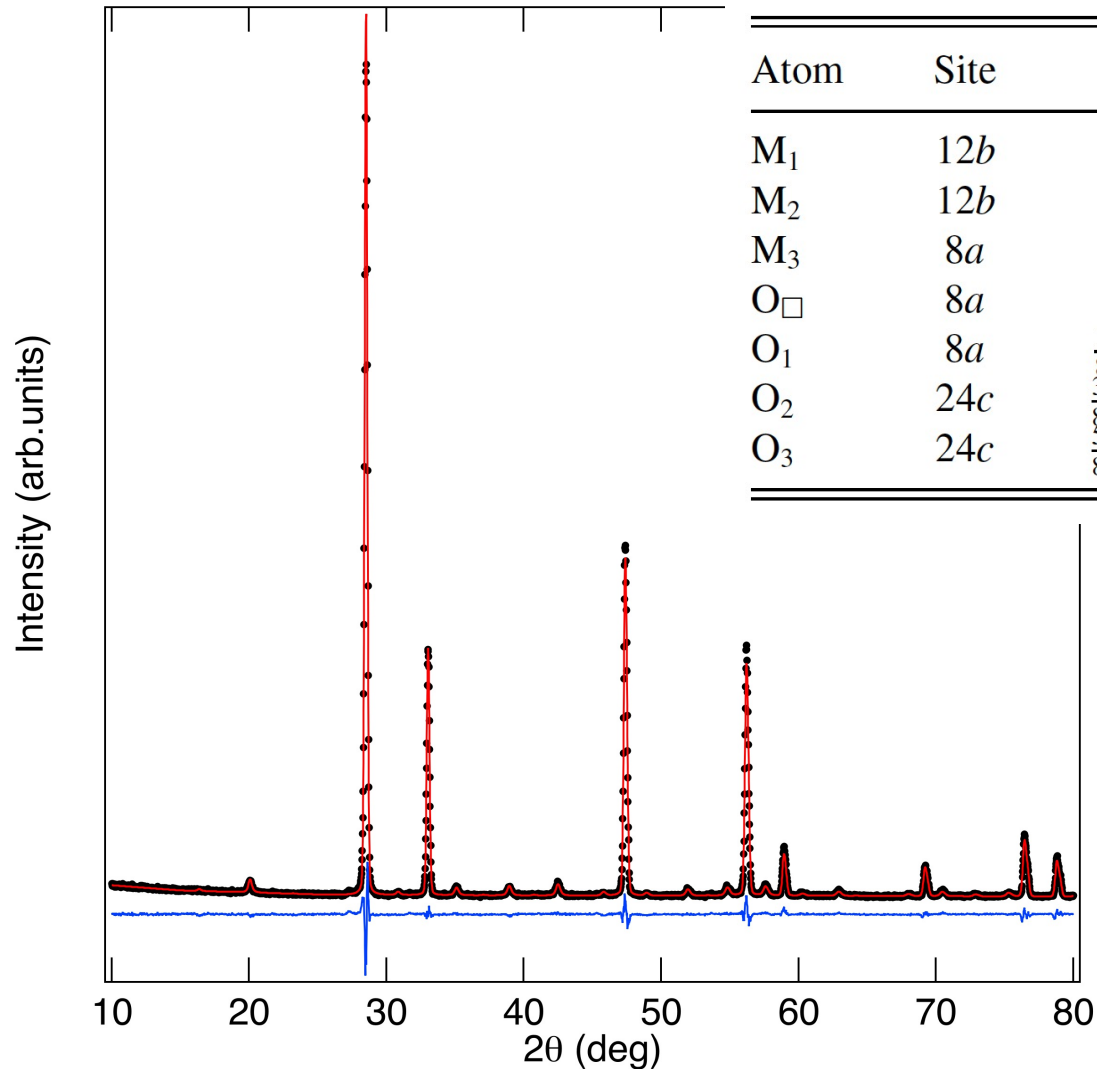
University of Liverpool, Los Alamos National Lab. and Université Paris-Saclay, CentraleSupélec

Recap on fitting XRD patterns $\text{Gd}_2\text{Ce}_2\text{O}_7$



Cations randomly distributed over two sites in an ideal disordered bixbyite
Space Group $Ia\bar{3}$

Rietveld refinements of $\text{Gd}_2\text{Ce}_2\text{O}_7$



Atom	Site	x/a	y/a	z/a	Occupancy
M_1	$12b$	$-\beta$	0	$\frac{1}{4}$	1
M_2	$12b$	β	0	$\frac{3}{4}$	1
M_3	$8a$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	1
O_{\square}	$8a$	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$	0
O_1	$8a$	$\frac{1}{8} + \gamma$	$\frac{1}{8} + \gamma$	$\frac{1}{8} + \gamma$	1
O_2	$24c$	$\frac{1}{8} + \delta_1$	$\frac{1}{8} + \delta_2$	$\frac{1}{8} + \delta_3$	1
O_3	$24c$	$\frac{1}{8} - \delta_1$	$\frac{1}{8} - \delta_2$	$\frac{1}{8} - \delta_3$	1

