Chapter 4: Crystal Lattices

1913 : - W and L. Bragg showed experimentally that atoms are arranged periodically in crystals

- X-ray crystallography is founded

Bravais lattice

2 Definitions

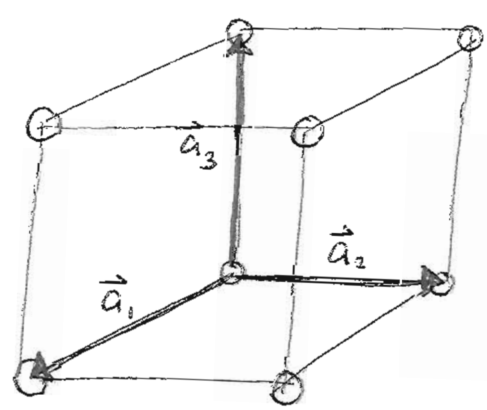
1) an infinite array of discreet points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed.

2) A (3-D) Bravais lattice consists of all points with position vectors $\vec{R}$ of the form

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

where $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ are any 3 vectors not all in the same plane, and n_1, n_2, and n_3 range through all integral values.

$\vec{a}_1, \vec{a}_2, \vec{a}_3$ are called primitive vectors
" " "
"generate or span" the lattice

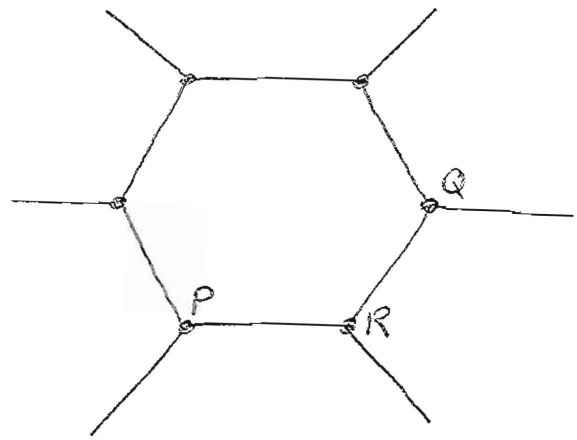


simple cubic

$\vec{a}_1 \perp \vec{a}_2 \perp \vec{a}_3$

$|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3|$

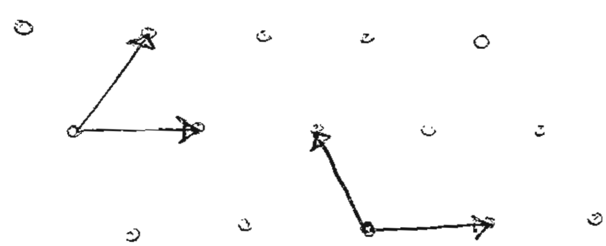
Not all lattices are Bravais lattices



P and Q : lattice looks same from either of these

P and R : lattice looks different from these

For ~~[illegible]~~ a given Bravais lattice, the primitive vectors are not unique



Some set of primitive vectors may be more convenient, however, for a given circumstance

→ some freedom to pick the most advantageous set at a given time

Important Types of Bravais lattices

simple Cubic (sc)	body-centered cubic (bcc)	face-centered cubic (fcc)

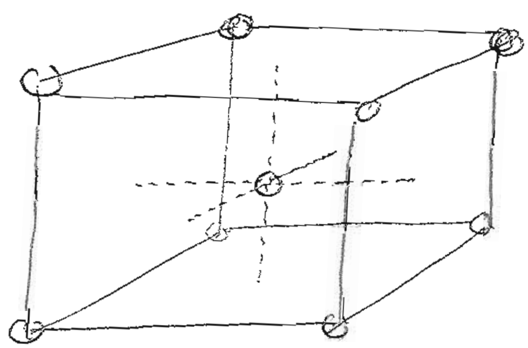
Some Cubic Types

simple cubic

possible set of primitive vectors:

$$\boxed{\vec{a}_1 = a\hat{x} \qquad \vec{a}_2 = a\hat{y} \qquad \vec{a}_3 = a\hat{z}}$$

body-centered cubic



corner and body-centered atoms are equivalent

possible set of primitive vectors

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

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

or

more symmetric set

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

To check if a given set of vectors composes a primitive set, one can think:

a) can 2 of the vectors span all the points within a single 2-D plane of the crystal?

b) does the 3rd vector connect 2 points on adjacent planes of the crystal?

If both answers are yes, then the set is indeed a primitive vector set

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exercise: show yourself that both sets given above for bcc span the lattice

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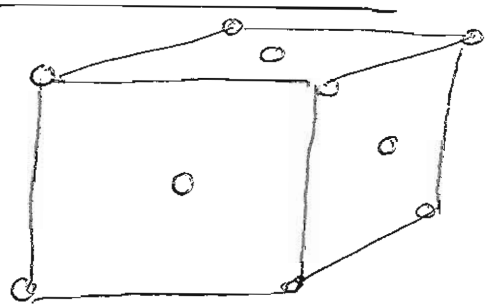
face-centered cubic (fcc)



- corner atoms
- face-center atoms

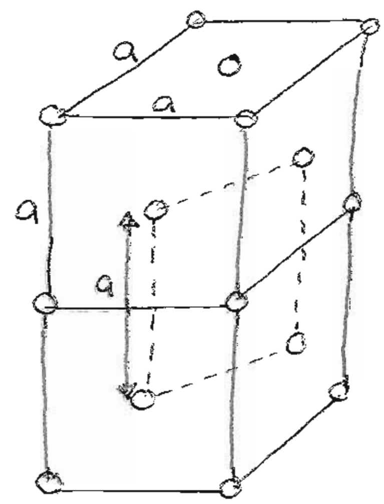
⇒ equivalent

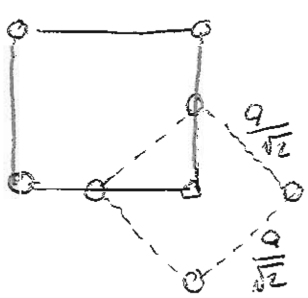
a primitive set

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$





fcc $\Leftrightarrow$ bct

$(a \times a \times a)$

$(a = b = c)$

$\left(\frac{a}{\sqrt{2}}, \frac{a}{\sqrt{2}}, a\right)$

$(a = b \neq c)$

bcc $\Leftrightarrow$ fct

(a, a, a)

$(\sqrt{2}a, \sqrt{2}a, a)$