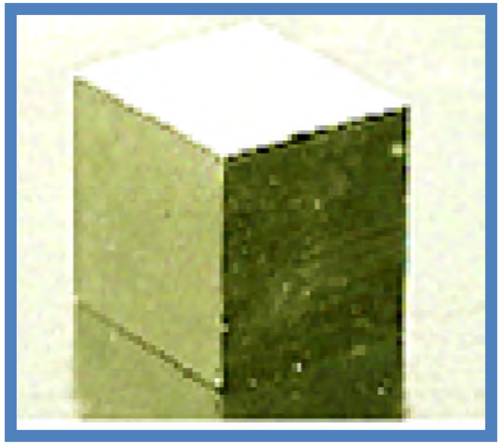
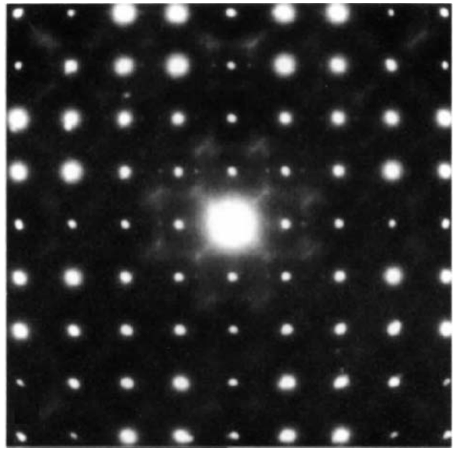
Lecture 3 Jan 14 2013



$$\mathbf{K}\cdot\mathbf{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

$$[\mathbf{b}_1\,\mathbf{b}_2\mathbf{b}_3]^T = 2\pi\,[\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3]^{-1}\,.$$

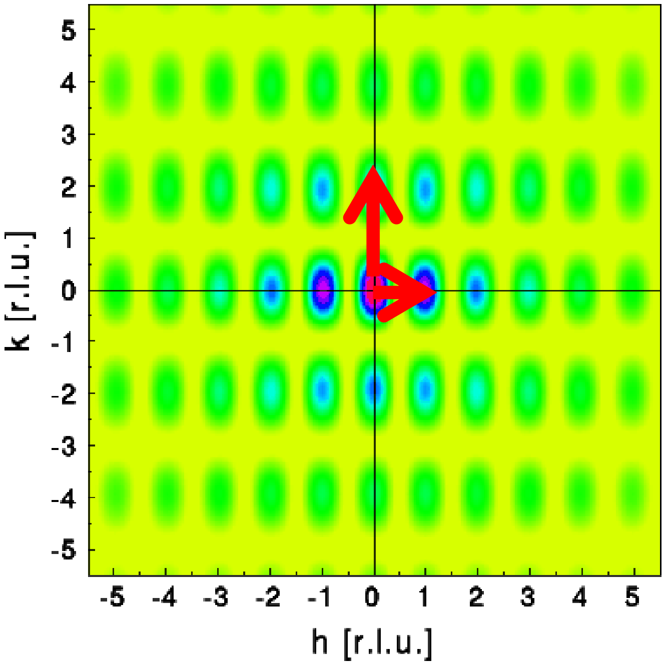


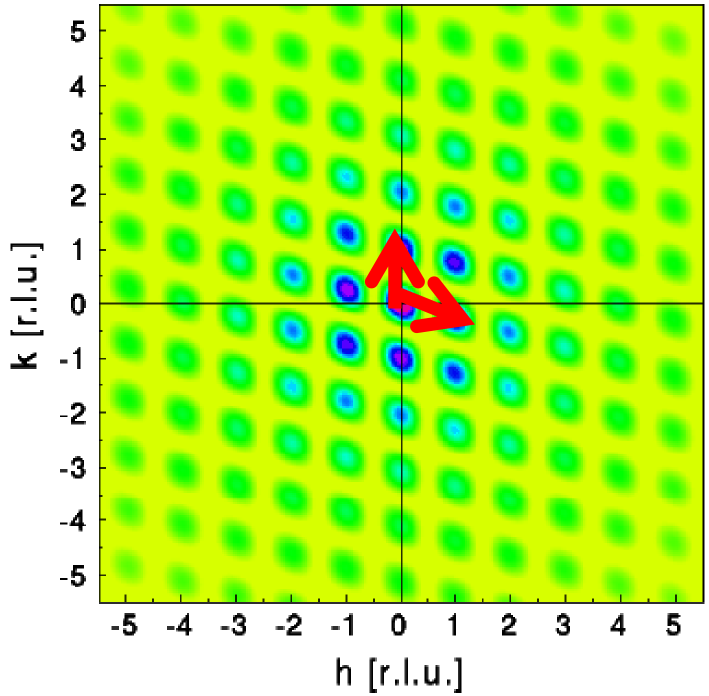
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

