Today's Outline - March 12, 2015

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- Structure factors

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Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Tuesday, March 24, 2015

BCC structure factor

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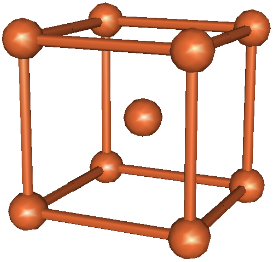

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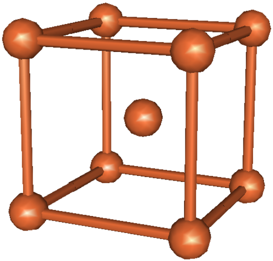

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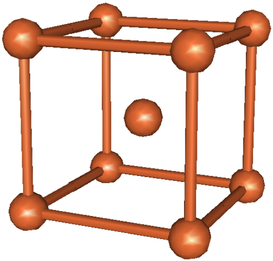

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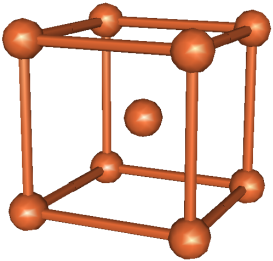

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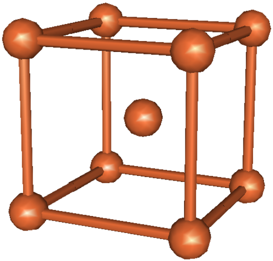

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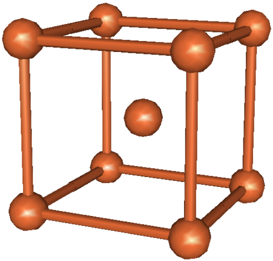

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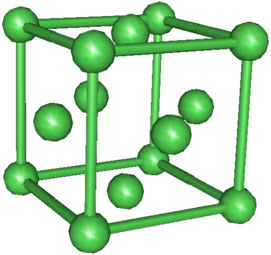

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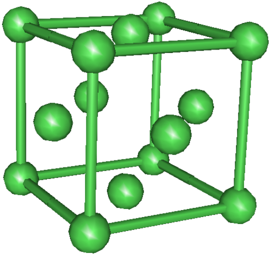

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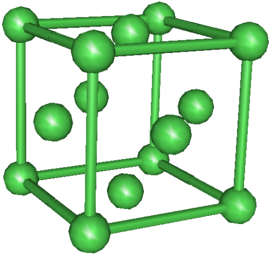

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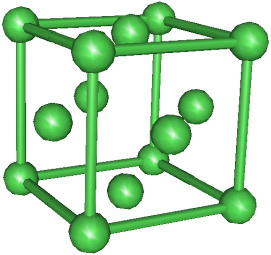

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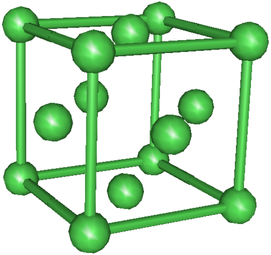

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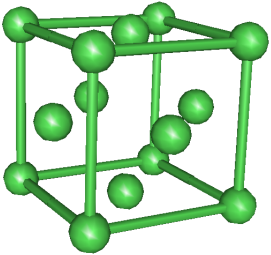

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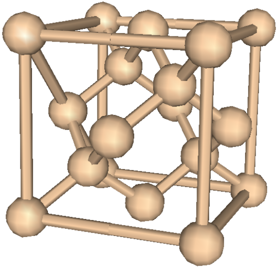

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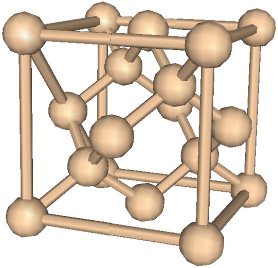

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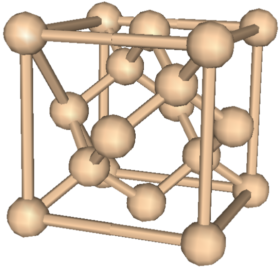

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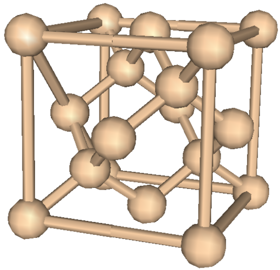
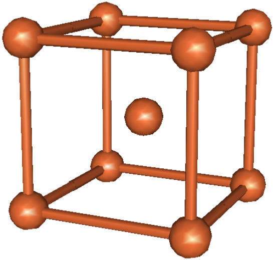
This is non-zero when h,k,l all even and $h+k+l=4n$ or h,k,l all odd



