Today's Outline - October 12, 2016

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Reading assignment: Chapter 5.2

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Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Monday, October 24, 2016

SAXS review

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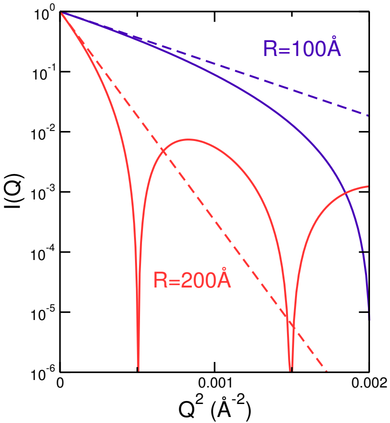

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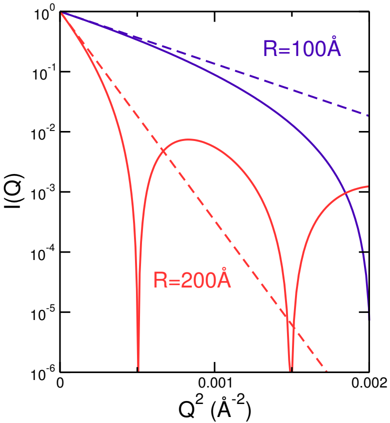

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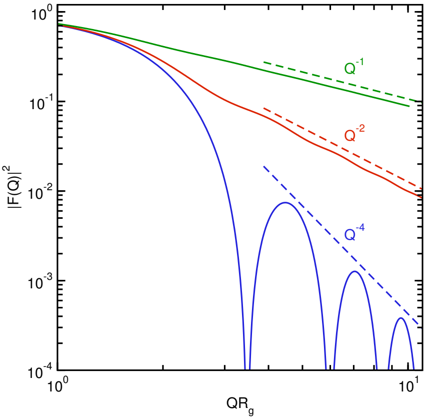

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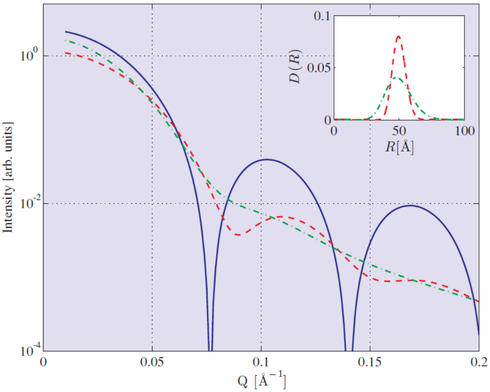
p = 0
p = 10%
p = 20%



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- Nucleation and growth of & glycine crystals

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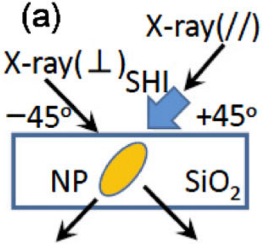

Expt. geometry

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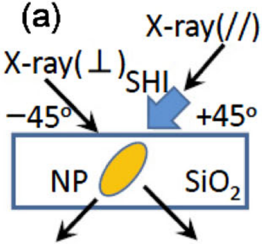

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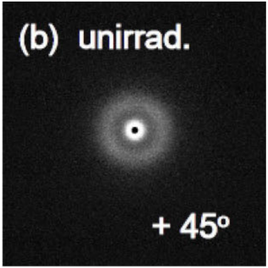

Unirradiated

"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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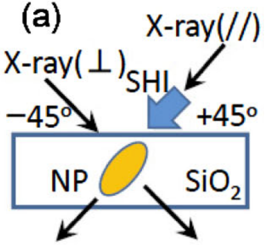

