Today's outline - October 05, 2021

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- Information about:

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  (a) Final presentation

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Reading Assignment: Chapter 5.2–5.3

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Reading Assignment: Chapter 5.2–5.3

Homework Assignment #04:
Chapter 4: 2,4,6,7.10
due Tuesday, October 19, 2021

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Reading Assignment: Chapter 5.2–5.3

Homework Assignment #04:
Chapter 4: 2,4,6,7.10
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Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

Final presentation

1. Choose paper for presentation

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2. Clear it with me!

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4. Prepare a 15 minute presentation

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5. Be ready for questions!

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6. Make sure to give reasonable answers forall the questions
7. Put me as one of the investigators of the proposal

SAXS review

The SAXS scattered intensity from a dilute solution depends on the single particle form factor, $\mathcal{F}(\vec{Q})$, the volume of the particle, V_p, and the density difference from the solvent, $\Delta\rho = (\rho_{sl,p} - \rho_{sl,0})$

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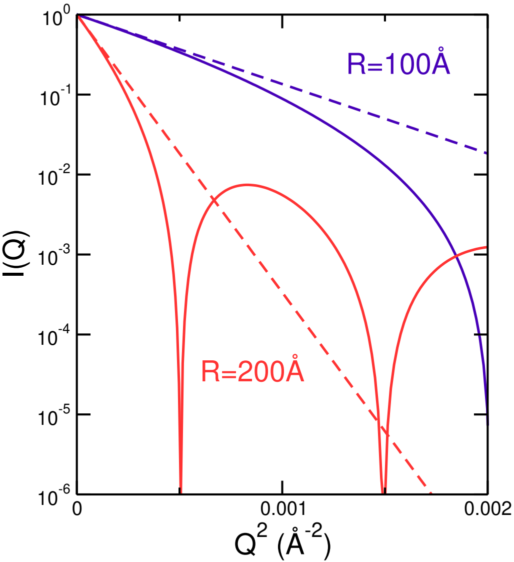

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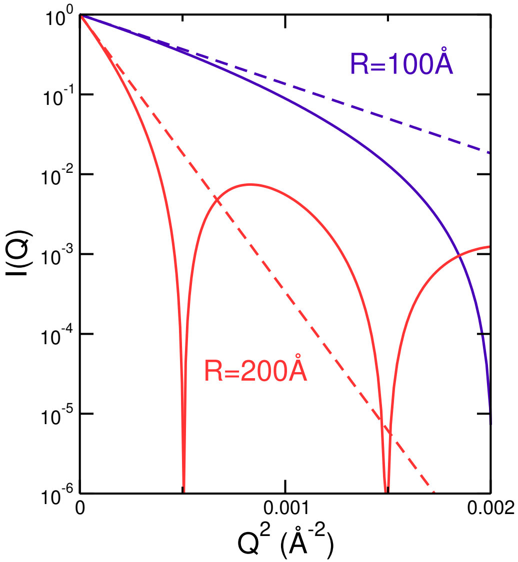
$$R_g^2 = \frac{\int_{V_p} \rho_{sl,p}(\vec{r}) r^2 dV_p}{\int_{V_p} \rho_{sl,p}(\vec{r}) dV_p}$$



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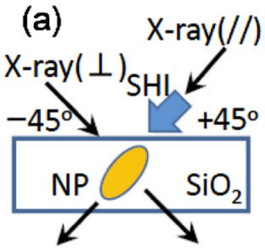

Expt. geometry

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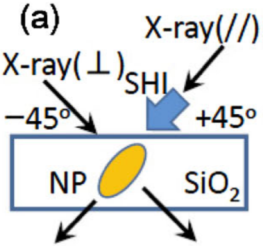

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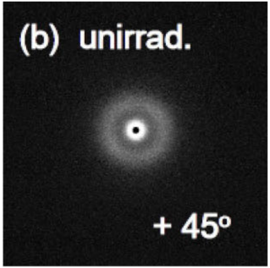

Unirradiated

"Shape elongation of embedded Zn nanoparticles induced by swift heavy ion irradiation: A SAXS study", H. Amekura, K. Kono, N. Okubo, and N. Ishikawa, *Phys. Status Solidi B* **252**, 165-169 (2015).

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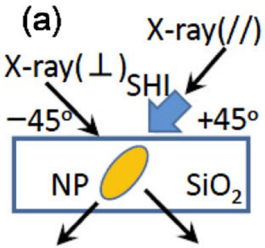

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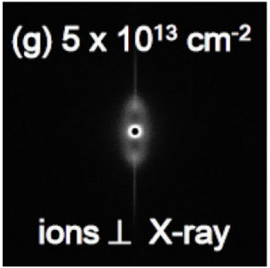
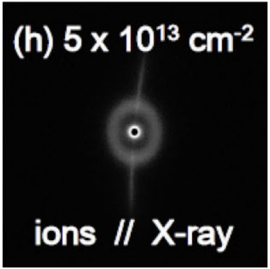


Irradiated $\perp$ x-rays



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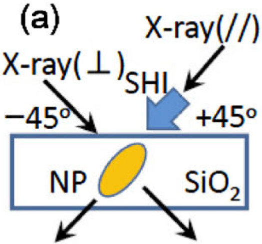

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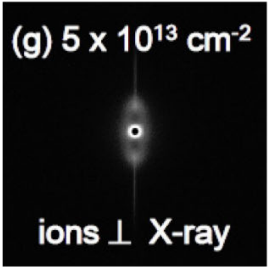

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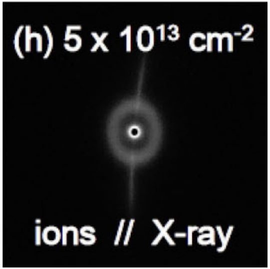

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Straight lines from ion tracks, seen in both directions and which persist to the highest fluences.

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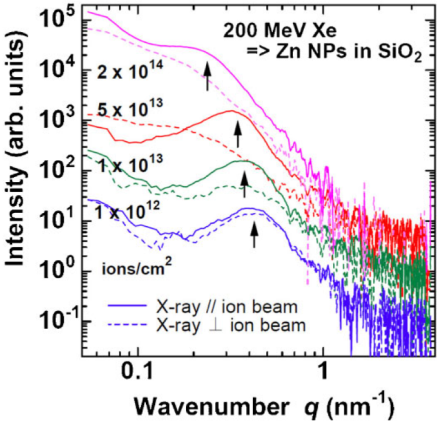

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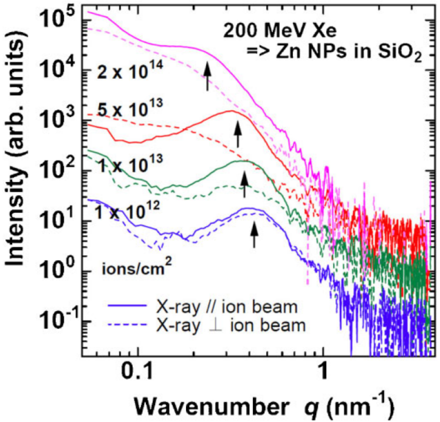