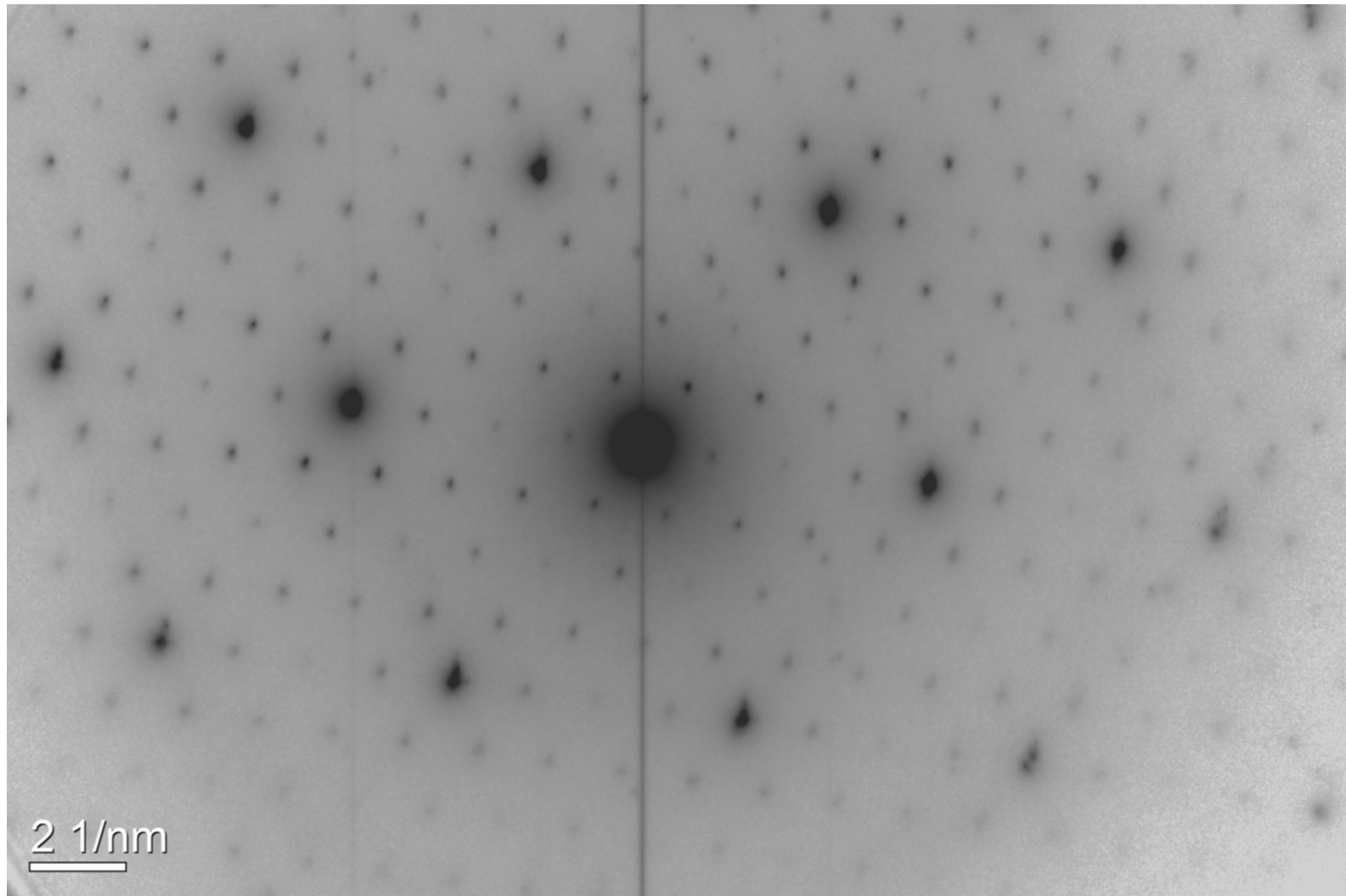
Space Group $I2_13$

$a \approx 10.85 \text{ \AA}$

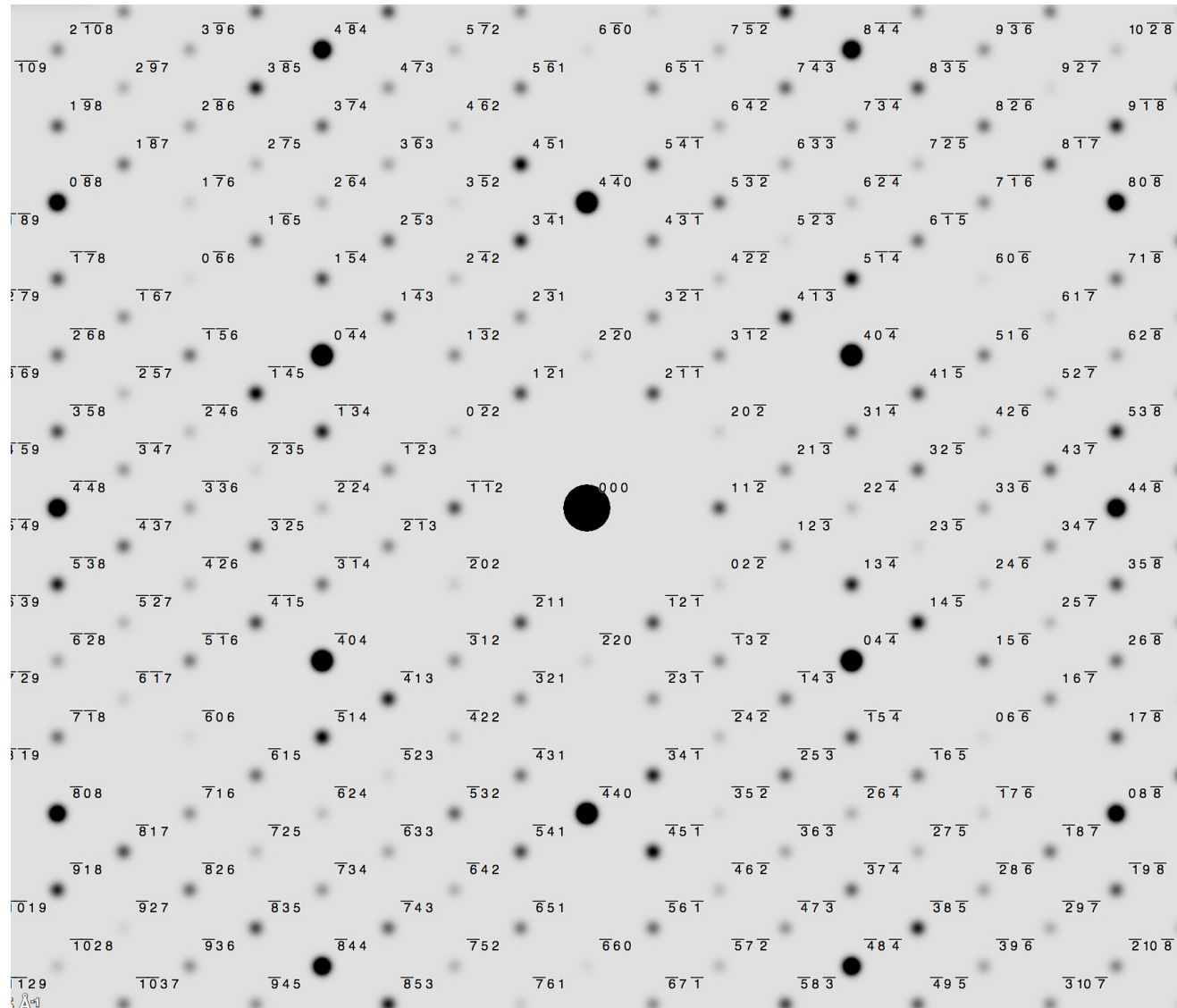
$Z = 32$

Diffused scattering by correlated microdomains