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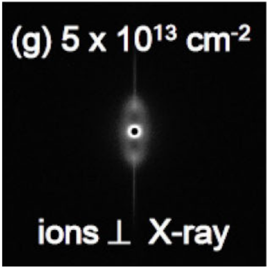
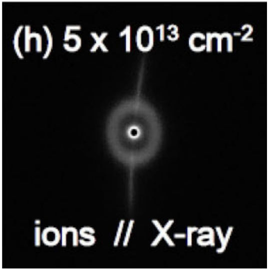


Irradiated $\parallel$ x-rays



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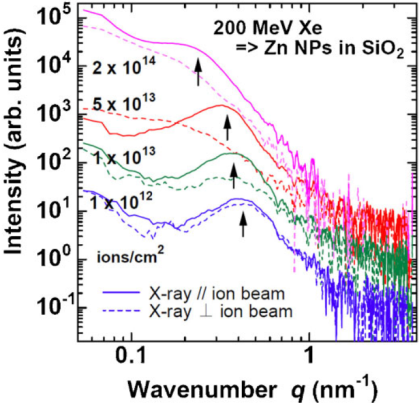

SAXS intensity for $\parallel$ and $\perp$ x-ray incidence

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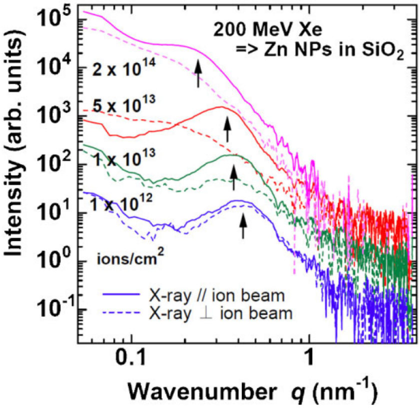

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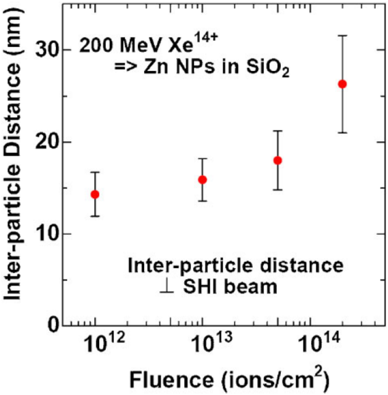

Interparticle distance as a function of irradiation fluence

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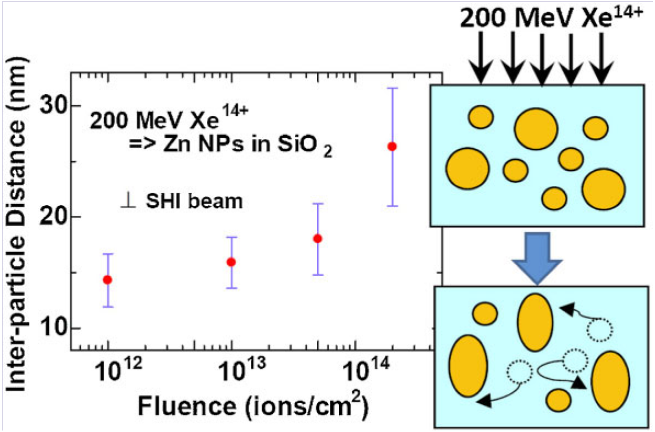

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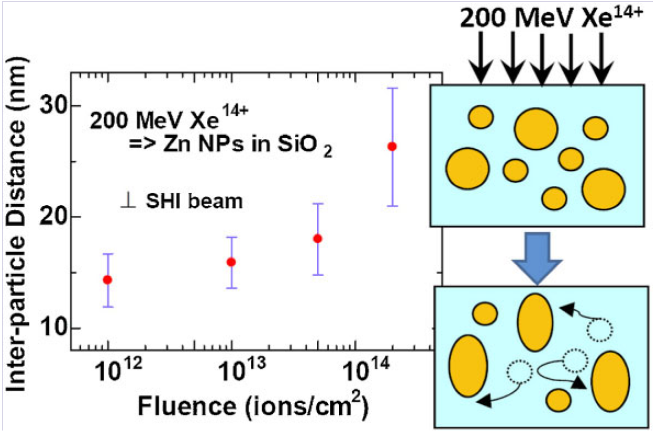

growth of interparticle spacing is due to dissolution and re-agglomeration with fluence