Heteroatomic structures



$\leftarrow$ bcc

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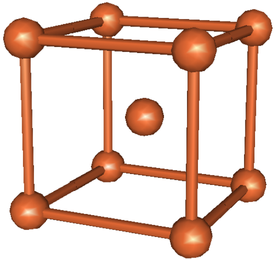
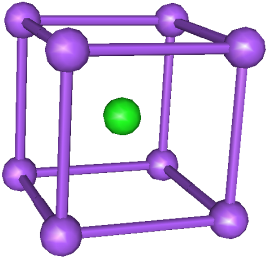


← bcc

sc →



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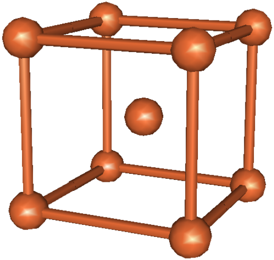

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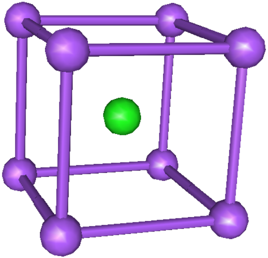

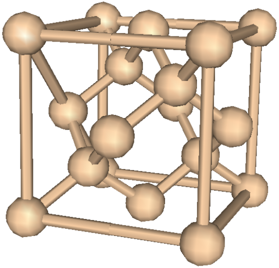

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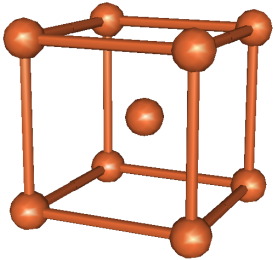

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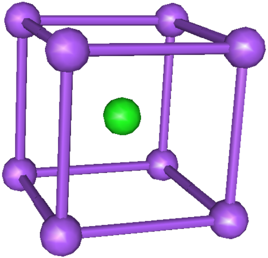

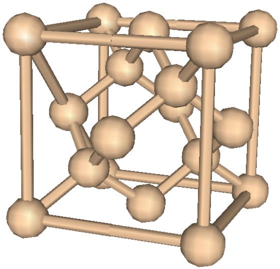

← diamond

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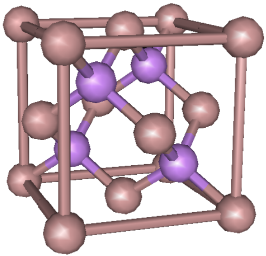

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http://phillips-lab.biochem.wisc.edu/software.html

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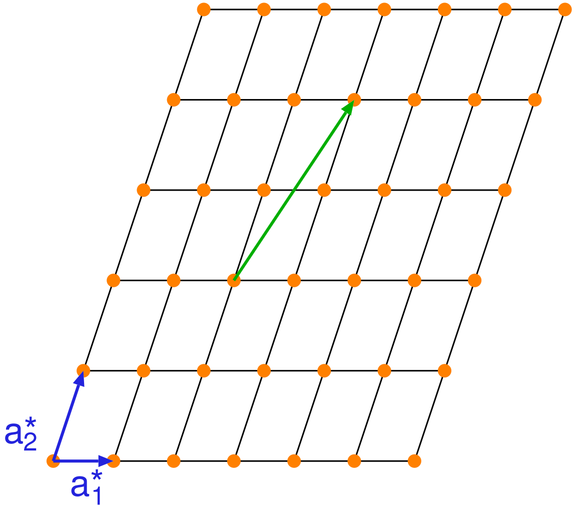

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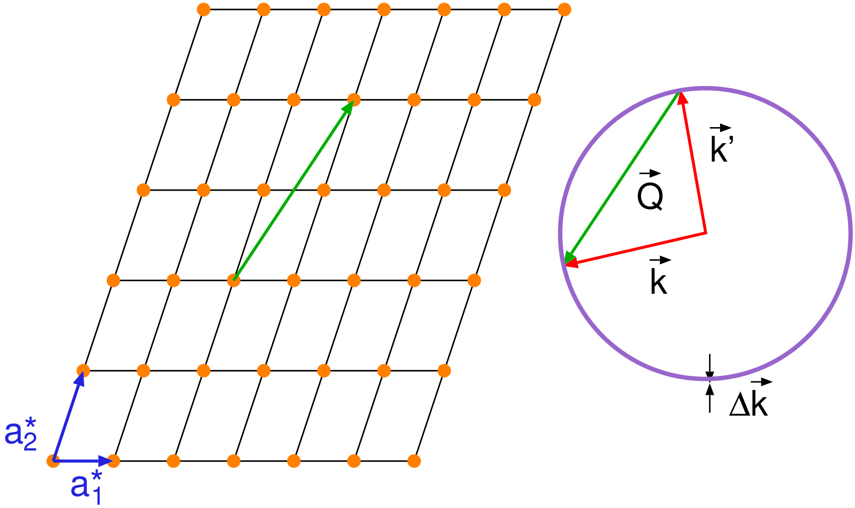