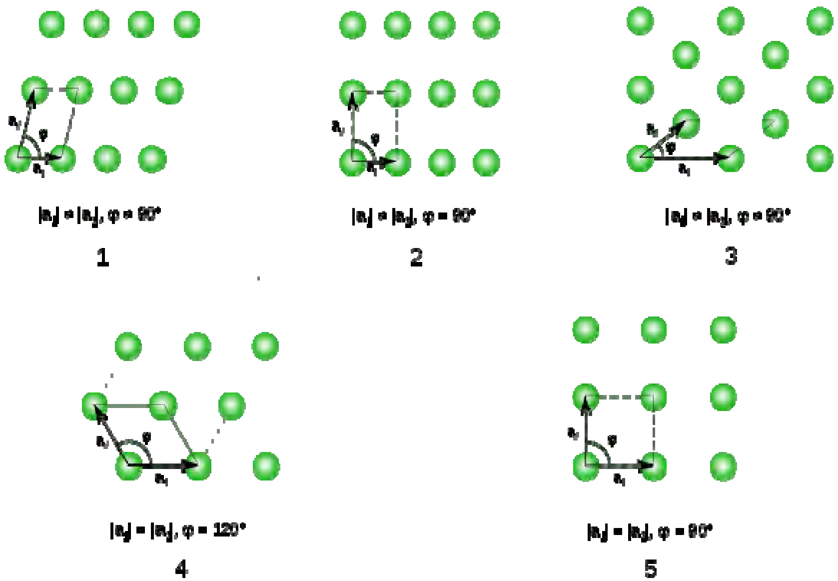
$$\mathbf{K} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$$

Primitive cell
Wigner-Seitz cell (WS)