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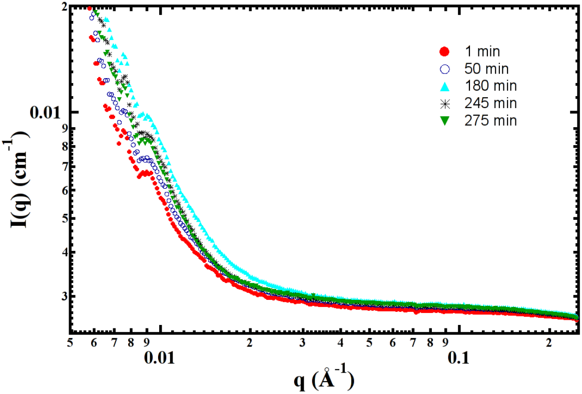
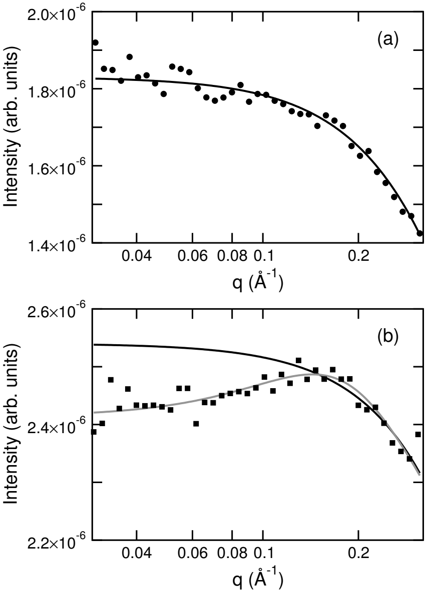
Nucleation & growth of glycine

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



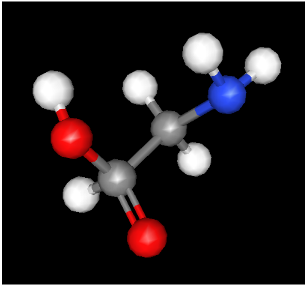
initial studies at 12 keV show change but no crystallization

Glycine nucleation



change to 25 keV x-rays

study neutral (top) and acidic (bottom) solutions



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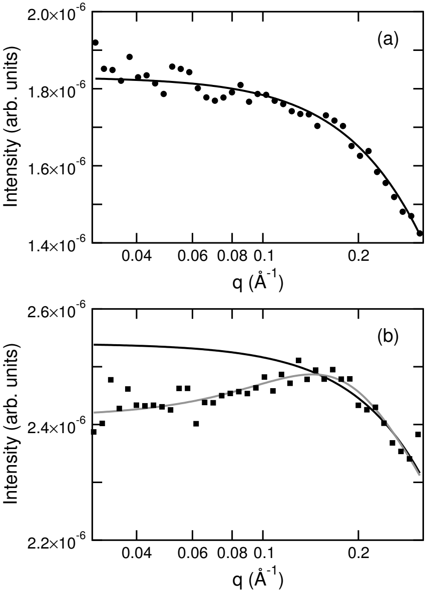