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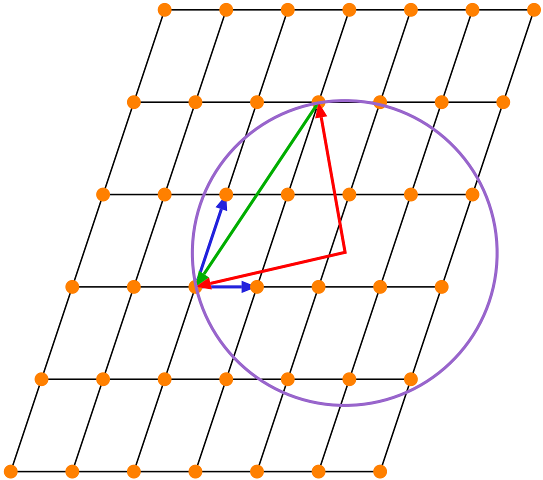

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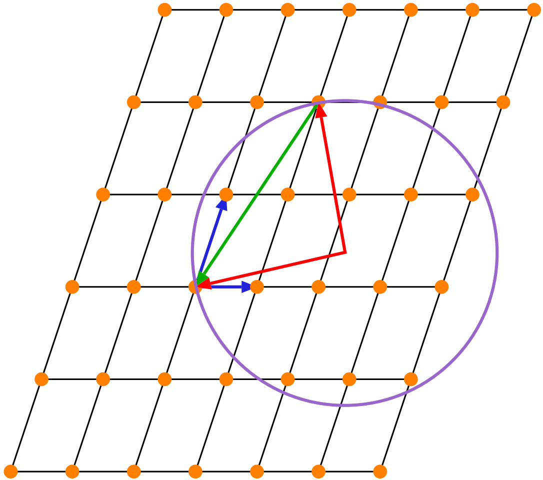

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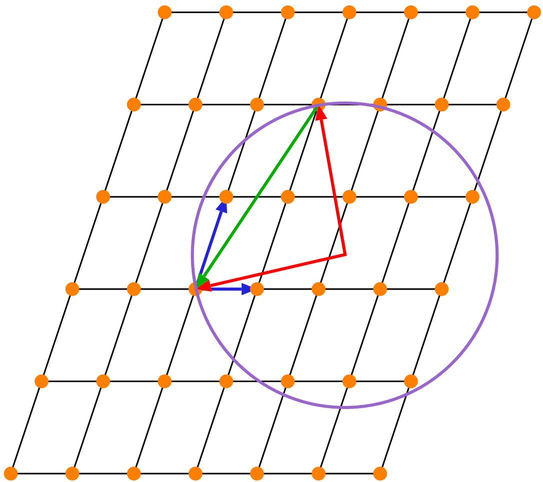

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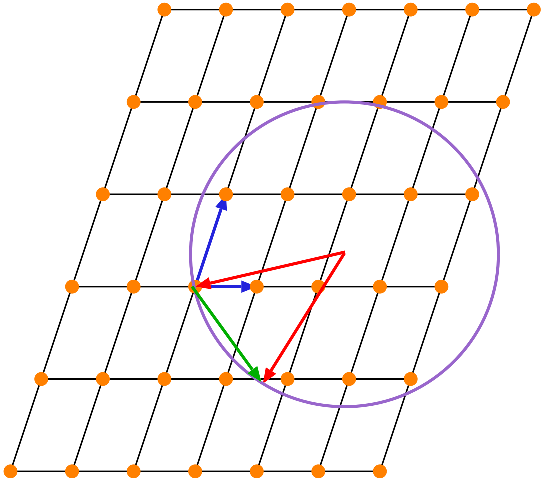
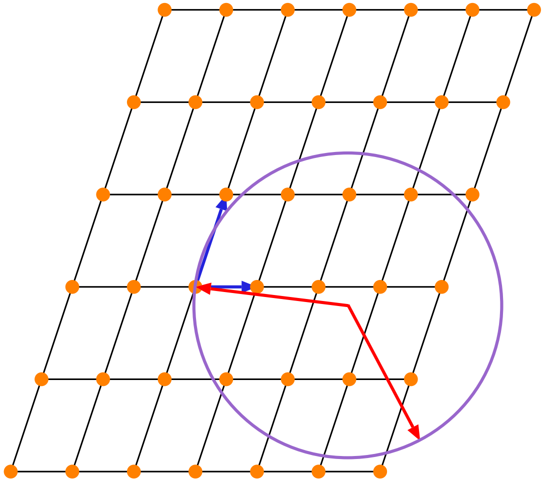
If the Ewald sphere (circle) lies on a reciprocal lattice point, a reflection can occur for that specific orientation of $\vec{k}$ to the reciprocal lattice (the physical crystal).