R. B. Neder et.al. Acta Cryst. A 46 (1990) 792

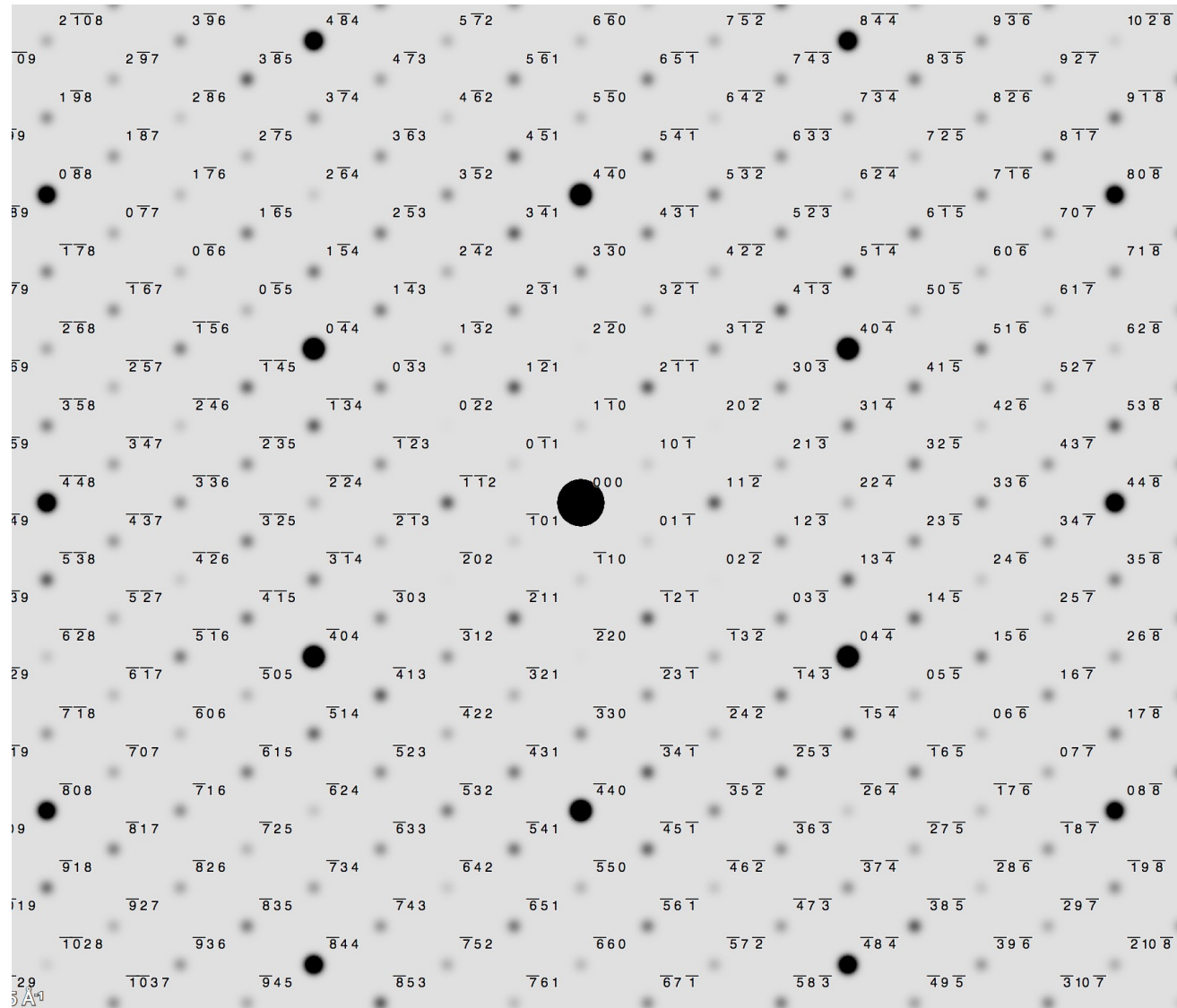
SAED from powdered $\text{Gd}_2\text{Ce}_2\text{O}_7$