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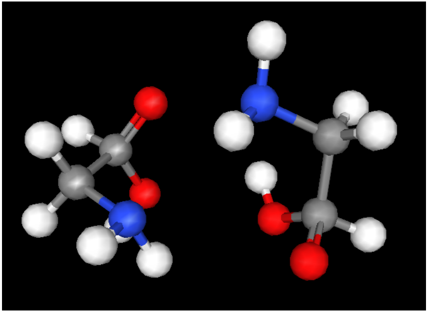
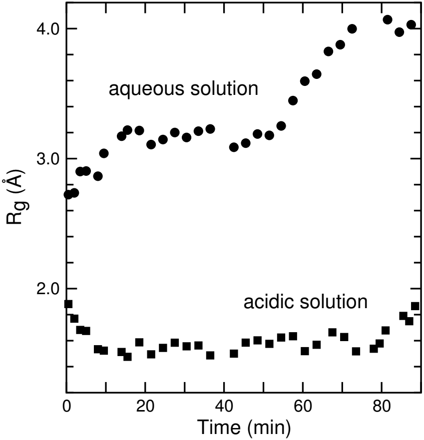


Glycine R_g



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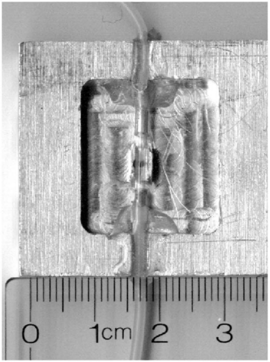
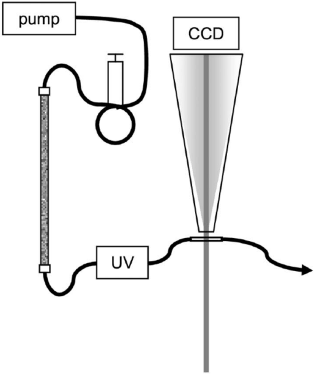
Matthew, Mirza & Menhart, "liquid-chromatography-coupled SAXS for accurate sizing of aggregating proteins," *J. Synchrotron Rad.* **11**, 314-318 (2004) developed a technique which is now being used routinely in biological SAXS, called Size Exclusion Chromatography SAXS.

Size exclusion chromatography SAXS





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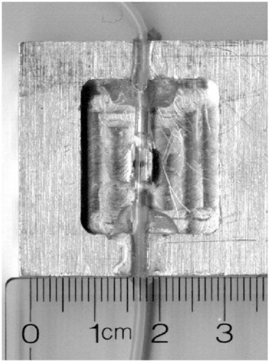
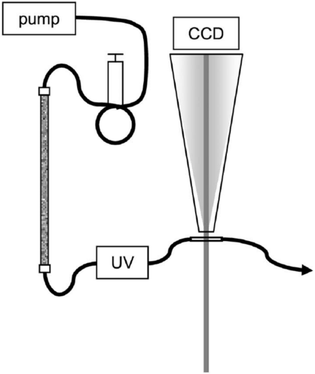
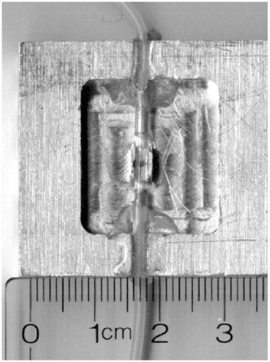
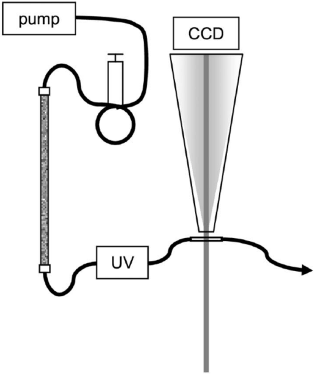




2m SAXS camera, 1.03Å(12 keV) x-rays were used

Size exclusion chromatography SAXS





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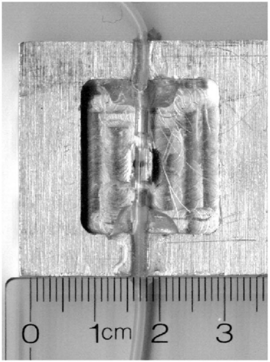