Ewald Construction



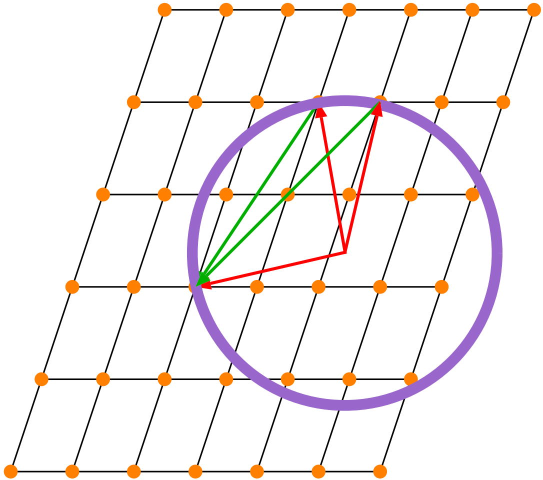
In directions of $\vec{k}'$ (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.

Ewald Construction



If the crystal is rotated slightly with respect to the incident beam, $\vec{k}$, there may be no Bragg reflections possible at all.

Polychromatic Radiation



If $\Delta\vec{k}$ is large enough, there may be more than one reflection lying on the Ewald sphere.

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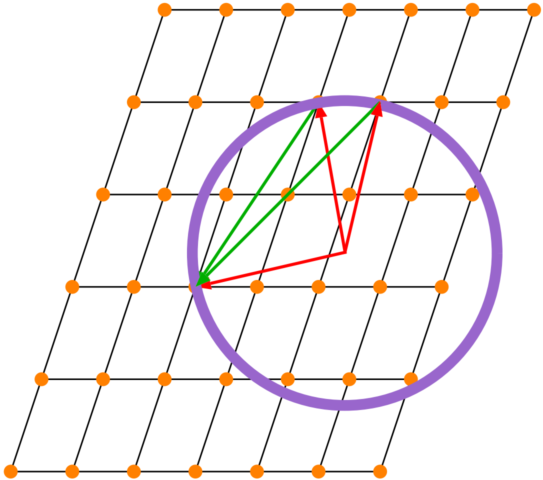

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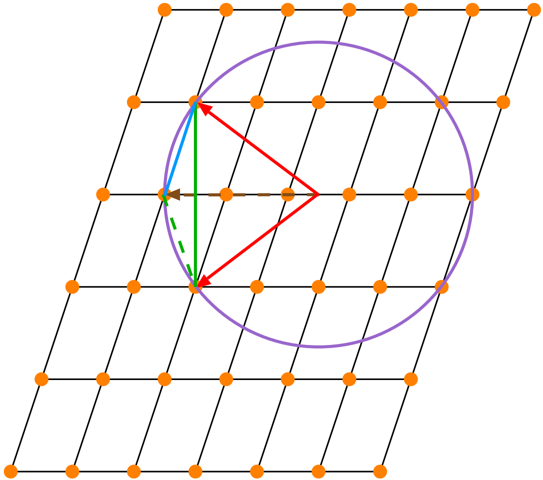
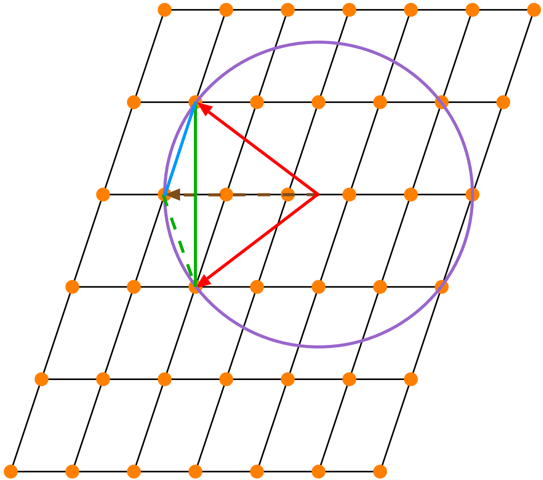
With an area detector, there may then be multiple reflections appear for a particular orientation (very common with protein crystals where the unit cell is very large).



Alternatively, scattering can occur internal to the crystal along $\vec{k}_{int}$ and then along another reciprocal lattice vector $\vec{G}$ to the detector at $\vec{k}'$.

