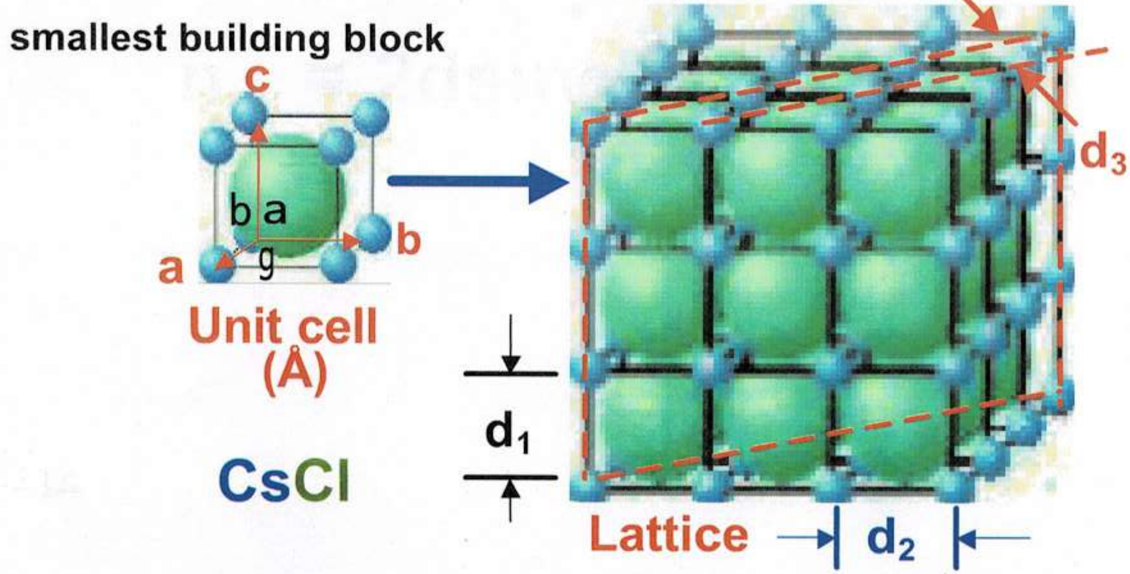
2.0 Basics of Crystallography



A crystal consists of a periodic arrangement of the unit cell into a lattice. The unit cell can contain a single atom or atoms in a fixed arrangement.

Crystals consist of planes of atoms that are spaced a distance d apart, but can be resolved into many atomic planes, each with a different d-spacing.

a,b **and** c **(length) and** α, β **and** γ **angles between a,b and c are lattice constants or parameters which can be determined by XRD.**

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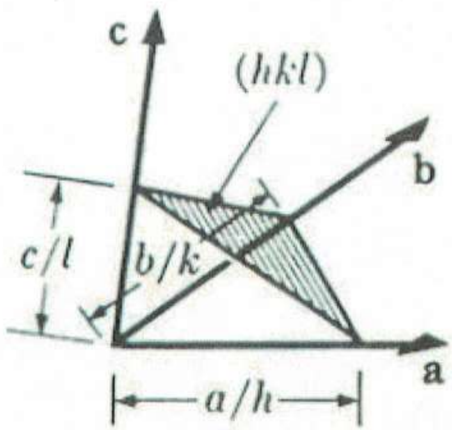
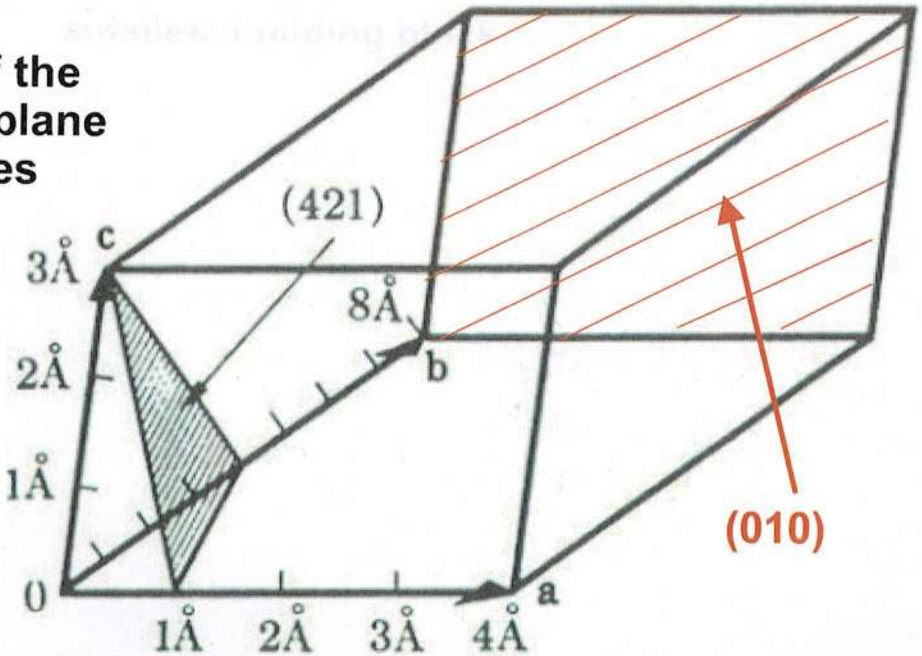
Seven Crystal Systems - Review