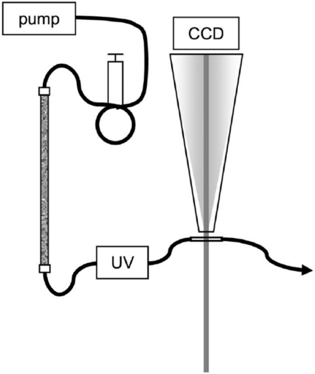

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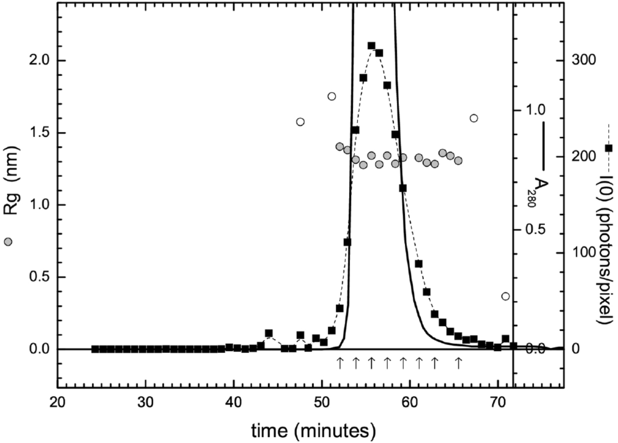
samples of (1) cytochrome c, (2) plasminogen, (3) mixture of cytochrome c bovine serum albumin, and blue dextran

SEC-SAXS experimental setup



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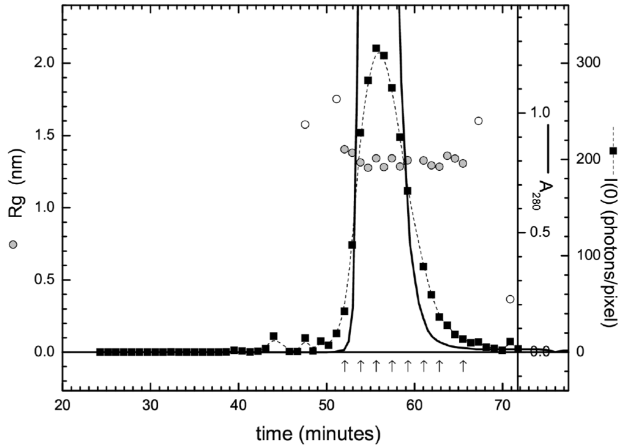
Cytochrome c



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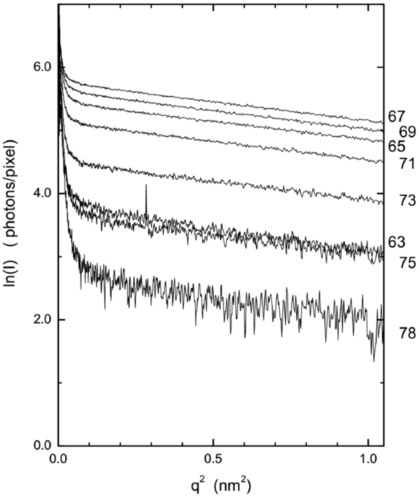
Cytochrome c - Guinier plots



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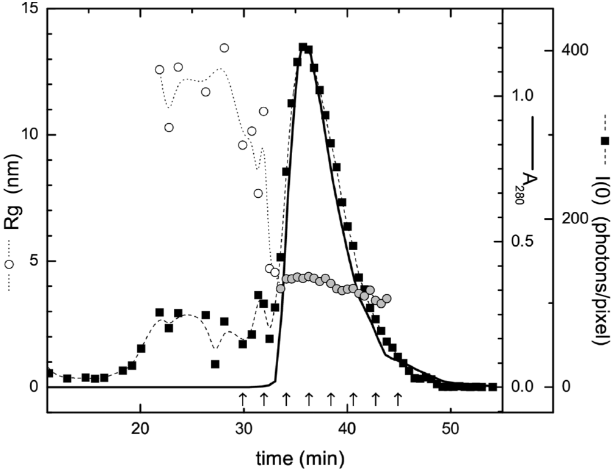
Plasminogen