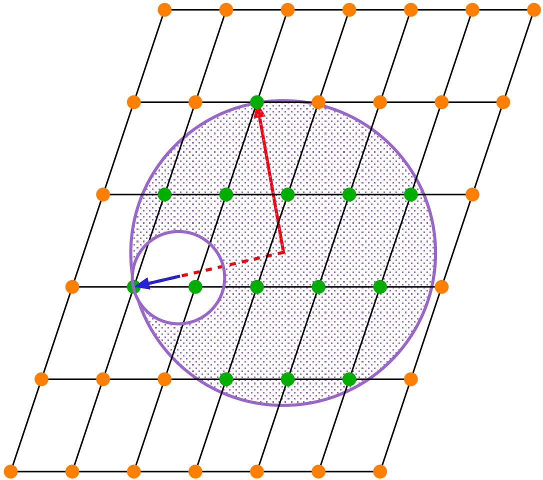
Multiple Scattering



Alternatively, scattering can occur internal to the crystal along $\vec{k}_{int}$ and then along another reciprocal lattice vector $\vec{G}$ to the detector at $\vec{k}'$.

This is the cause of monochromator glitches which sometimes remove intensity but can also add intensity.

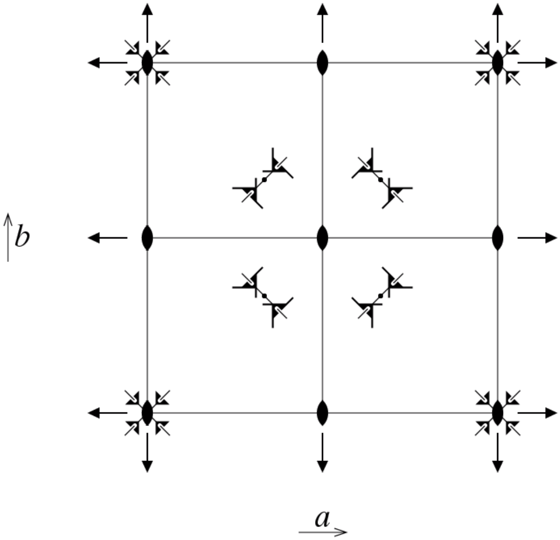
Laue Diffraction



The Laue diffraction technique uses a wide range of radiation from $\vec{k}_{min}$ to $\vec{k}_{max}$

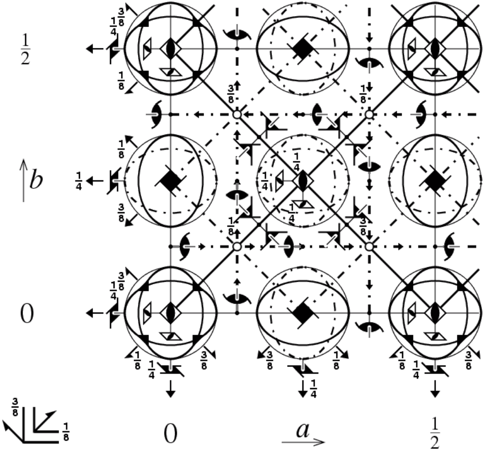
These define two Ewald spheres and a volume between them such that any reciprocal lattice point which lies in the volume will meet the Laue condition for reflection.

$P23$ $P\,2\,3$ 23 No. 195



1 x, y, z
2 $x, \bar{y}, \bar{z}$
3 $\bar{x}, y, \bar{z}$
4 $\bar{x}, \bar{y}, z$
5 z, x, y
6 $\bar{z}, \bar{x}, y$
7 $z, \bar{x}, \bar{y}$
8 $\bar{z}, x, \bar{y}$
9 y, z, x
10 $\bar{y}, z, \bar{x}$
11 $\bar{y}, \bar{z}, x$
12 $y, \bar{z}, \bar{x}$

$Fd\bar{3}m$ $\quad$ $F\,4_1/d\,\bar{3}\,2/m$ $\quad$ $m\bar{3}m$ $\quad$ No. 227