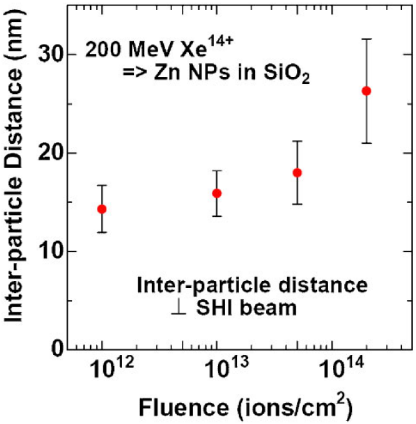

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Interparticle distance increases as a function of irradiation fluence

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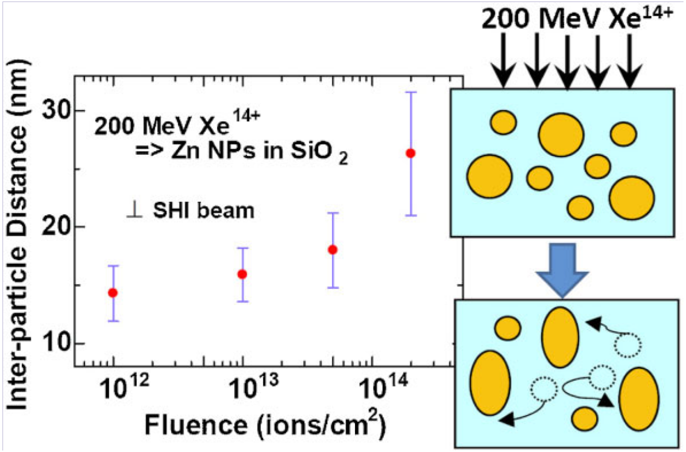

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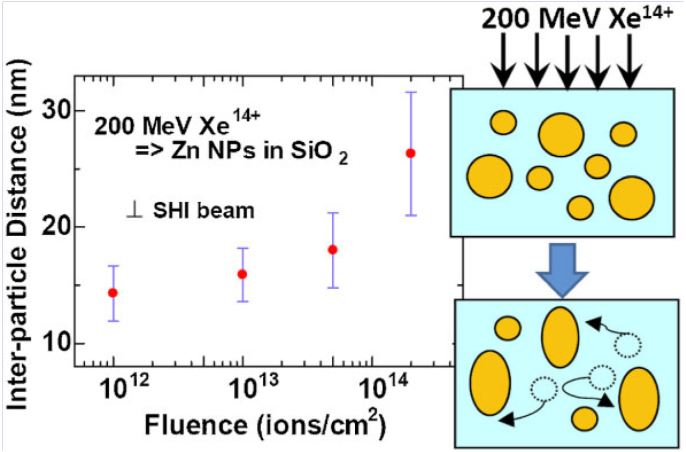
Growth of interparticle spacing is due to dissolution and re-agglomeration with fluence leading to larger interparticle spacings



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Nucleation & growth of glycine

Can SAXS help us understand the nucleation and growth of a simple molecule which is the prototype for pharmaceutical compounds?

"SAXS study of the nucleation of glycine crystals from a supersaturated solution," S. Chattopadhyay et al. *Crystal Growth Design* **5**, 523-527 (2004)

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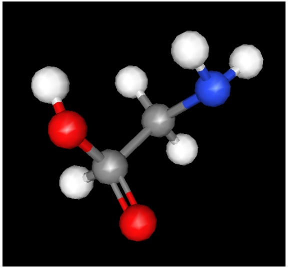

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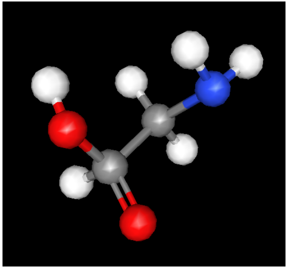

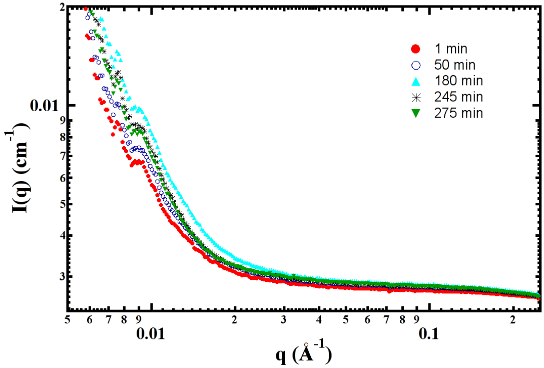

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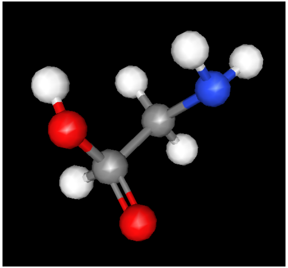

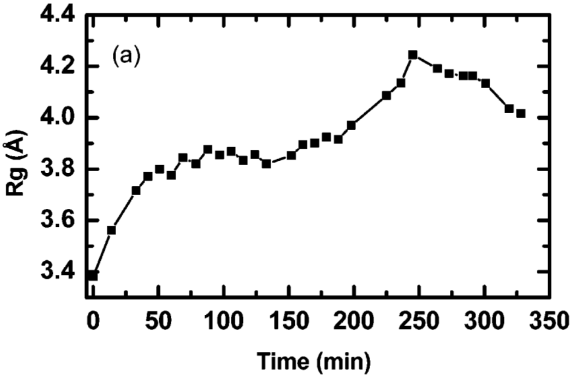

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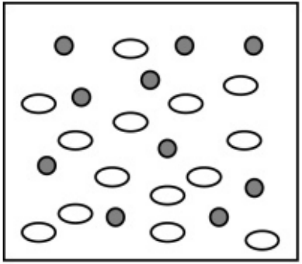

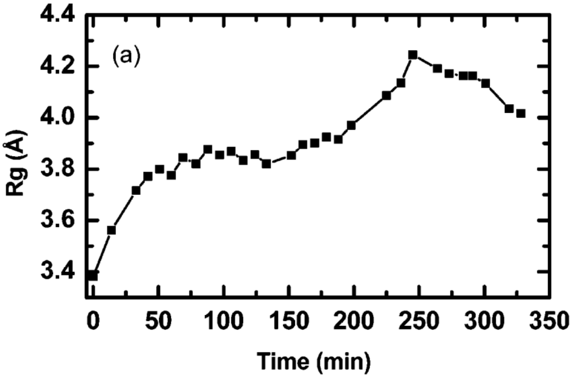

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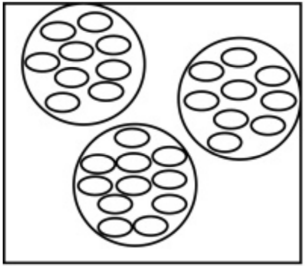