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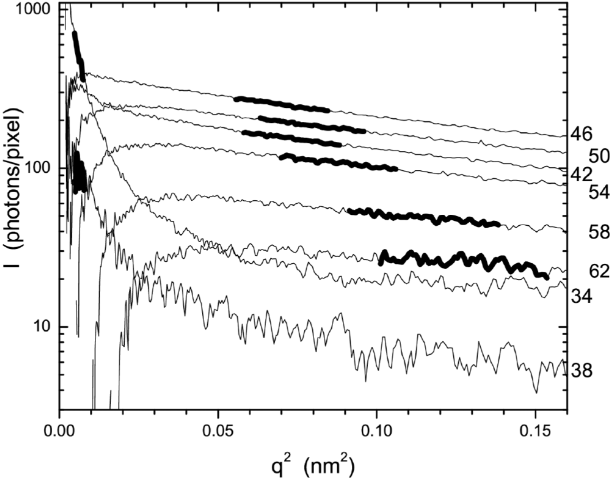

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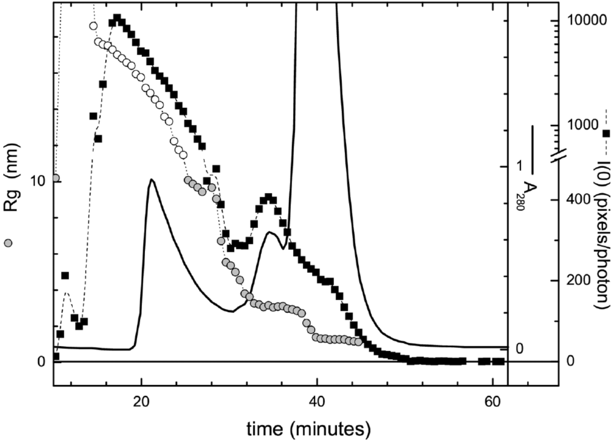
Three component mixture



Matthew, Mirza & Menhart, "liquid-chromatography-coupled SAXS for accurate sizing of aggregating proteins," *J. Synchrotron Rad.* **11**, 314-318 (2004).

Types of lattice vectors

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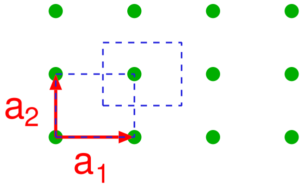

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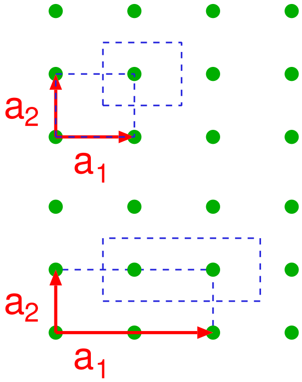

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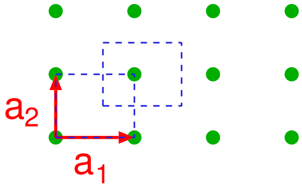

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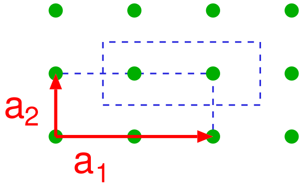
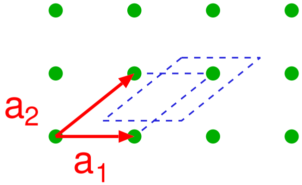
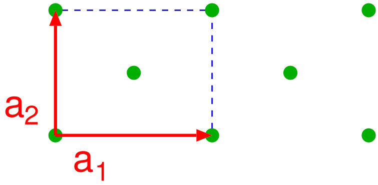


non-primitive



non-conventional

More about lattice vectors



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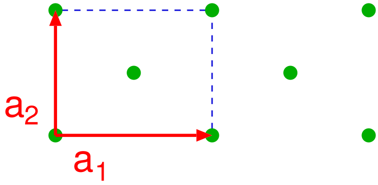