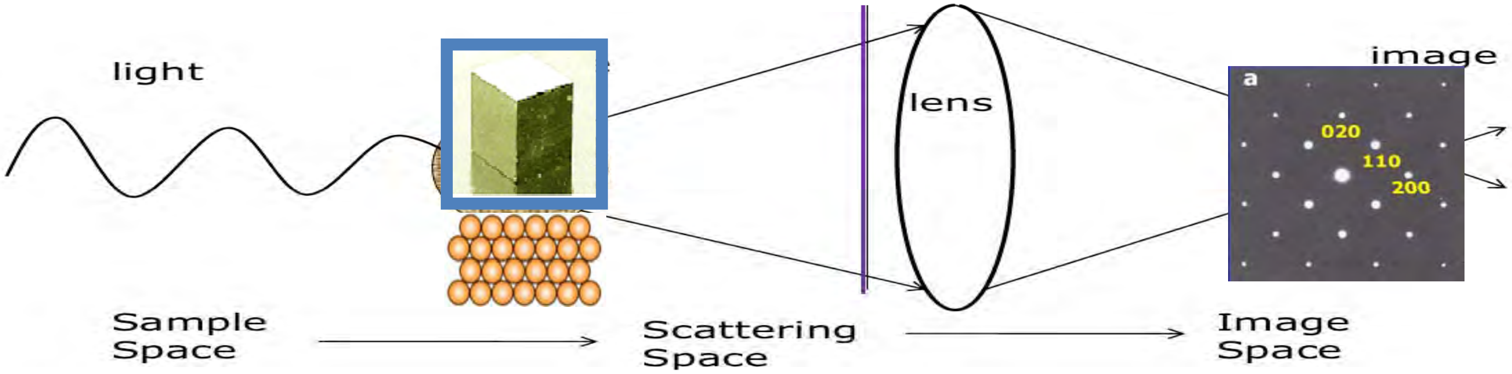
Primitive cell

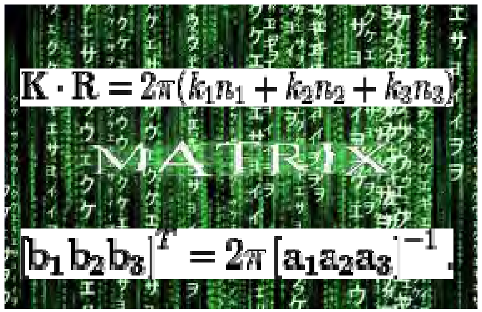

k [r.l.u.]
h [r.l.u.]
5
4
3
2
1
0
-1
-2
-3
-4
-5

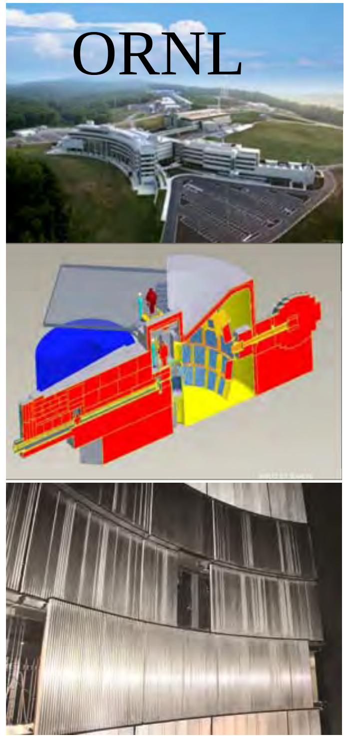

k [r.l.u.]
h [r.l.u.]
5
4
3
2
1
0
-1
-2