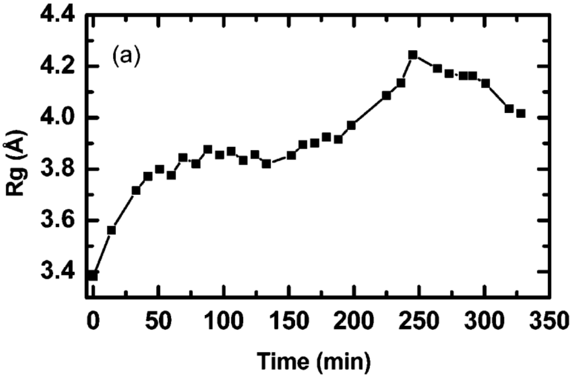

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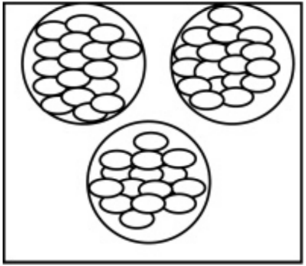

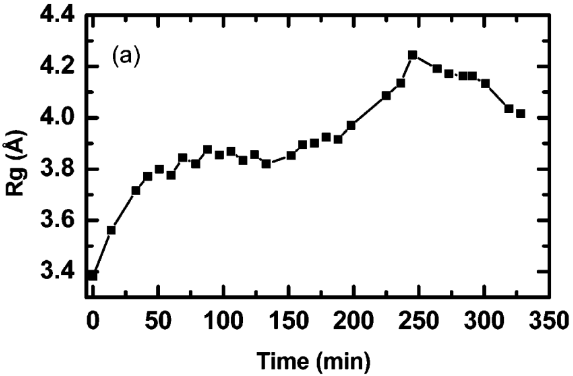

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Different polymorphs are produced under varying conditions so study extended to both neutral and acidic solutions

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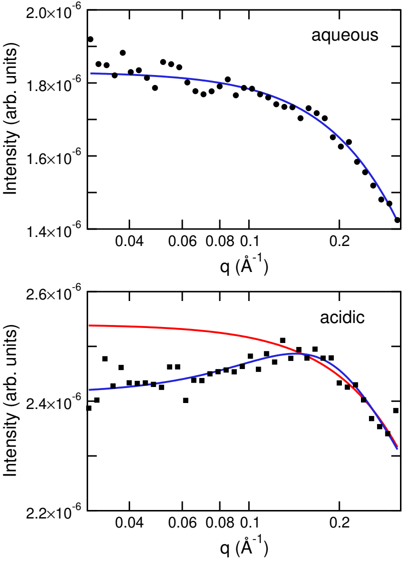

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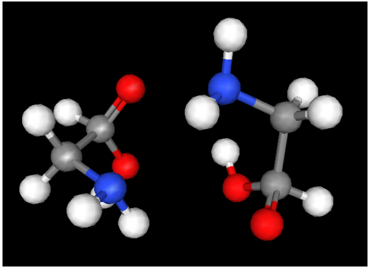

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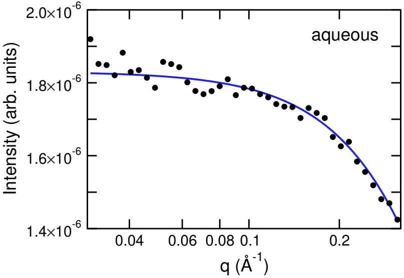

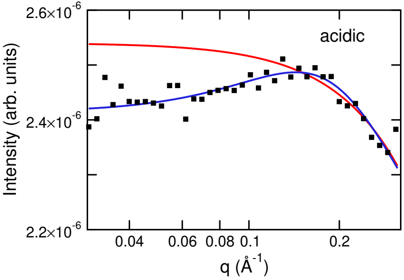

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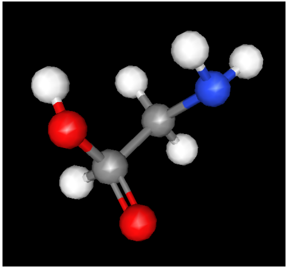

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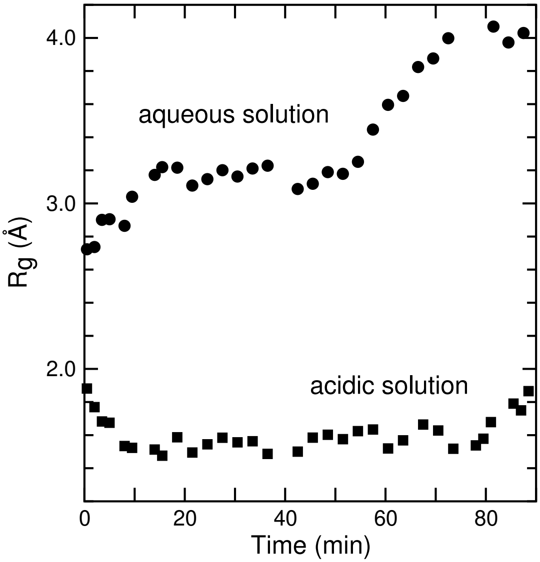

In aqueous solution, R_g implies dimerization and increases due to aggregation until crystallization

"Relationship between self-sssociation of glycine molecules in supersaturated solution and solid state outcome",
D. Erdemir et al. *Phys. Rev. Lett.* **99**, 115702 (2007)

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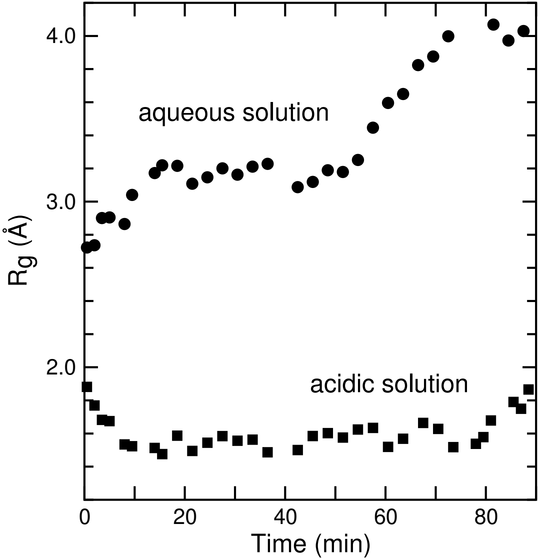

In aqueous solution, R_g implies dimerization and increases due to aggregation until crystallization

In acidic solution, Rg remains small and implies that no dimerization or aggregation occurs before nucleation

"Relationship between self-sssociation of glycine molecules in supersaturated solution and solid state outcome",
D. Erdemir et al. *Phys. Rev. Lett.* **99**, 115702 (2007)

Size exclusion chromatography SAXS

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Mathew, Mirza & Menhart, "Liquid-chromatography-coupled SAXS for accurate sizing of aggregating proteins," *J. Synchrotron Rad.* **11**, 314-318 (2004) developed a technique which is now being used routinely in biological SAXS, called Size Exclusion Chromatography SAXS.