1	x, y, z	25	$\frac14-x, \frac14-y, \frac14-z$
2	$x, \bar{y}, \bar{z}$	26	$\frac14-x, \frac14+y, \frac14+z$
3	$\bar{x}, y, \bar{z}$	27	$\frac14+x, \frac14-y, \frac14+z$
4	$\bar{x}, \bar{y}, z$	28	$\frac14+x, \frac14+y, \frac14-z$
5	z, x, y	29	$\frac14-z, \frac14-x, \frac14-y$
6	$\bar{z}, \bar{x}, y$	30	$\frac14+z, \frac14+x, \frac14-y$
7	$z, \bar{x}, \bar{y}$	31	$\frac14-z, \frac14+x, \frac14+y$
8	$\bar{z}, x, \bar{y}$	32	$\frac14+z, \frac14-x, \frac14+y$
9	y, z, x	33	$\frac14-y, \frac14-z, \frac14-x$
10	$\bar{y}, z, \bar{x}$	34	$\frac14+y, \frac14-z, \frac14+x$
11	$\bar{y}, \bar{z}, x$	35	$\frac14+y, \frac14+z, \frac14-x$
12	$y, \bar{z}, \bar{x}$	36	$\frac14-y, \frac14+z, \frac14+x$
13	$\frac14+x, \frac14-z, \frac14+y$	37	$\bar{x}, z, \bar{y}$
14	$\frac14+x, \frac14+z, \frac14-y$	38	$\bar{x}, \bar{z}, y$
15	$\frac14-x, \frac14-z, \frac14-y$	39	x, z, y
16	$\frac14-x, \frac14+z, \frac14+y$	40	$x, \bar{z}, \bar{y}$
17	$\frac14+z, \frac14+y, \frac14-x$	41	$\bar{z}, \bar{y}, x$
18	$\frac14-z, \frac14+y, \frac14+x$	42	$z, \bar{y}, \bar{x}$
19	$\frac14-z, \frac14-y, \frac14-x$	43	z, y, x
20	$\frac14+z, \frac14-y, \frac14+x$	44	$\bar{z}, y, \bar{x}$
21	$\frac14-y, \frac14+x, \frac14+z$	45	$y, \bar{x}, \bar{z}$
22	$\frac14+y, \frac14-x, \frac14+z$	46	$\bar{y}, x, \bar{z}$
23	$\frac14-y, \frac14-x, \frac14-z$	47	y, x, z
24	$\frac14+y, \frac14+x, \frac14-z$	48	$\bar{y}, \bar{x}, z$

$+(0,\frac12,\frac12), (\frac12,0,\frac12), (\frac12,\frac12,0)$

Wyckoff Positions of Group 195 (*P*23)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
12	j	1	(x,y,z) (-x,-y,z) (-x,y,-z) (x,-y,-z) (z,x,y) (z,-x,-y) (-z,-x,y) (-z,x,-y) (y,z,x) (-y,z,-x) (y,-z,-x) (-y,-z,x)
6	i	2..	(x,1/2,1/2) (-x,1/2,1/2) (1/2,x,1/2) (1/2,-x,1/2) (1/2,1/2,x) (1/2,1/2,-x)
6	h	2..	(x,1/2,0) (-x,1/2,0) (0,x,1/2) (0,-x,1/2) (1/2,0,x) (1/2,0,-x)
6	g	2..	(x,0,1/2) (-x,0,1/2) (1/2,x,0) (1/2,-x,0) (0,1/2,x) (0,1/2,-x)
6	f	2..	(x,0,0) (-x,0,0) (0,x,0) (0,-x,0) (0,0,x) (0,0,-x)
4	e	.3.	(x,x,x) (-x,-x,x) (-x,x,-x) (x,-x,-x)
3	d	222 . .	(1/2,0,0) (0,1/2,0) (0,0,1/2)
3	c	222 . .	(0,1/2,1/2) (1/2,0,1/2) (1/2,1/2,0)
1	b	23.	(1/2,1/2,1/2)
1	a	23.	(0,0,0)