-3
-4
-5


1
2
3
4
5

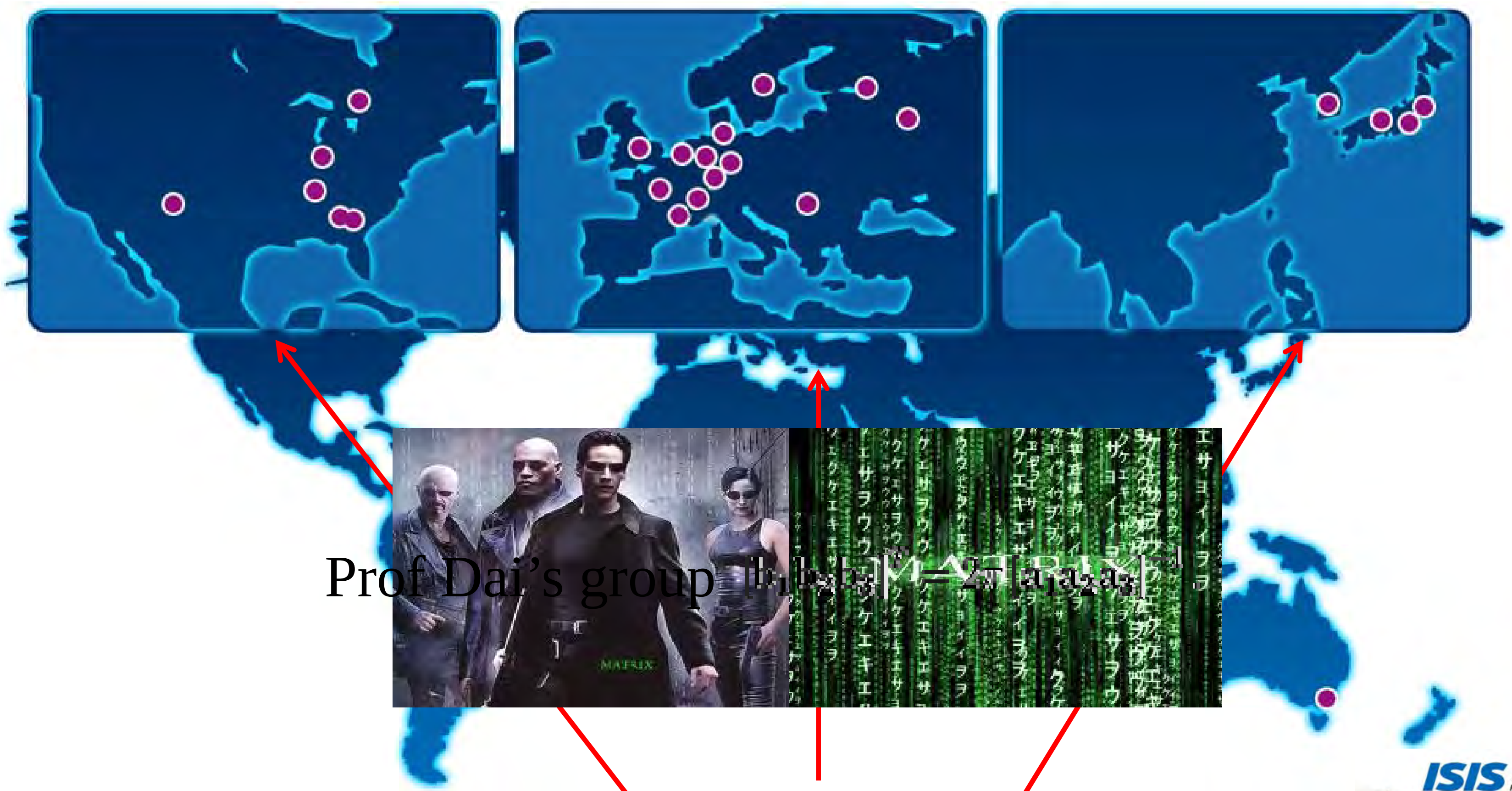
Thinking in Reciprocal space





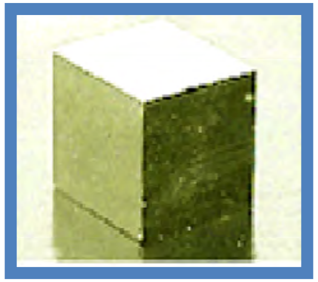


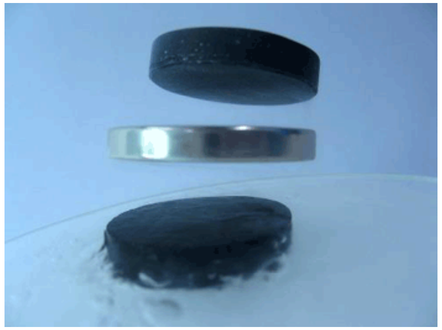
Where are the reciprocal space stations on earth?