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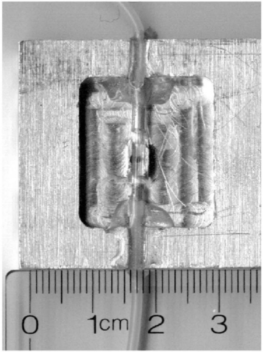

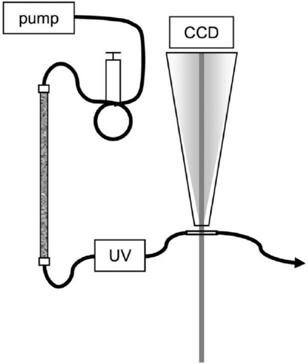

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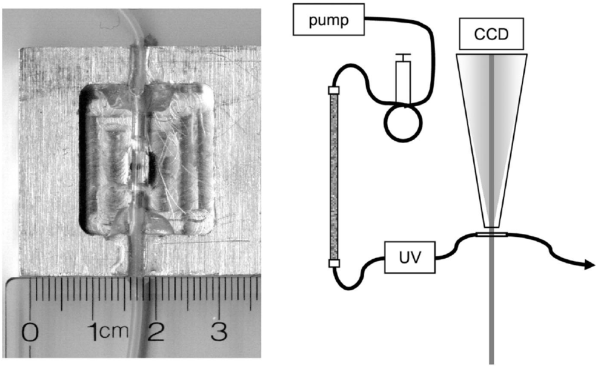

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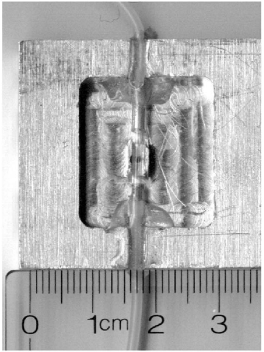

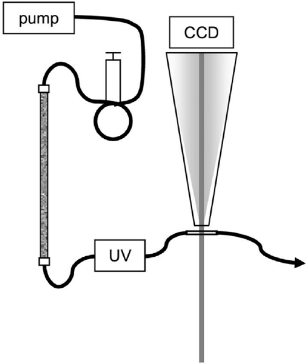

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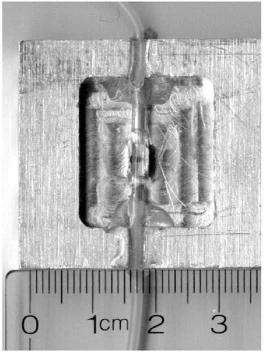

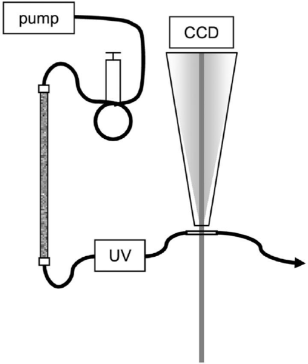

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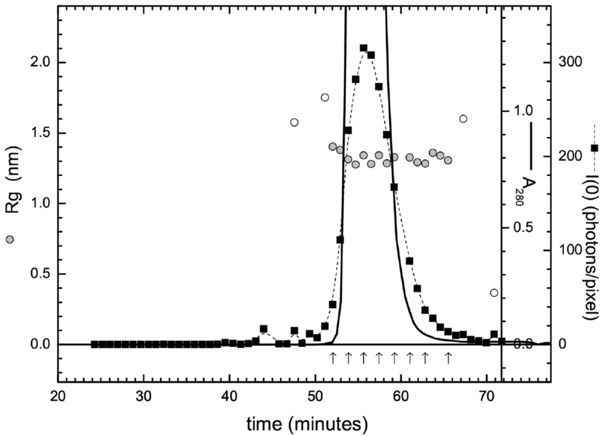

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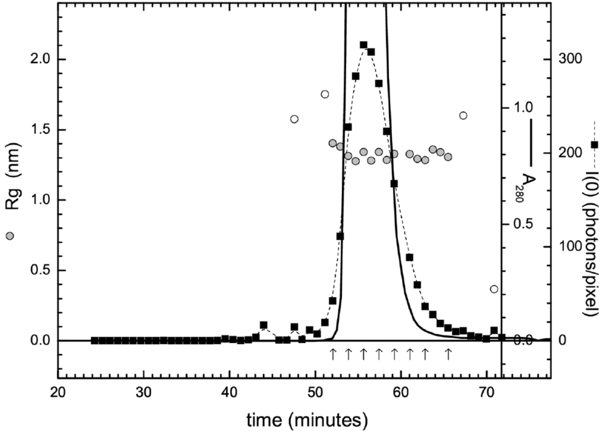

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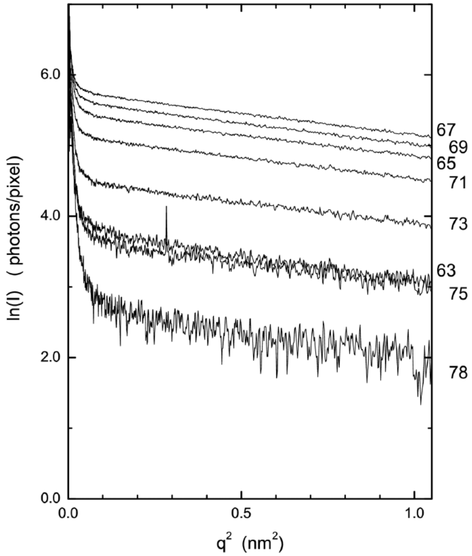

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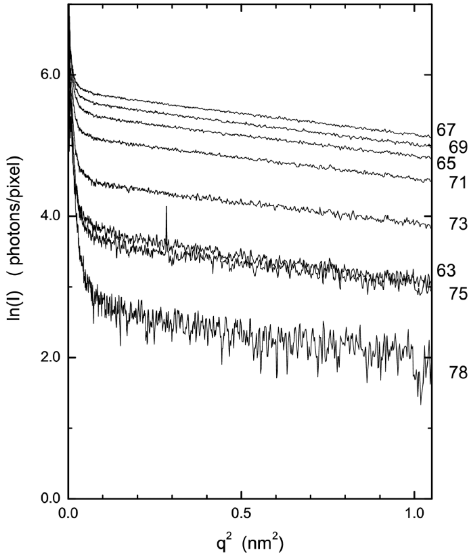

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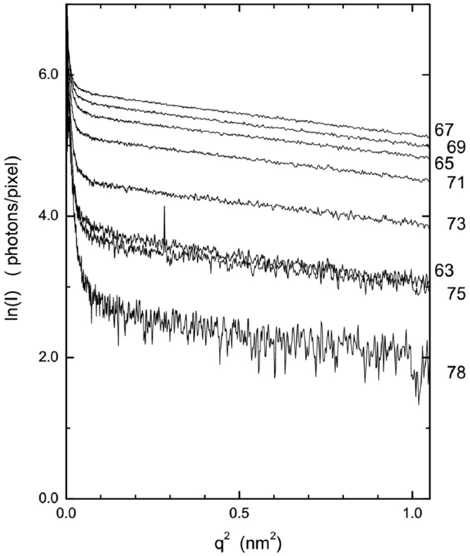

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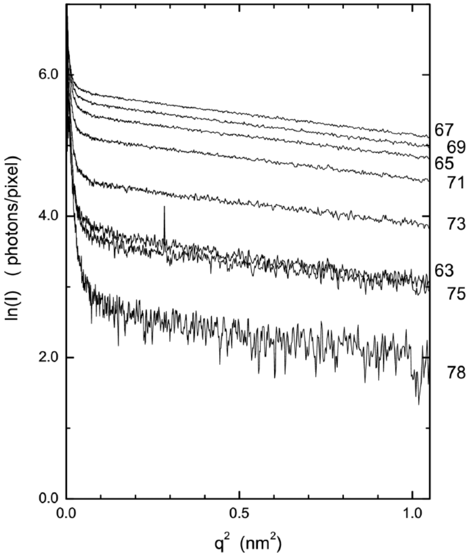

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Even lowest intensity data set gives a consistent R_g.