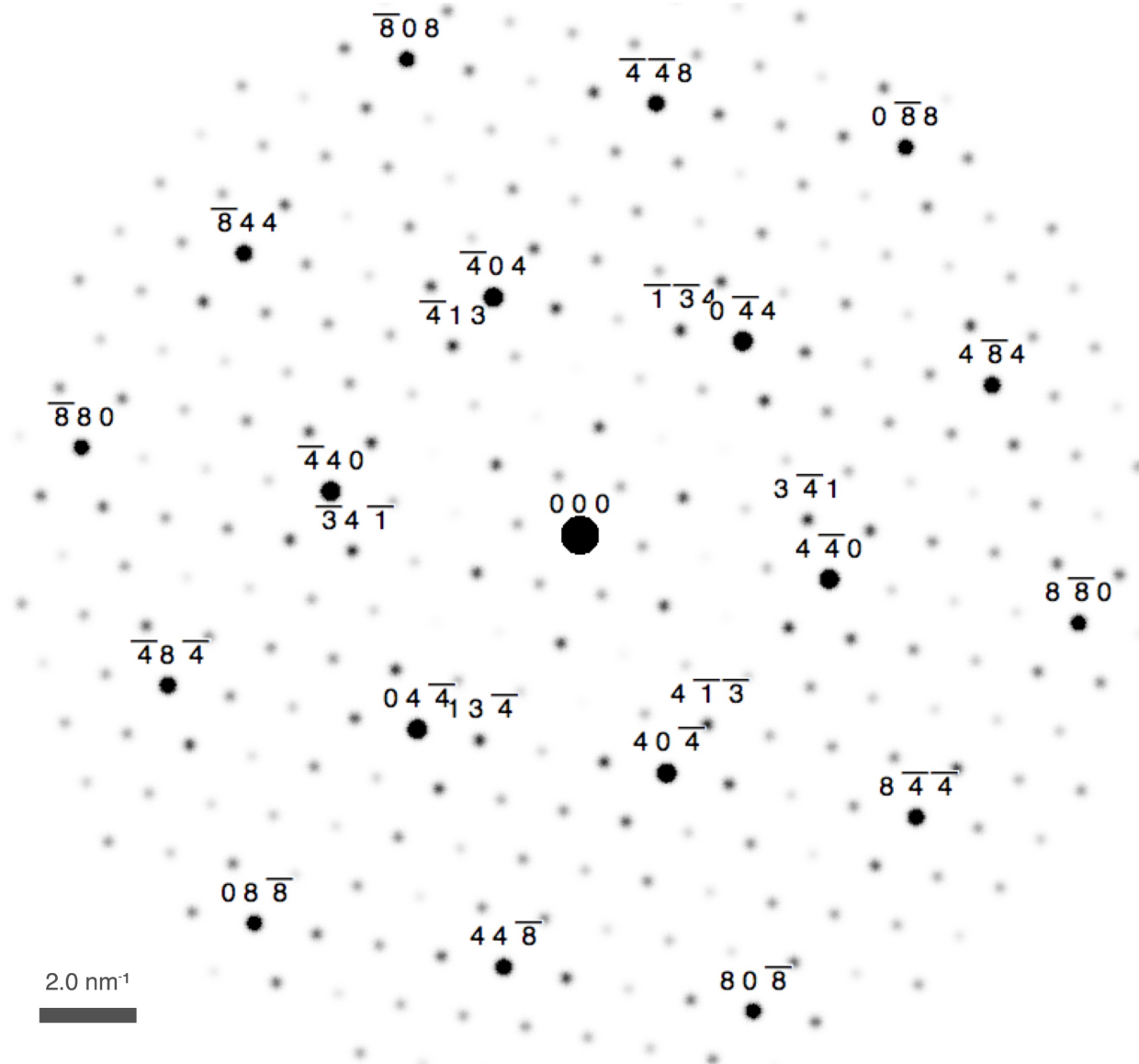
True Bixbyite



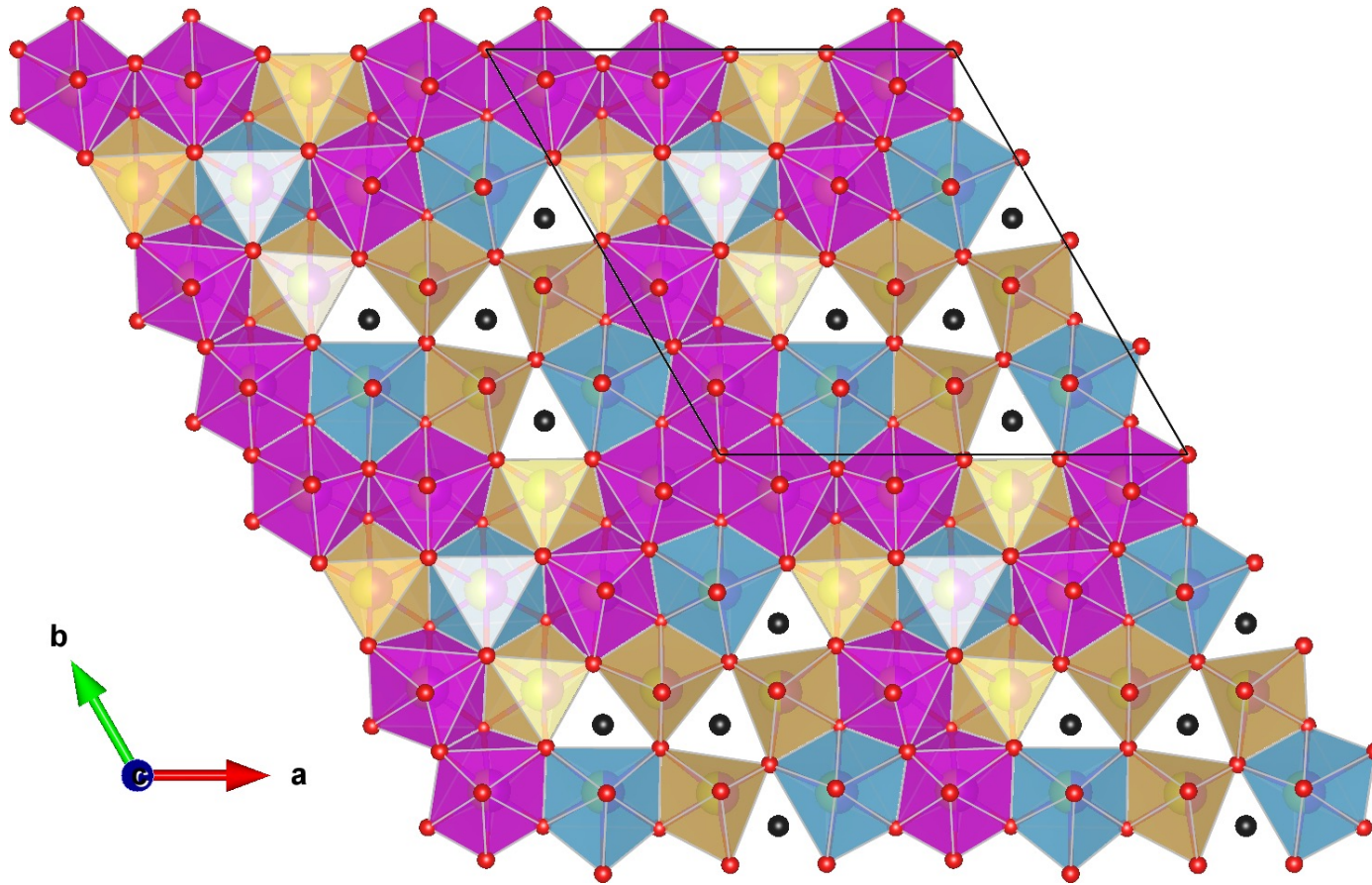