Wyckoff Positions of Group 227 (*Fd*-3*m*) [origin choice 1]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates			
			(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +			
192	i	1	(x,y,z)	(-x,-y+1/2,z+1/2)	(-x+1/2,y+1/2,-z)	(x+1/2,-y,-z+1/2)
			(z,x,y)	(z+1/2,-x,-y+1/2)	(-z,-x+1/2,y+1/2)	(-z+1/2,x+1/2,-y)
			(y,z,x)	(-y+1/2,z+1/2,-x)	(y+1/2,-z,-x+1/2)	(-y,-z+1/2,x+1/2)
			(y+3/4,x+1/4,-z+3/4)	(-y+1/4,-x+1/4,-z+1/4)	(y+1/4,-x+3/4,z+3/4)	(-y+3/4,x+3/4,z+1/4)
			(x+3/4,z+1/4,-y+3/4)	(-x+3/4,z+3/4,y+1/4)	(-x+1/4,-z+1/4,-y+1/4)	(x+1/4,-z+3/4,y+3/4)
			(z+3/4,y+1/4,-x+3/4)	(z+1/4,-y+3/4,x+3/4)	(-z+3/4,y+3/4,x+1/4)	(-z+1/4,-y+1/4,-x+1/4)
			(-x+1/4,-y+1/4,-z+1/4)	(x+1/4,y+3/4,-z+3/4)	(x+3/4,-y+3/4,z+1/4)	(-x+3/4,y+1/4,z+3/4)
			(-z+1/4,-x+1/4,-y+1/4)	(-z+3/4,x+1/4,y+3/4)	(z+1/4,x+3/4,-y+3/4)	(z+3/4,-x+3/4,y+1/4)
			(-y+1/4,-z+1/4,-x+1/4)	(y+3/4,-z+3/4,x+1/4)	(-y+3/4,z+1/4,x+3/4)	(y+1/4,z+3/4,-x+3/4)
			(-y+1/2,-x,z+1/2)	(y,x,z)	(-y,x+1/2,-z+1/2)	(y+1/2,-x+1/2,-z)
			(-x+1/2,-z,y+1/2)	(x+1/2,-z+1/2,-y)	(x,z,y)	(-x,z+1/2,-y+1/2)
			(-z+1/2,-y,x+1/2)	(-z,y+1/2,-x+1/2)	(z+1/2,-y+1/2,-x)	(z,y,x)
96	h	..2	(1/8,y,-y+1/4)	(7/8,-y+1/2,-y+3/4)	(3/8,y+1/2,y+3/4)	(5/8,-y,y+1/4)
			(-y+1/4,1/8,y)	(-y+3/4,7/8,-y+1/2)	(y+3/4,3/8,y+1/2)	(y+1/4,5/8,-y)
			(y,-y+1/4,1/8)	(-y+1/2,-y+3/4,7/8)	(y+1/2,y+3/4,3/8)	(-y,y+1/4,5/8)
			(1/8,-y+1/4,y)	(3/8,y+3/4,y+1/2)	(7/8,-y+3/4,-y+1/2)	(5/8,y+1/4,-y)
			(y,1/8,-y+1/4)	(y+1/2,3/8,y+3/4)	(-y+1/2,7/8,-y+3/4)	(-y,5/8,y+1/4)
			(-y+1/4,y,1/8)	(y+3/4,y+1/2,3/8)	(-y+3/4,-y+1/2,7/8)	(y+1/4,-y,5/8)
96	g	..m	(x,x,z)	(-x,-x+1/2,z+1/2)	(-x+1/2,x+1/2,-z)	(x+1/2,-x,-z+1/2)
			(z,x,x)	(z+1/2,-x,-x+1/2)	(-z,-x+1/2,x+1/2)	(-z+1/2,x+1/2,-x)
			(x,z,x)	(-x+1/2,z+1/2,-x)	(x+1/2,-z,-x+1/2)	(-x,-z+1/2,x+1/2)
			(x+3/4,x+1/4,-z+3/4)	(-x+1/4,-x+1/4,-z+1/4)	(x+1/4,-x+3/4,z+3/4)	(-x+3/4,x+3/4,z+1/4)
			(x+3/4,z+1/4,-x+3/4)	(-x+3/4,z+3/4,x+1/4)	(-x+1/4,-z+1/4,-x+1/4)	(x+1/4,-z+3/4,x+3/4)
			(z+3/4,x+1/4,-x+3/4)	(z+1/4,-x+3/4,x+3/4)	(-z+3/4,x+3/4,x+1/4)	(-z+1/4,-x+1/4,-x+1/4)
48	f	2.m m	(x,0,0)	(-x,1/2,1/2)	(0,x,0)	(1/2,-x,1/2)
			(0,0,x)	(1/2,1/2,-x)	(3/4,x+1/4,3/4)	(1/4,-x+1/4,1/4)
			(x+3/4,1/4,3/4)	(-x+3/4,3/4,1/4)	(3/4,1/4,-x+3/4)	(1/4,3/4,x+3/4)
32	e	.3m	(x,x,x)	(-x,-x+1/2,x+1/2)	(-x+1/2,x+1/2,-x)	(x+1/2,-x,-x+1/2)
			(x+3/4,x+1/4,-x+3/4)	(-x+1/4,-x+1/4,-x+1/4)	(x+1/4,-x+3/4,x+3/4)	(-x+3/4,x+3/4,x+1/4)
16	d	.-3m	(5/8,5/8,5/8)	(3/8,7/8,1/8)	(7/8,1/8,3/8)	(1/8,3/8,7/8)
16	c	.-3m	(1/8,1/8,1/8)	(7/8,3/8,5/8)	(3/8,5/8,7/8)	(5/8,7/8,3/8)
8	b	-43m	(1/2,1/2,1/2)	(1/4,3/4,1/4)		
8	a	-43m	(0,0,0)	(3/4,1/4,3/4)		

SAXS of irradiated Zn nanoparticles

Zn nanoparticles formed by ion implantation. SAXS measured after irradiation with high energy Xe^{+14} ions using 18 keV x-rays

"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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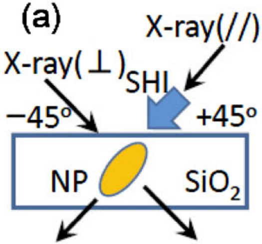

Expt. geometry

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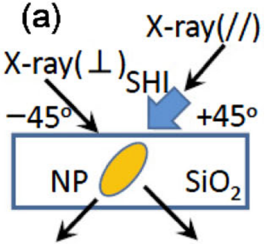
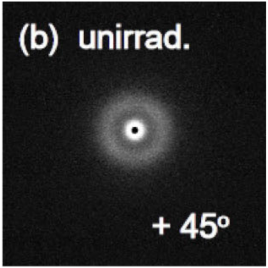