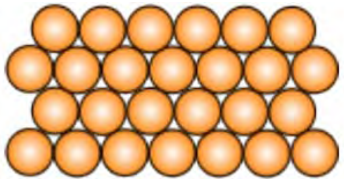


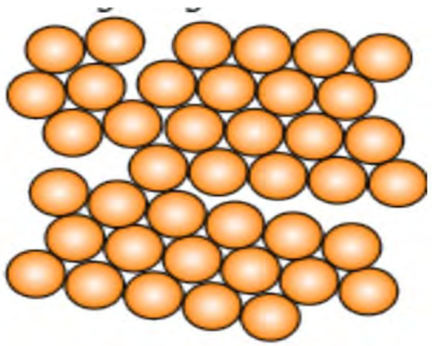
Prof Dai's group

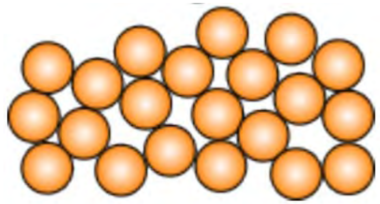
Which one is physicists' favorit?



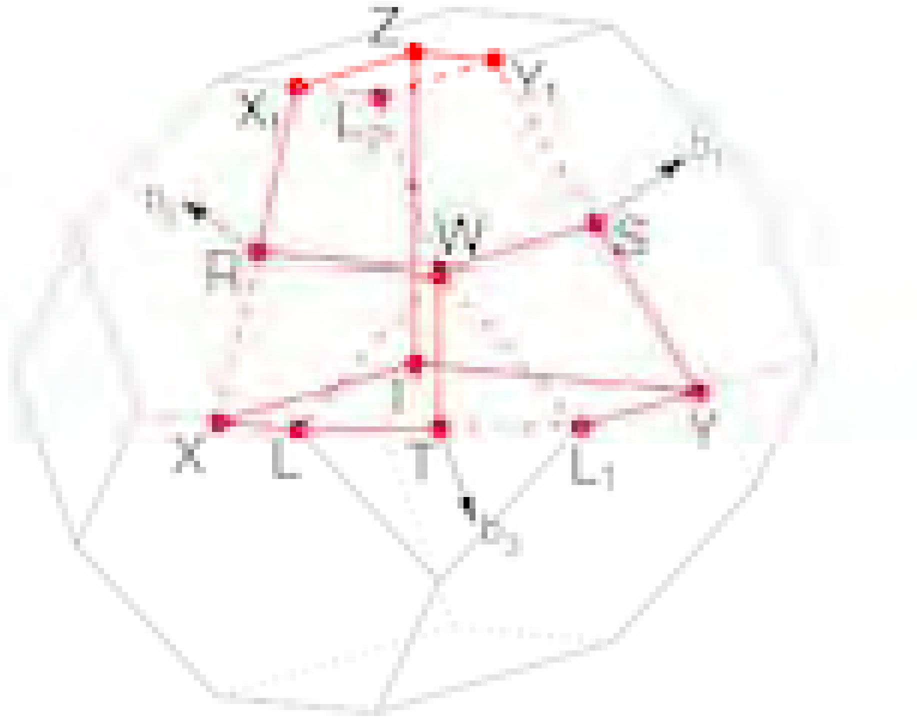






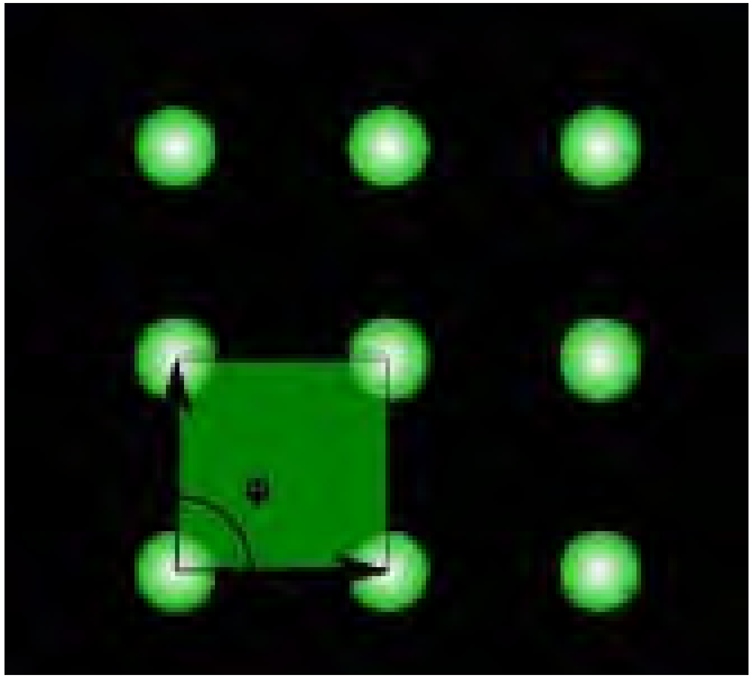


Brillouin zone

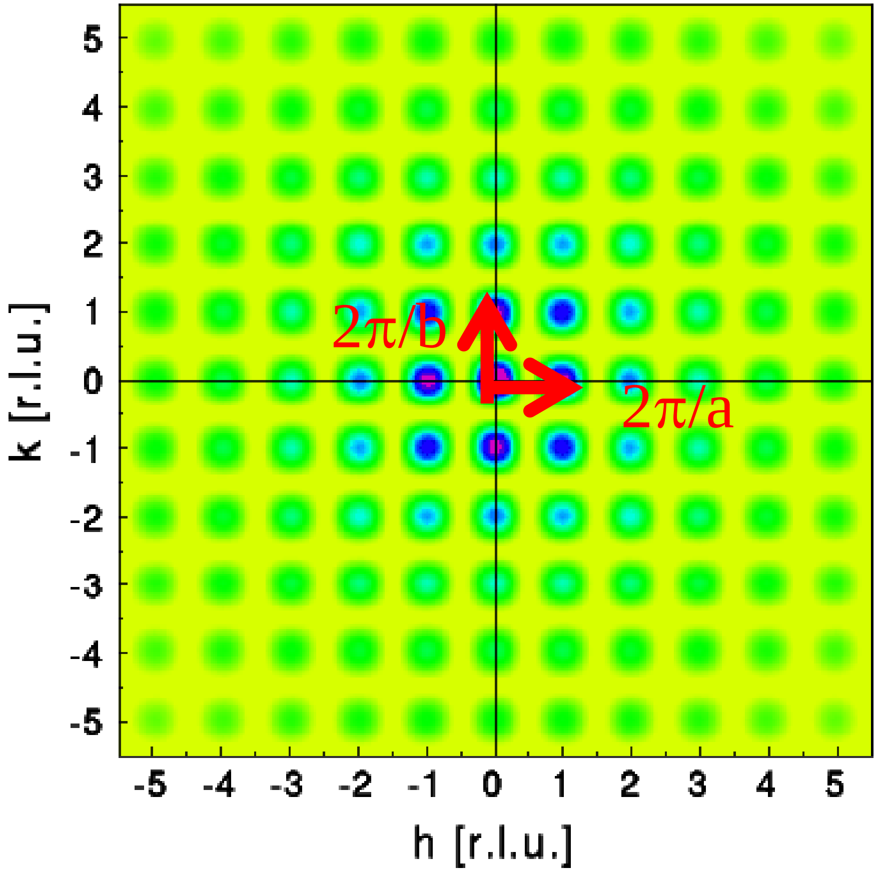


ORCI path: Γ-X-L-T-W-R-X_1-Z-Γ-Y-S-W|L_1-Y|Y_1-Z

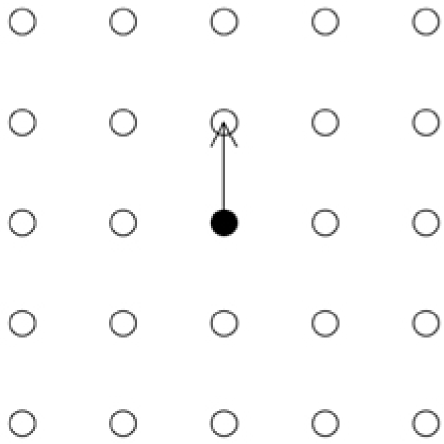
R space



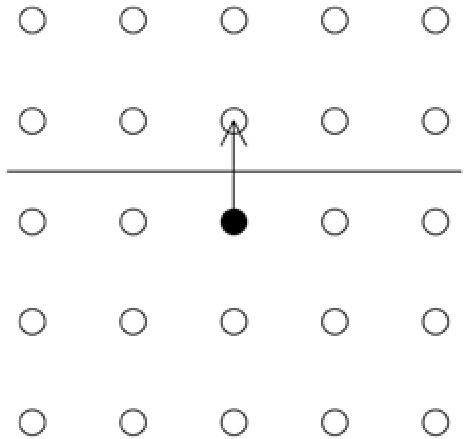