Anion excess Bixbyite



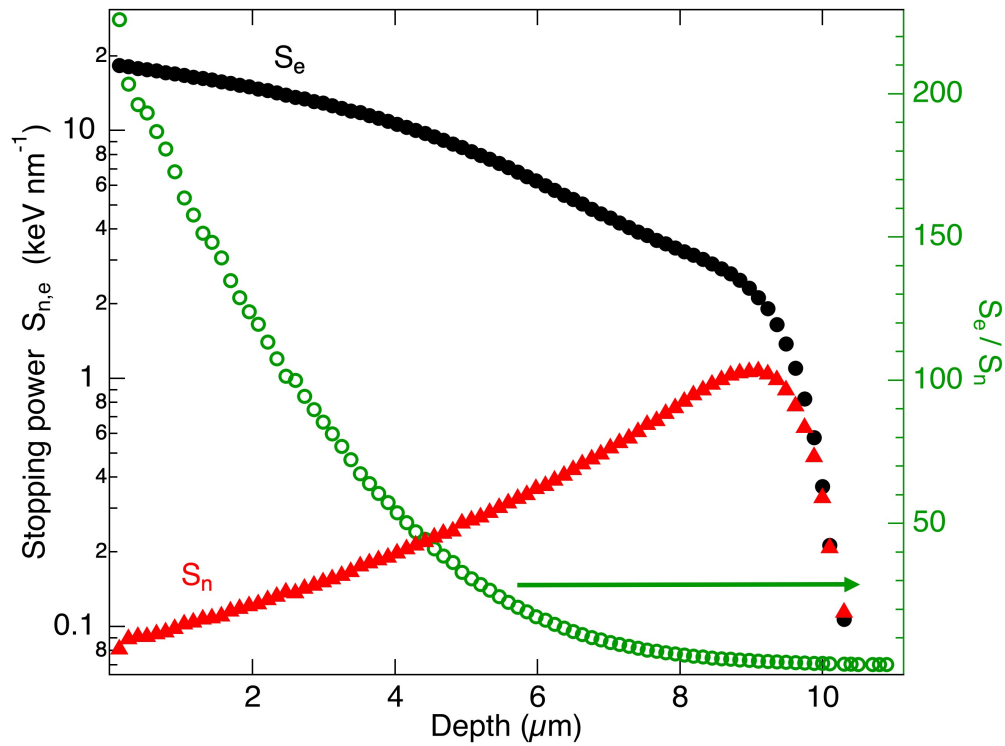
Simulated SAED $\text{Gd}_2\text{Ce}_2\text{O}_7$