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Plasminogen & 3-component mixture

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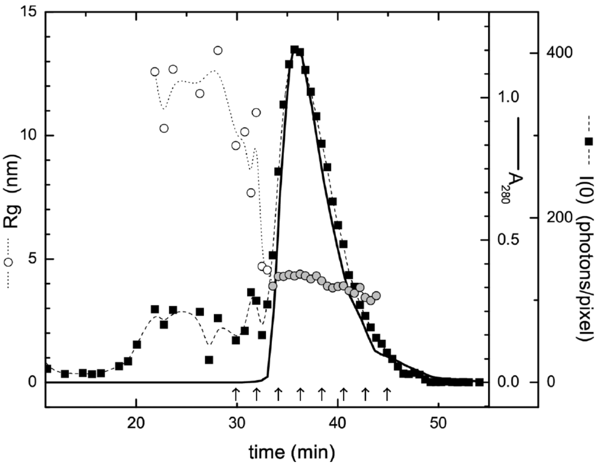

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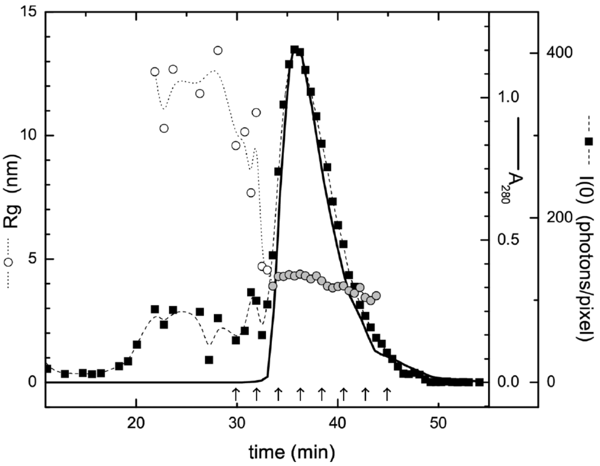

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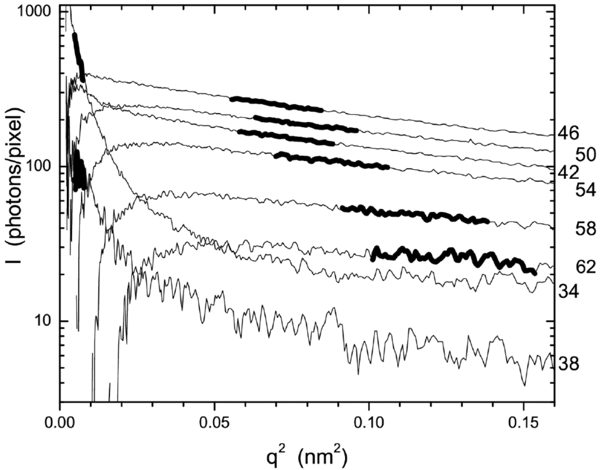

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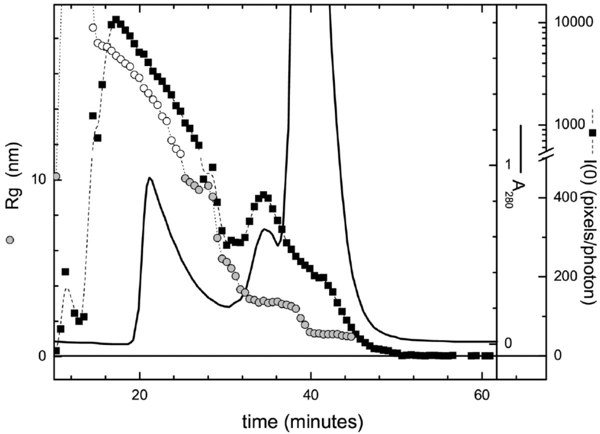
The three components show consistent R_g and can be individually identified despite the overlap.



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Porosity in CaO calcination

SAXS was used to study the nature of the porosity and particle sizes of CaO obtained by calcining $CaCO_3$.

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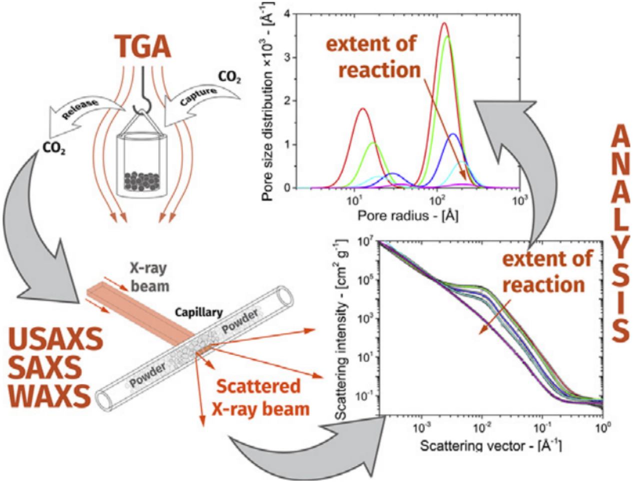

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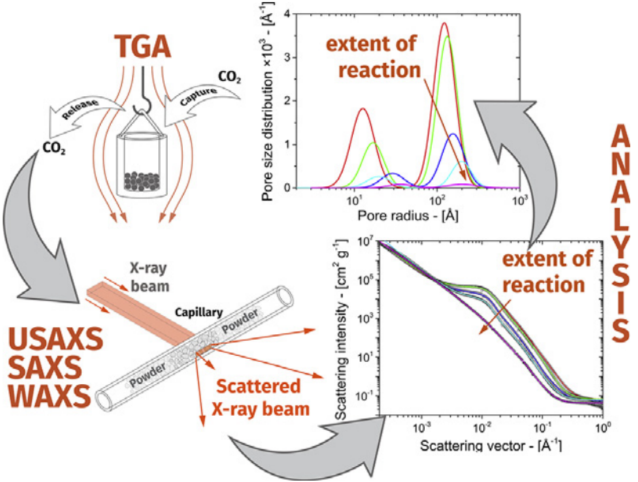

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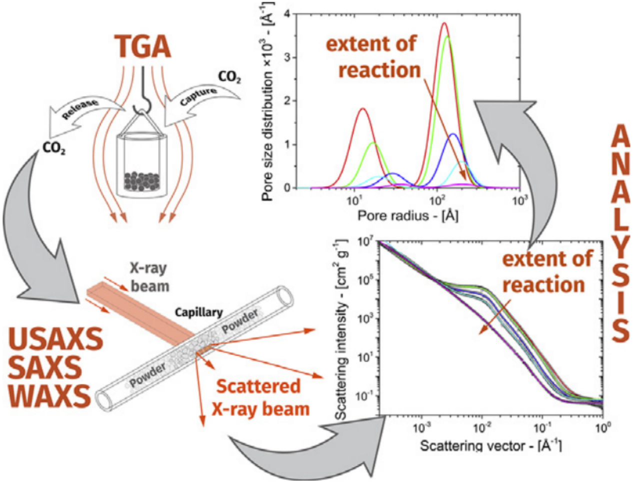
The samples were studied ex-situ at Sector 9-ID using USAXS and analyzed with a unified fit model