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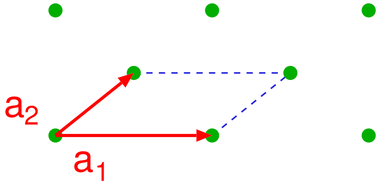
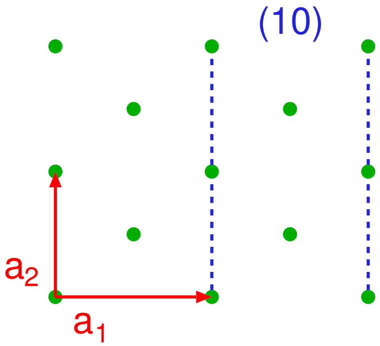


...are not primitive

Miller indices



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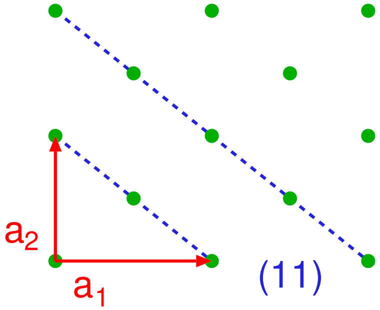

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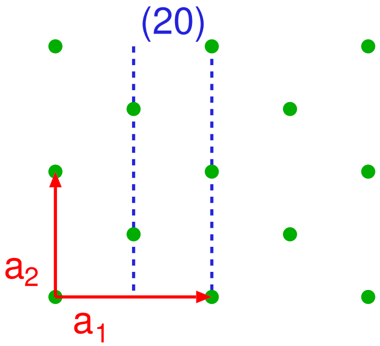

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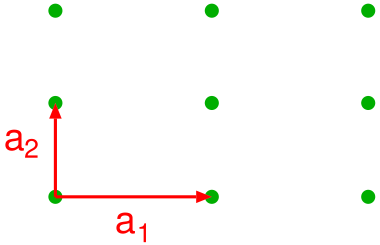
for a lattice with orthogonal unit vectors

$$\frac{1}{d_{hk}^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2}$$

Reciprocal lattice



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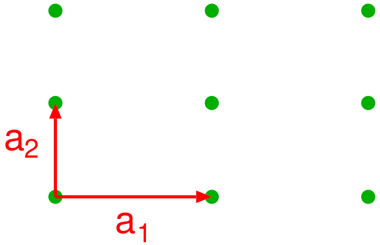

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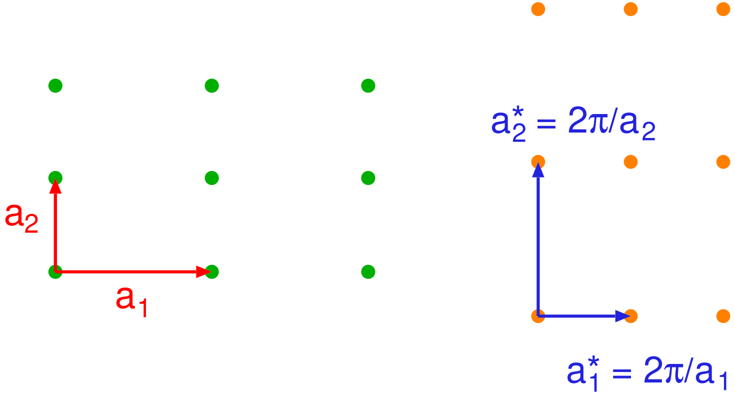

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$$\therefore\ \vec{Q} = \vec{G}_{hkl}$$

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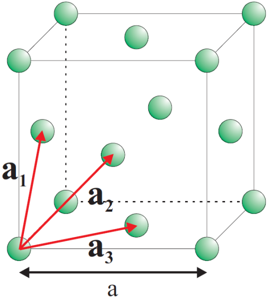
The primitive lattice vectors of the face-centered cubic lattice are