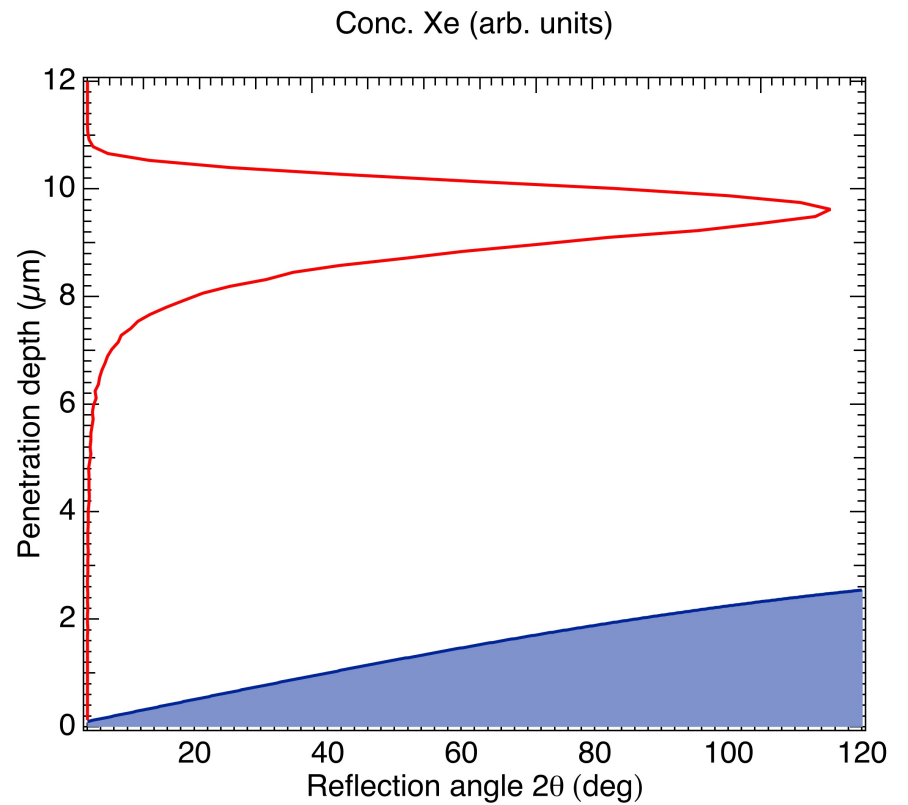
Polyhedral model: anion excess bixbyite



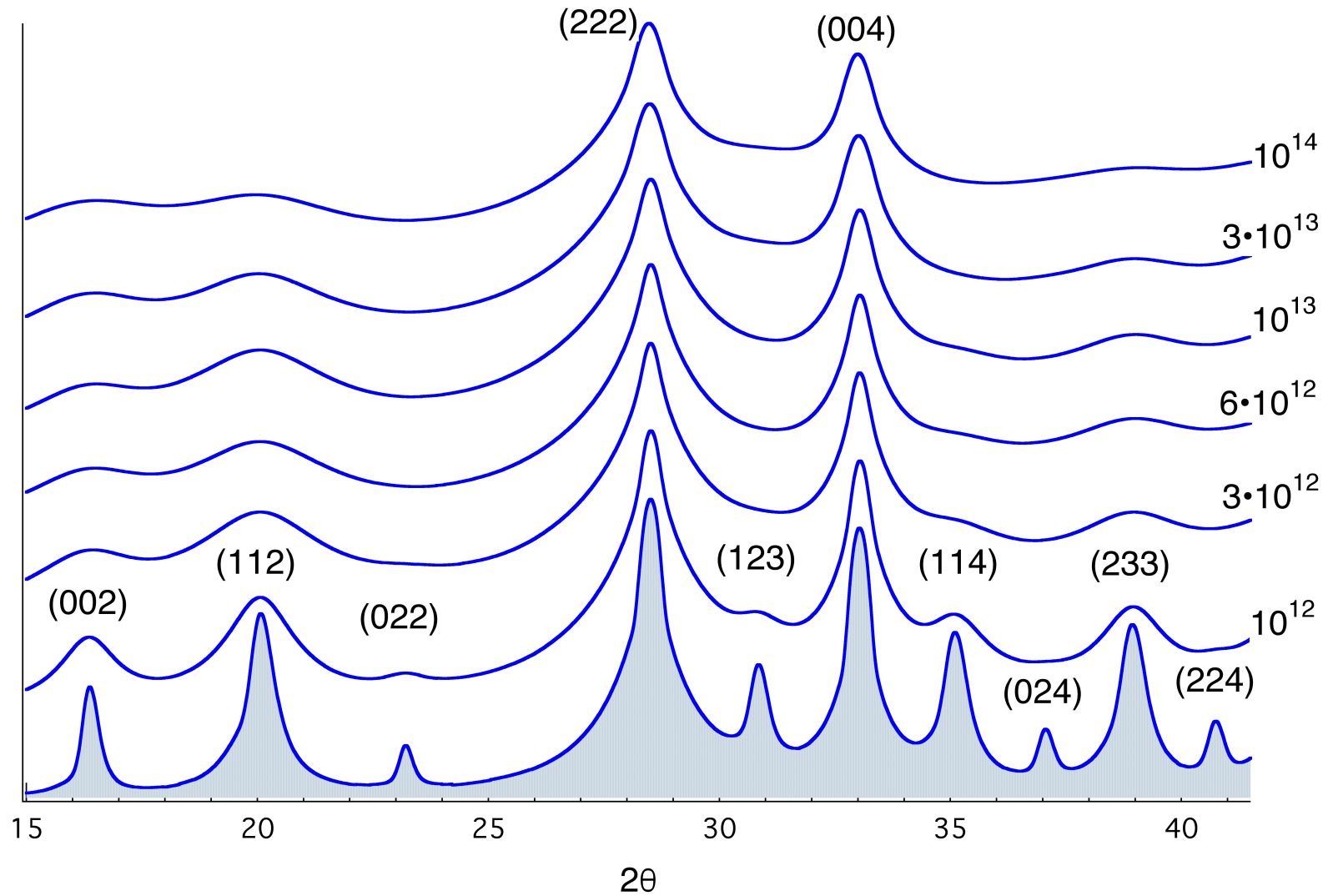
Swift Heavy Ion (SHI) irradiations