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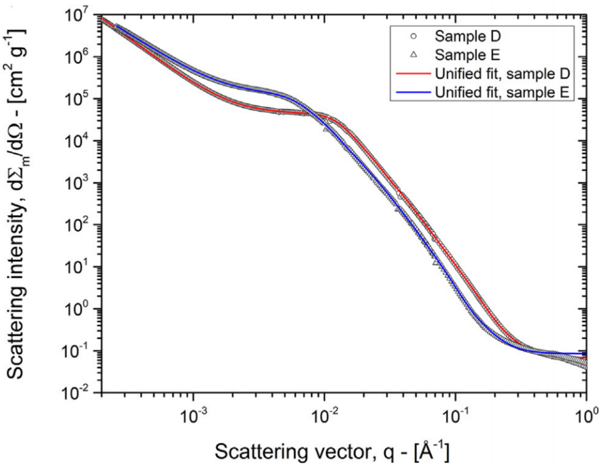
Sample D was calcined at 900 °C for 50 minutes while sample E was calcined at the same temperature for 240 minutes



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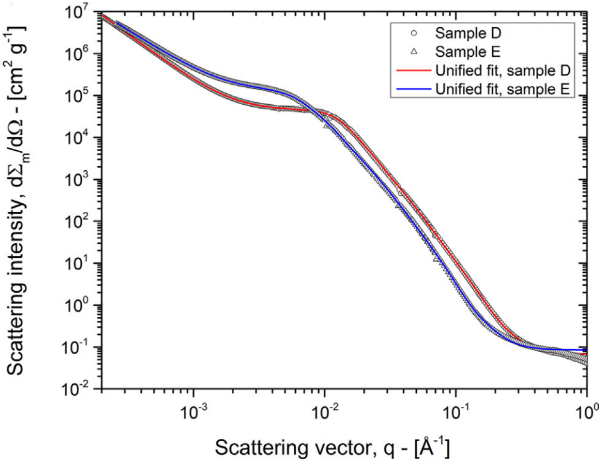
The SAXS shows the grain growth evolution between the two samples and it is clear that the samples need a multilevel unified fit



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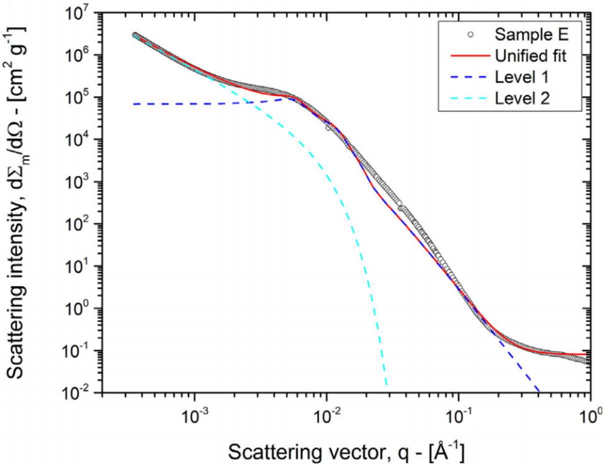

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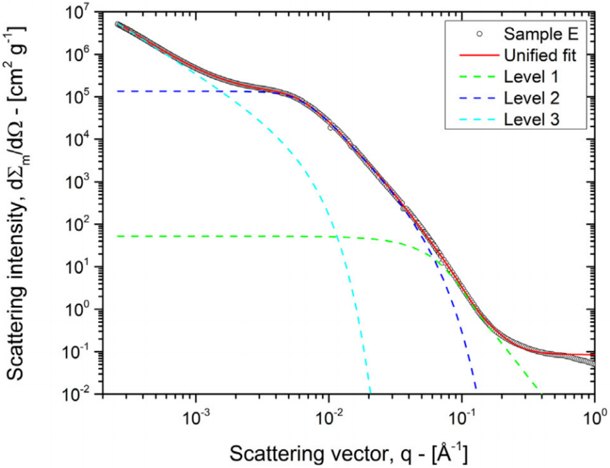
A three level fit works well for the calcined samples and from this one can extract the pore sizes for two different pore populations in the calcined samples



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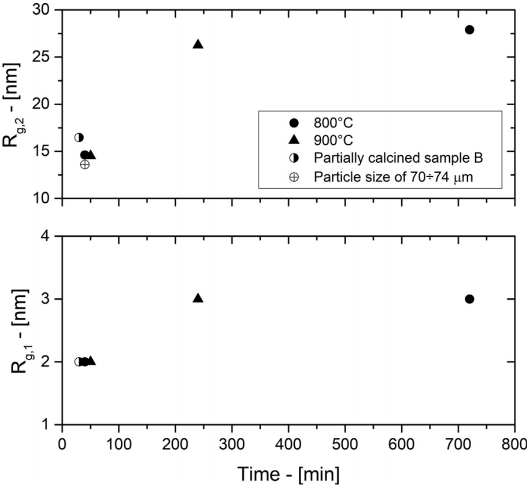

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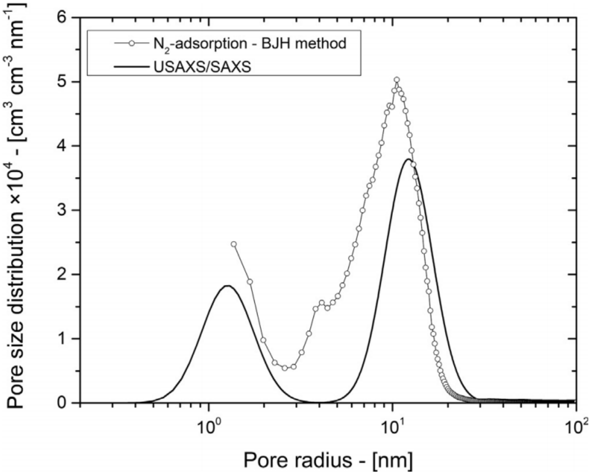
The resulting pore size distributions correspond well to those measured using gas adsorption methods



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We will now proceed to develop a model for this kind of scattering starting with some definitions in 2D space.