K space



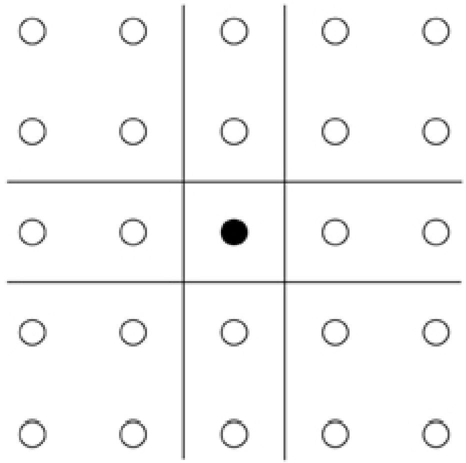
Square Lattice



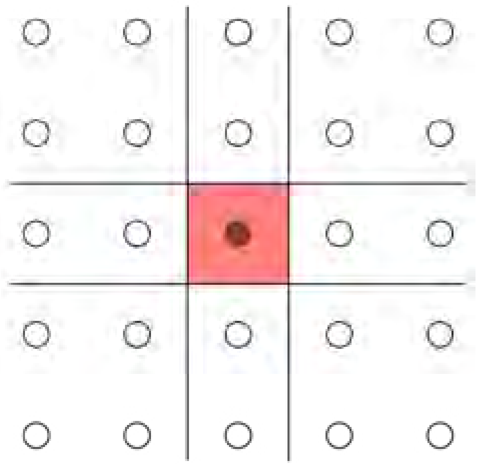
Square Lattice



Square Lattice

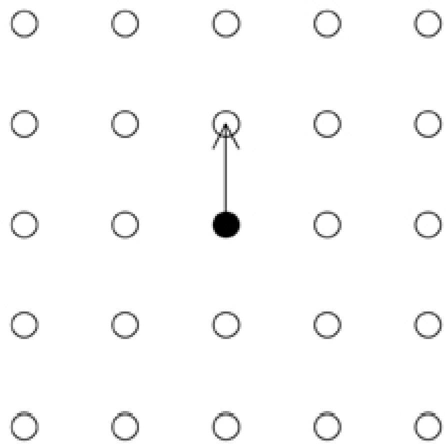


Square Lattice: 1st brillouin zone

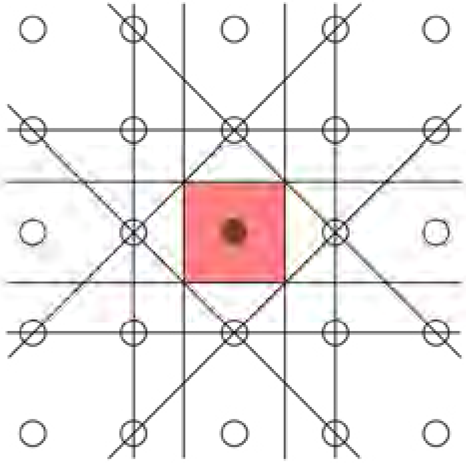


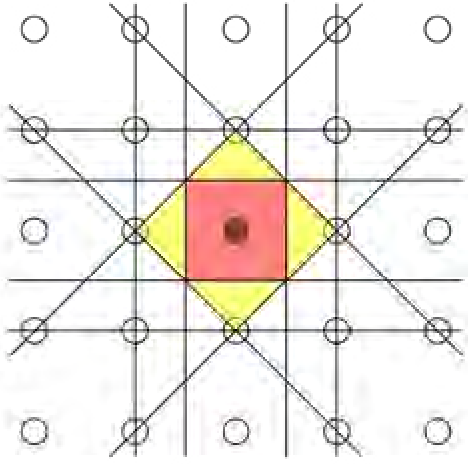
The locus of points in reciprocal space that have no Bragg Planes between them and the origin defines the first Brillouin Zone.

How to built the 2nd BZ?