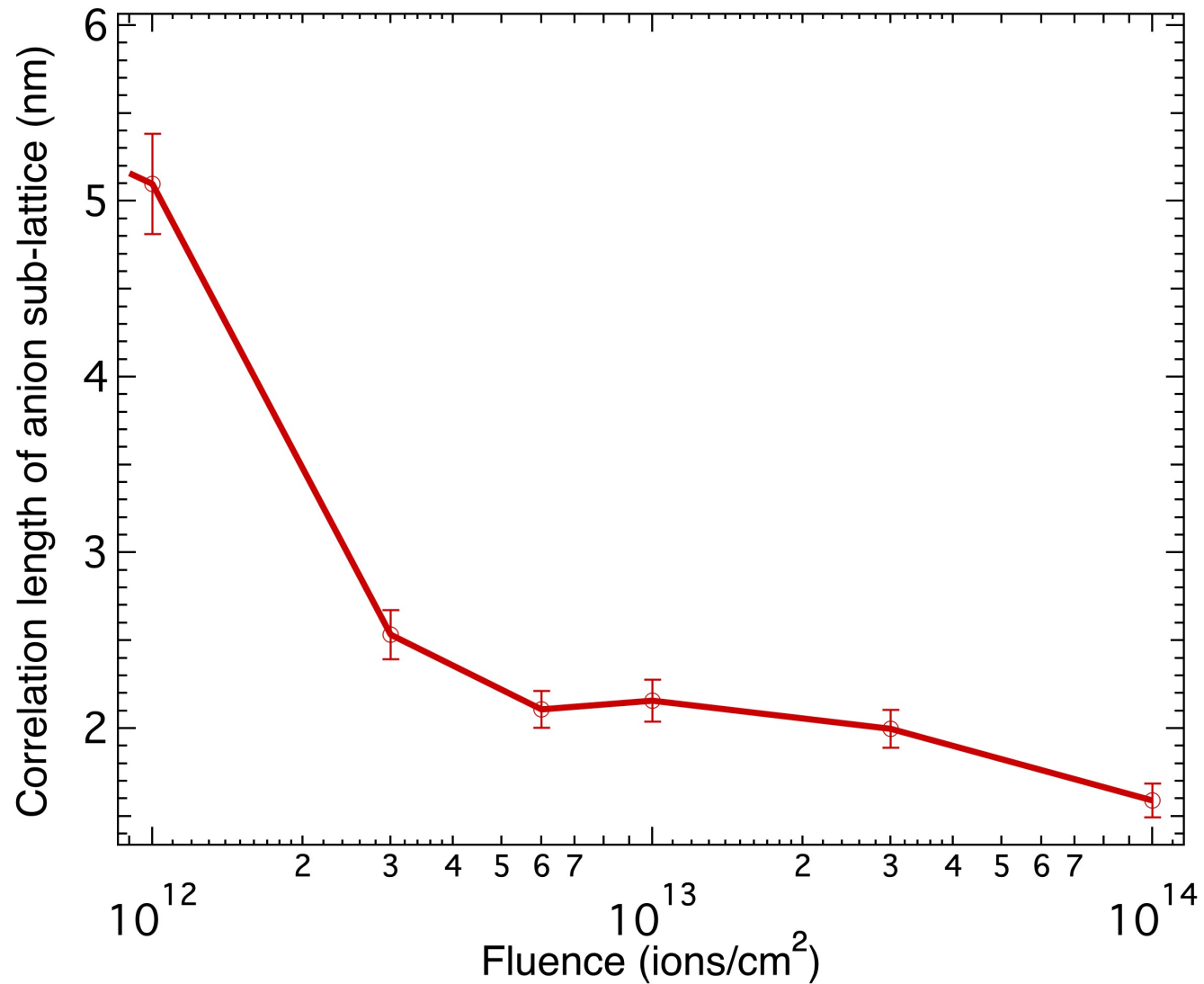
92 MeV Xe ions



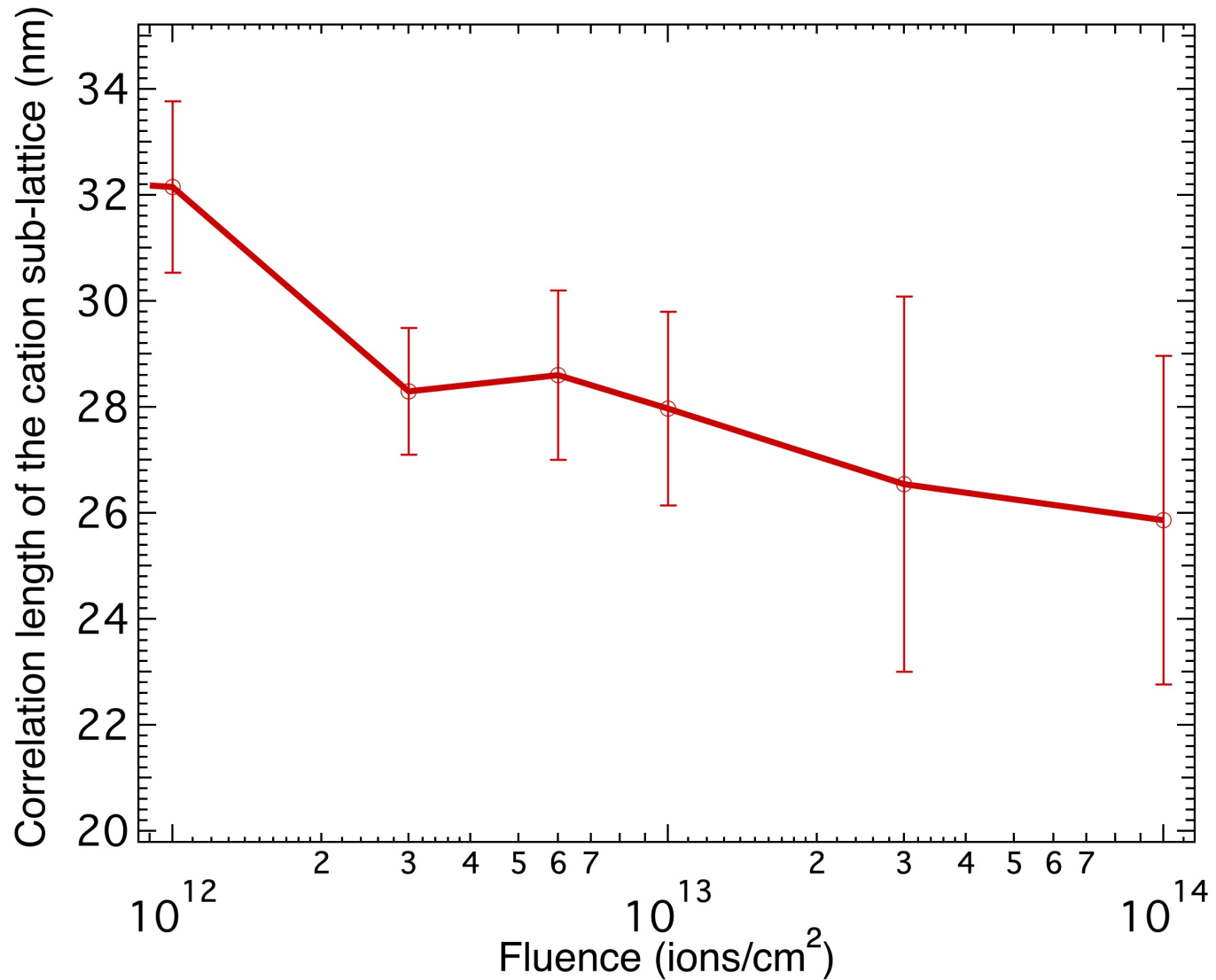
Raw XRD patterns as a function of fluence (ions/cm²)