Types of lattice vectors

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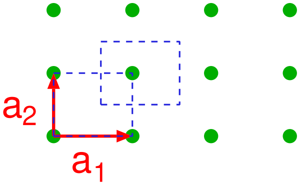

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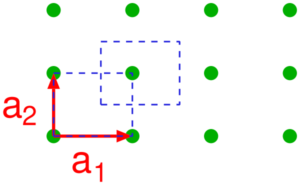

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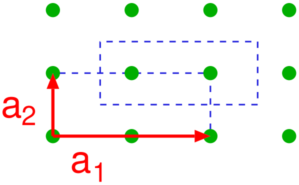

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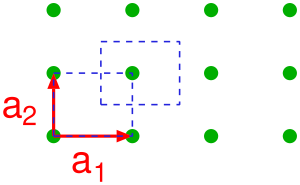

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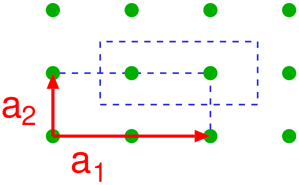

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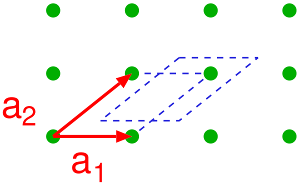

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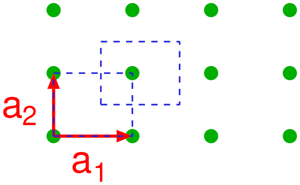

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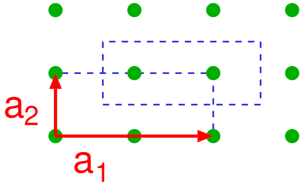

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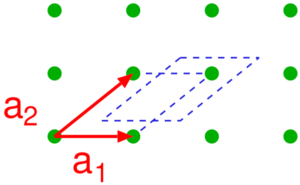

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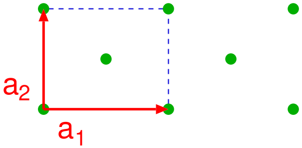

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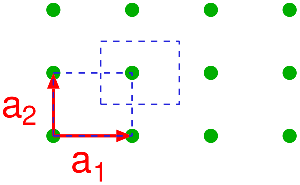

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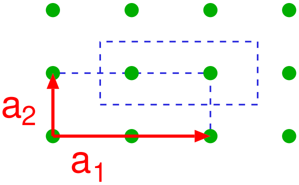

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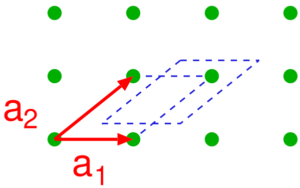

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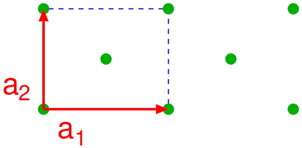

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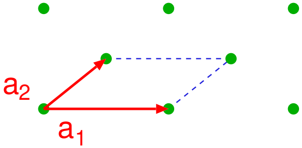
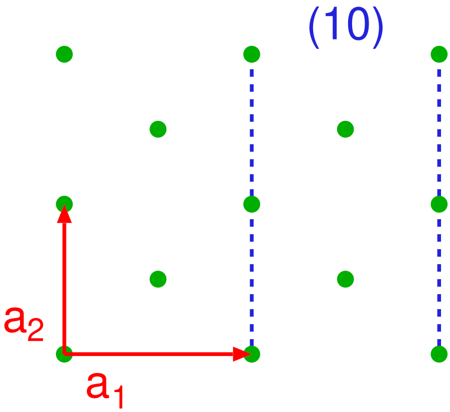


...are not primitive

Miller indices



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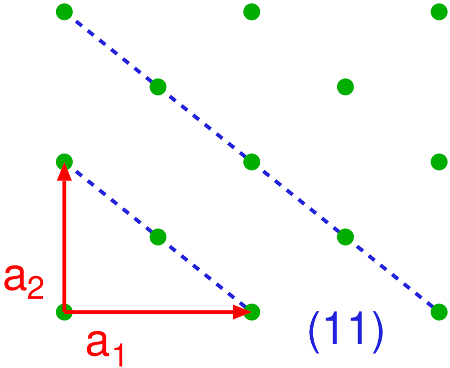

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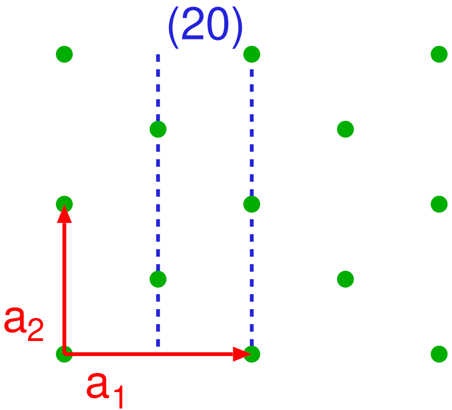

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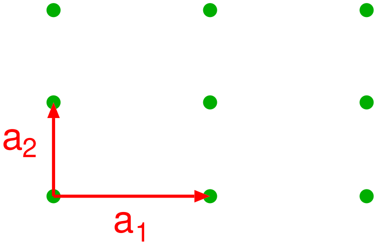
Reciprocal lattice



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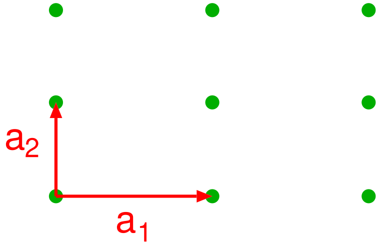

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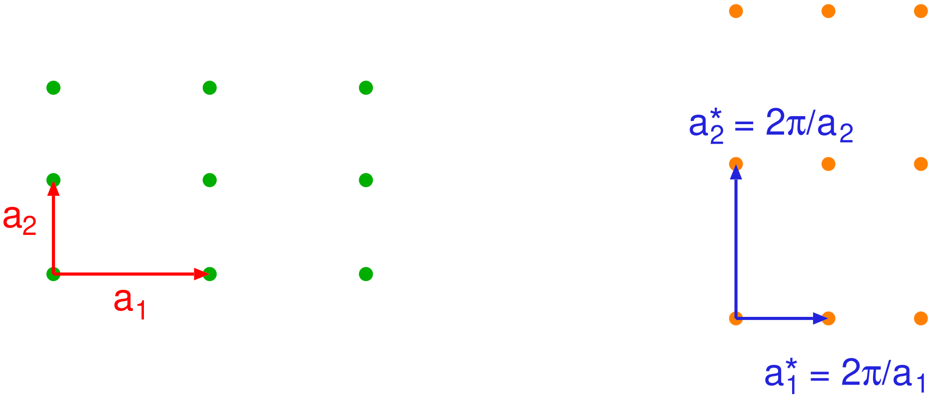

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$$\therefore\ \vec{Q} = \vec{G}_{hkl}$$

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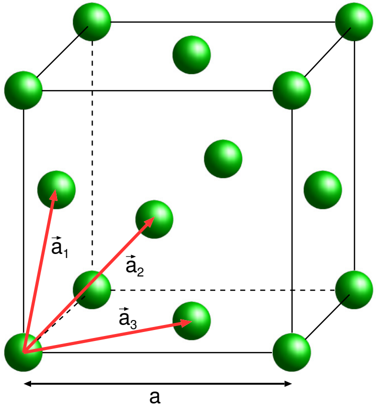
The primitive lattice vectors of the face-centered cubic lattice are



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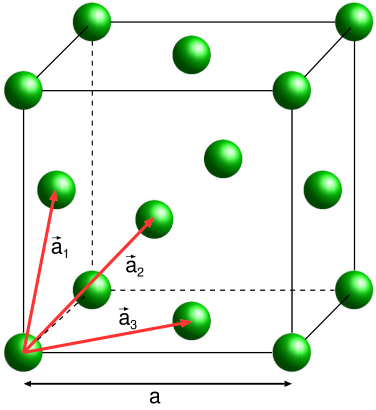