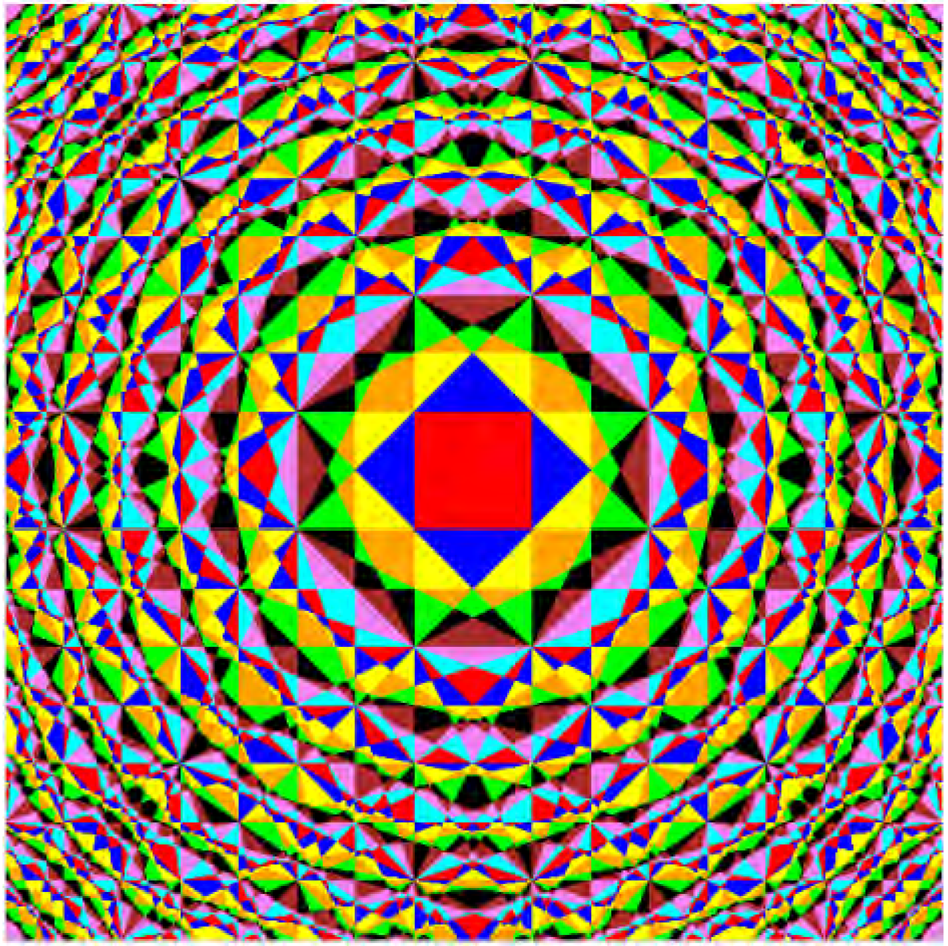
Square Lattice: 2^{nd} brillouin zone





http://nptel.iitm.ac.in/courses/113106040/Lecture30.pdf

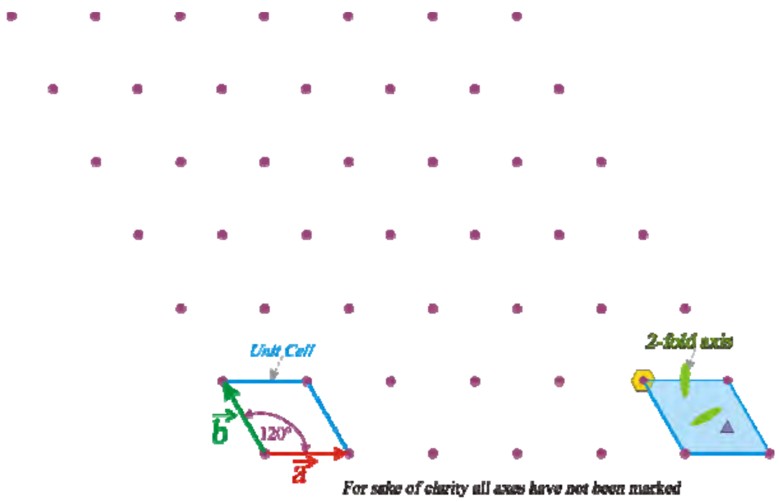
All Brillouin Zones: Square Lattice



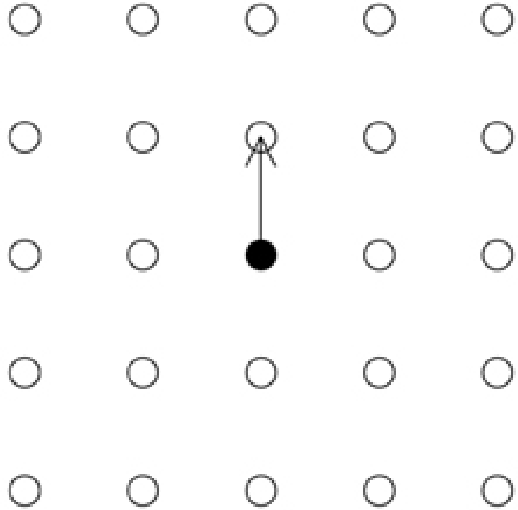
Zone folding

- http://www.doitpoms.ac.uk/tlplib/brillouin_zones/folding.php

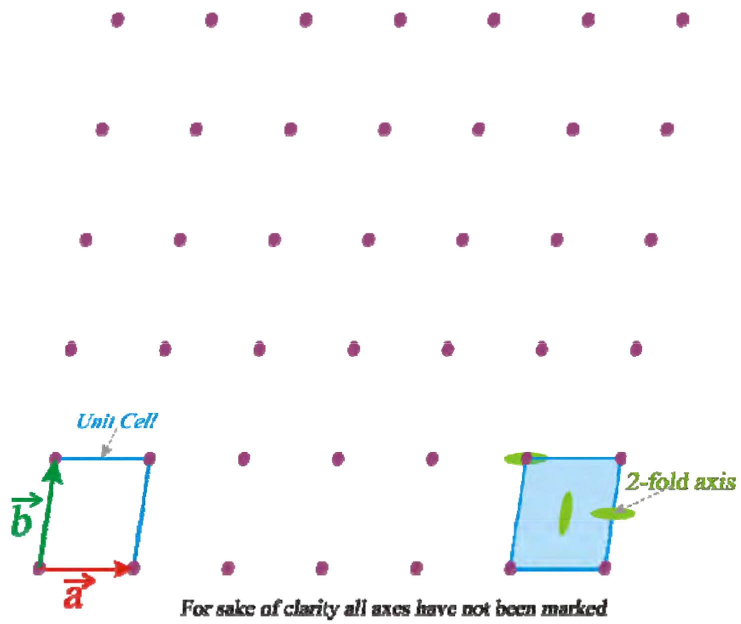
1^{st} BZ



2^{nd} BZ



1^{st} BZ

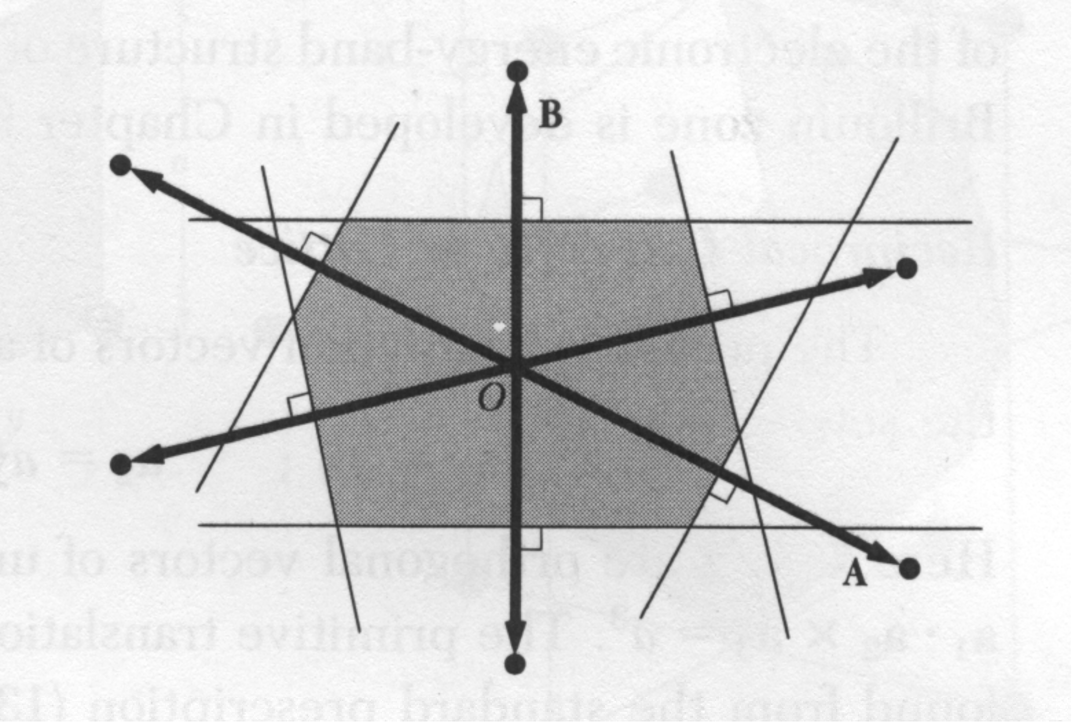


Zone folding

- http://www.doitpoms.ac.uk/tlplib/brillouin_zones/folding.php

First Brillouin zone

The Wigner-Seitz primitive cell of the reciprocal lattice is known as the first Brillouin zone. (Wigner-Seitz is real space concept while Brillouin zone is a reciprocal space idea).



3D Lattices (14)

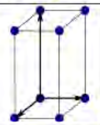
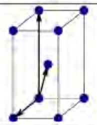
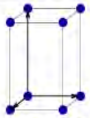
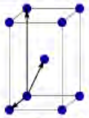
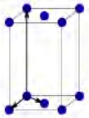
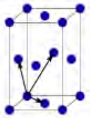
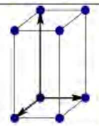
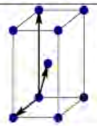
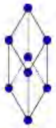
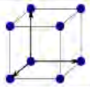
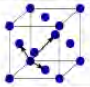
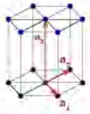
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90^\circ$ $\alpha_{12} \neq 90^\circ$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^\circ$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^\circ$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120^\circ$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^\circ$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120^\circ$ $\alpha_{23} = \alpha_{31} = 90^\circ$				

Table 1.1: Bravais lattices in three-dimensions.

3D BZ

http://lamp.tu-graz.ac.at/~hadley/ss1/bzones/

Acknowledge

- Pengcheng’s slides
- Profs in condensed matter physics
- internet