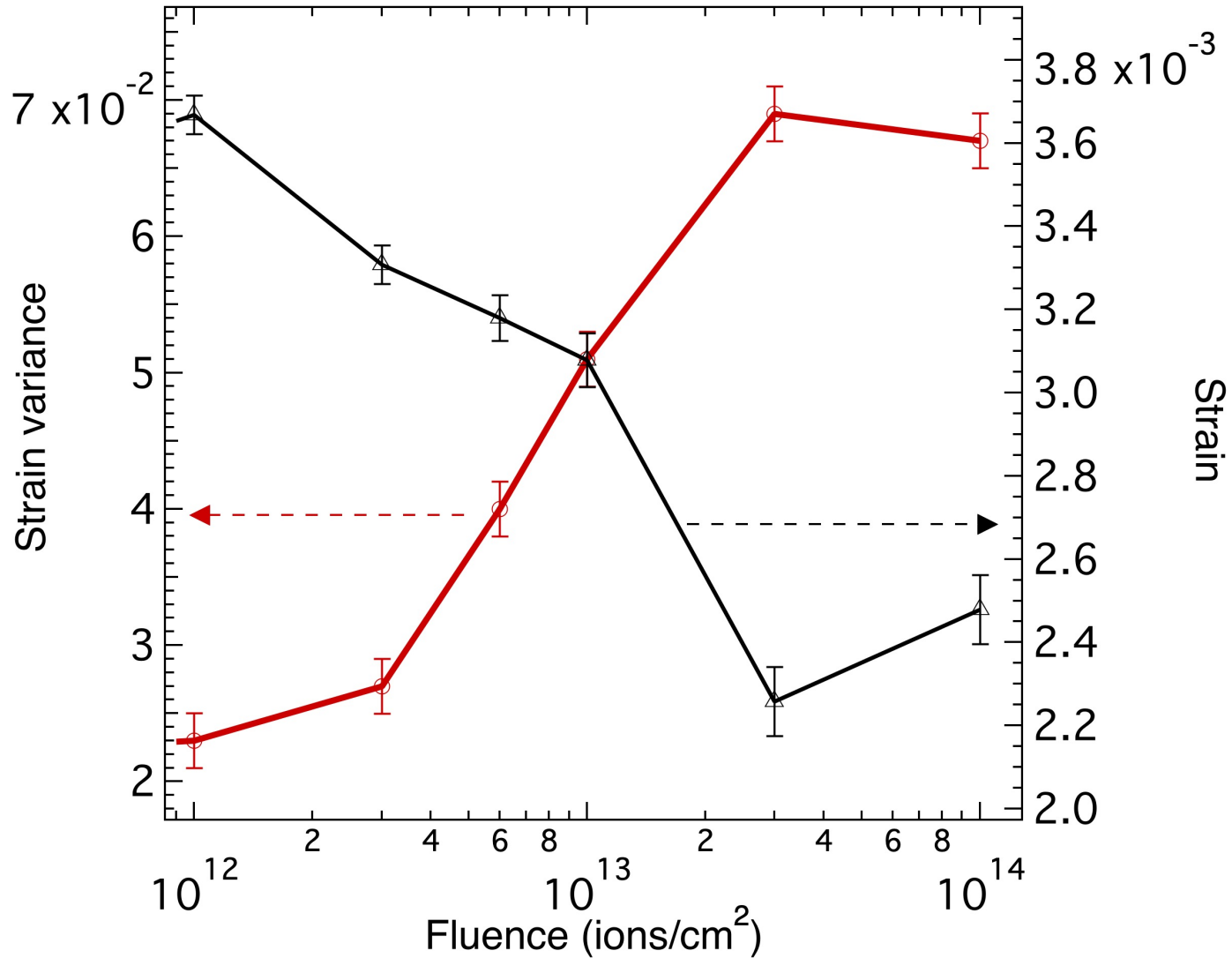
Anion sublattice (micro domain size)



Length scale for periodic arrangement of average cations



Lattice strain and microstrain



Conclusions

$\text{Gd}_2\text{Ce}_2\text{O}_7$ crystallizes in an anion 'excess' bixbyite structure

SHI studies to understand the behaviour of anion v/s cation sublattice

Topological disorder on the anion sublattice grows faster than that on the cation sublattice

The microstructural response at increasing radiation fluences leads to a decrease of the strain after an initial increase

While the variance of the strain increases following the increase of the microdomain wall density.

Thank you..

Apologies for not attending the meeting in-person

-Maulik