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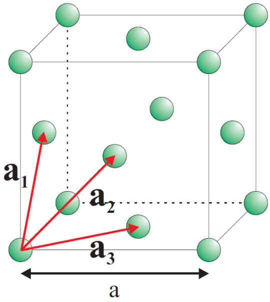

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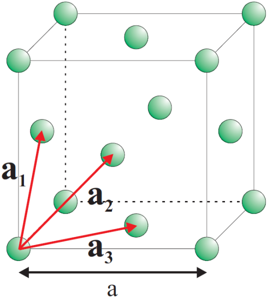

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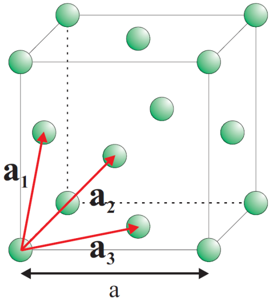

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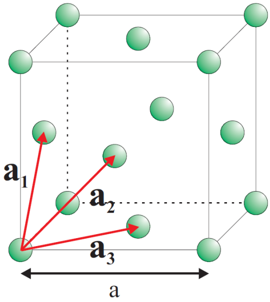

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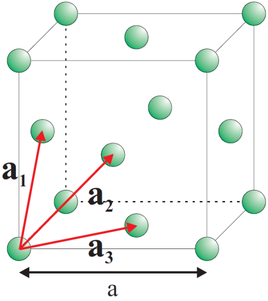

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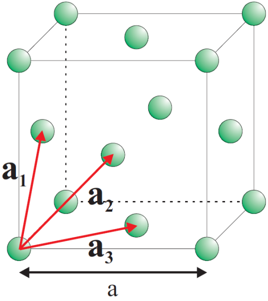

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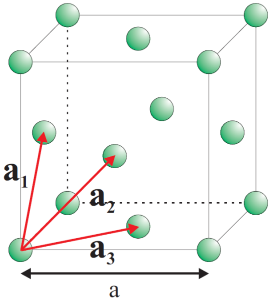

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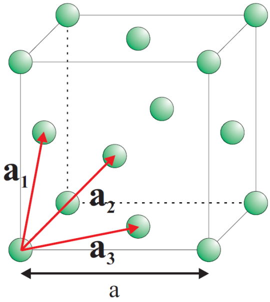
The FCC reciprocal lattice

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

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



The volume of the unit cell is

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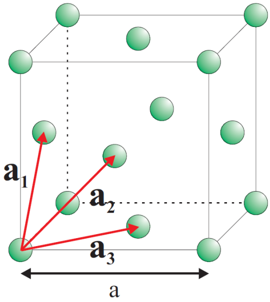

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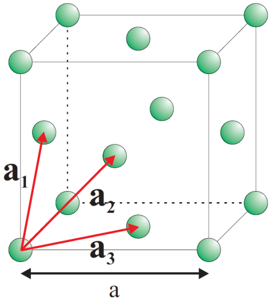

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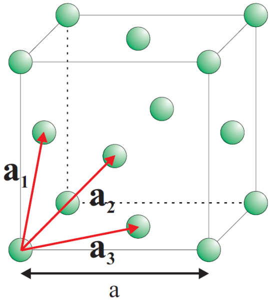

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$$\vec{a}_3^* = \frac{4\pi}{a}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}-\frac{\hat{z}}{2}\right)$$

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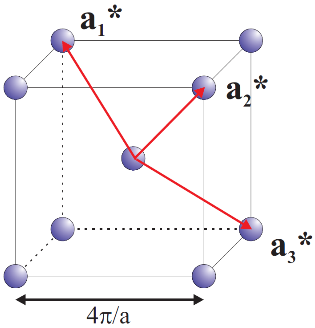

which is a body-centered cubic lattice

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