Expt. geometry



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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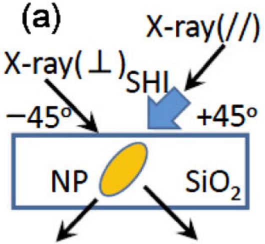
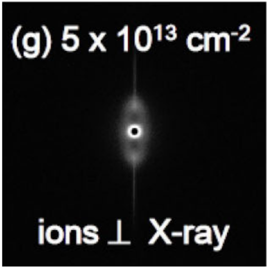


Expt. geometry



Irradiated $\parallel$ x-rays

"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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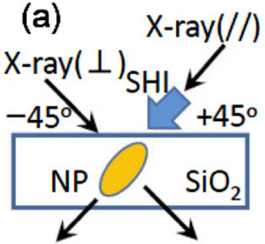
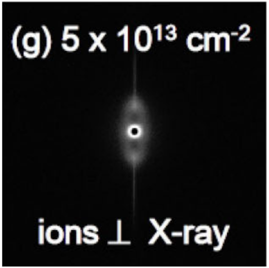
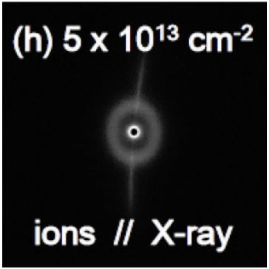


Expt. geometry



Irradiated ∥ x-rays



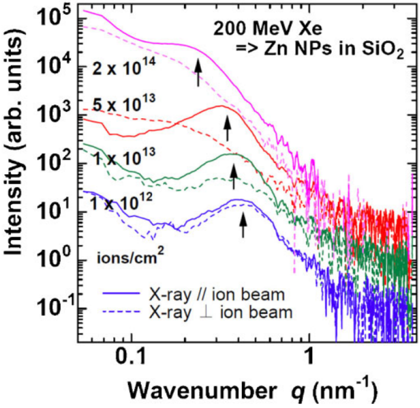
Irradiated ⊥ x-rays

“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).

SAXS of irradiated Zn nanoparticles

"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).

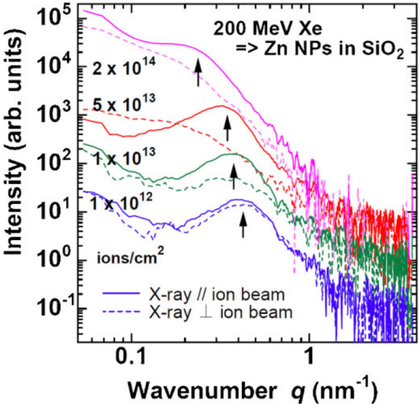
SAXS of irradiated Zn nanoparticles



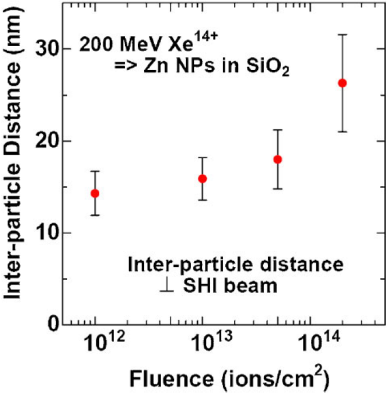
SAXS intensity for $\parallel$ and $\perp$ x-ray incidence

"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).

SAXS of irradiated Zn nanoparticles



SAXS intensity for ∥ and ⊥ x-ray incidence



Interparticle distance as a function of irradiation fluence

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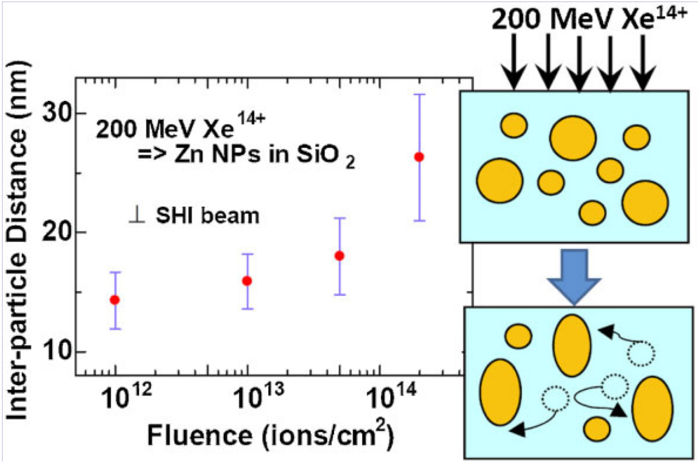

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