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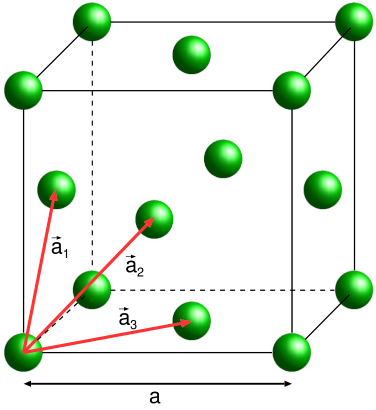

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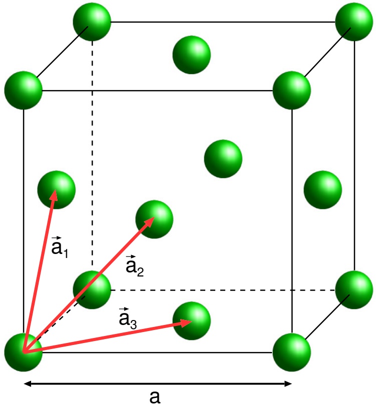

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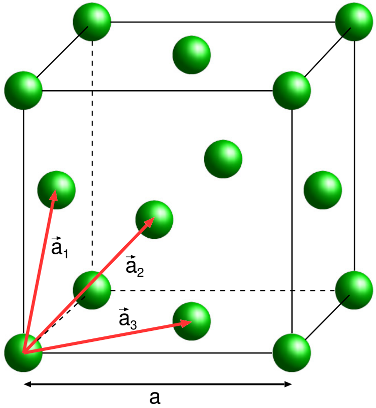

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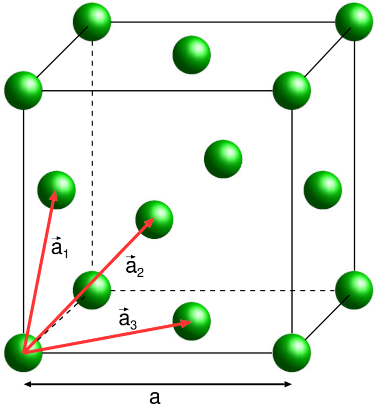

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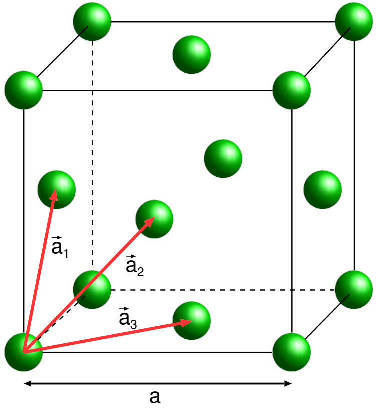

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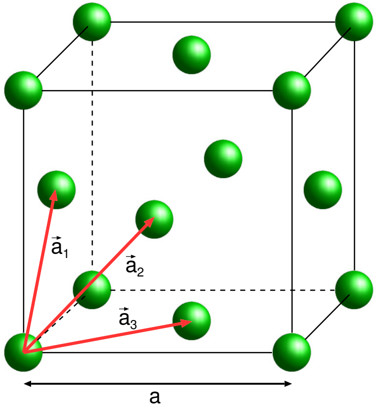

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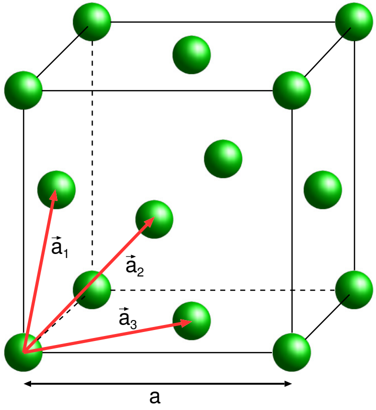

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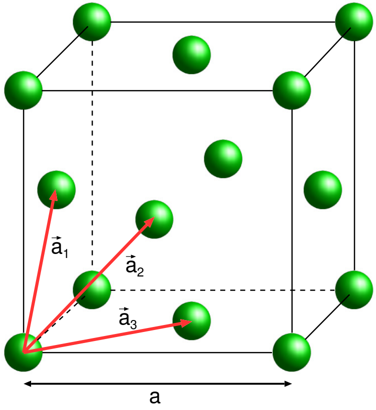

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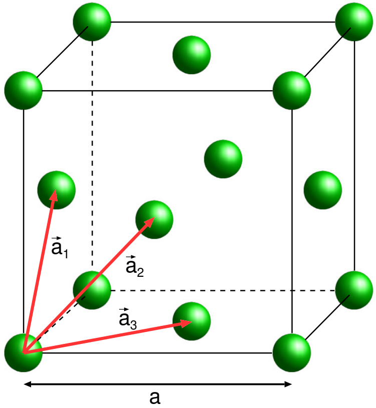

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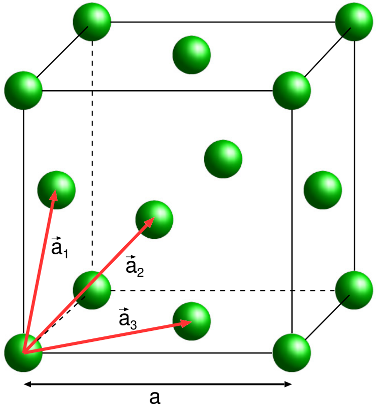
$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}), \qquad \vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x}), \qquad \vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$



The volume of the unit cell is

$$v_c = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \vec{a}_1 \cdot \frac{a^2}{4}\left(\hat{y} + \hat{z} - \hat{x}\right) = \frac{a^3}{4}$$

$$\vec{a}_1^* = \frac{2\pi}{v_c}\vec{a}_2 \times \vec{a}_3 = \frac{2\pi}{v_c}\frac{a^2}{4}\left(\hat{y} + \hat{z} - \hat{x}\right) = \frac{4\pi}{a}\left(\frac{\hat{y}}{2} + \frac{\hat{z}}{2} - \frac{\hat{x}}{2}\right)$$

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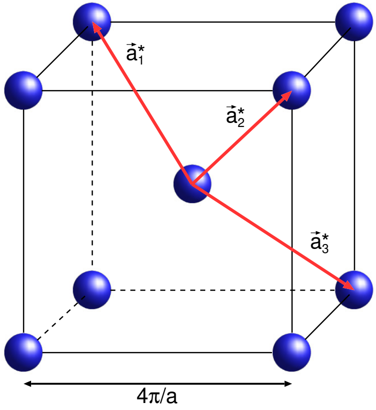

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which is a body-centered cubic lattice

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since $\delta(a^*\xi) = \delta(\xi)/a^*$

Lattice sum modulus

the 1D modulus squared

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and similarly in 3D

$$\left|S_N(\vec{Q})\right|^2 \rightarrow NV_c^* \sum_{\vec{G}_{hkl}} \delta(\vec{Q} - \vec{G}_{hkl})$$