Crystal class	Axis system
Cubic	$a = b = c,\ \alpha = \beta = \gamma = 90^\circ$
Tetragonal	$a = b \neq c,\ \alpha = \beta = \gamma = 90^\circ$
Hexagonal	$a = b \neq c,\ \alpha = \beta = 90^\circ,\ \gamma = 120^\circ$
Rhombohedral	$a = b = c,\ \alpha = \beta = \gamma \neq 90^\circ$
Orthorhombic	$a \neq b \neq c,\ \alpha = \beta = \gamma = 90^\circ$
Monoclinic	$a \neq b \neq c,\ \alpha = \gamma = 90^\circ,\ \beta \neq 90^\circ$
Triclinic	$a \neq b \neq c,\ \alpha \neq \beta \neq \gamma \neq 90^\circ$

Miller Indices: hkl - Review

Miller indices-the reciprocals of the fractional intercepts which the plane makes with crystallographic axes





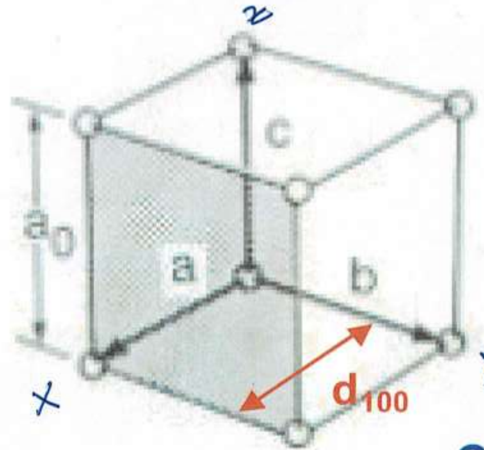
	a	b	c
Axial length	4Å	8Å	3Å
Intercept lengths	1Å	4Å	3Å
Fractional intercepts	¼	½	1
Miller indices	4	2	1
	h	k	l

a	b	c
4Å	8Å	3Å
¥	8Å	¥
0	1	0
0	1	0
h	k	l

4/ ¥ =0

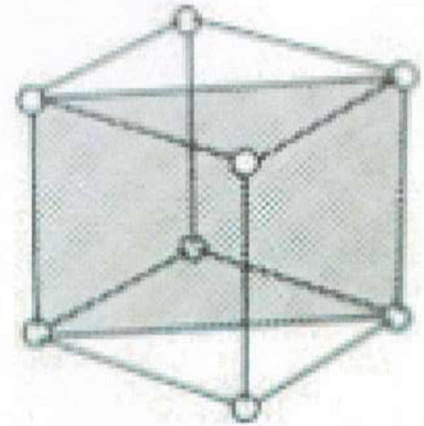
Several Atomic Planes and Their d-spacings in a Simple Cubic - Review

a	b	c
1	0	0
1	0	0



(100)

Cubic
$a=b=c=a_0$



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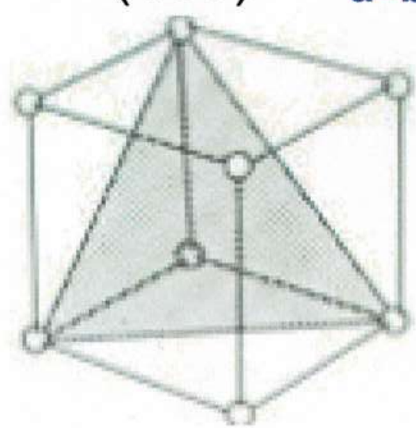
a	b	c
1	1	0
1	1	0

a	b	c
1	1	1
1	1	1



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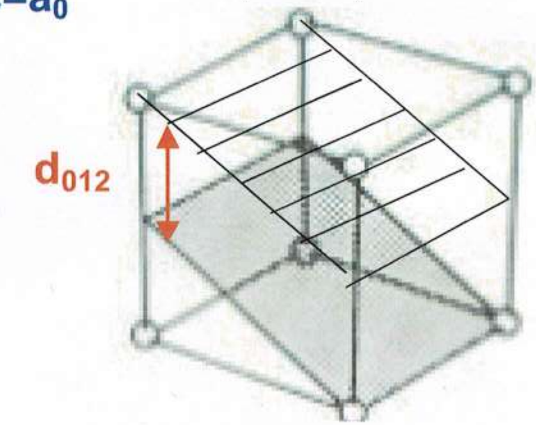


(012)

a	b	c
0	1	½
0	1	2

Black numbers-fractional intercepts, Blue numbers-Miller indices

Peak Position

d-spacings and lattice parameters

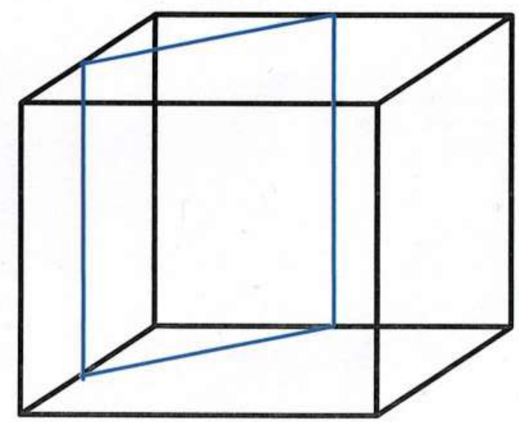
l = 2d_{hkl}sinq_{hkl}

Fix l (Cu ka) = 1.54Å **d_{hkl} = 1.54Å/2sinq_{hkl}**

(Most accurate d-spacings are those calculated from high-angle peaks)

For a simple cubic (a = b = c = a_0)

$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$



→ **a_0 = d_{hkl} /$(h^2+k^2+l^2)^{1/2}$**

e.g., for NaCl, 2q_{220}=46°, q_{220}=23°,

d_{220} =1.9707Å, a_0=5.5739Å

Bragg's Law and Diffraction:

How waves reveal the atomic structure of crystals

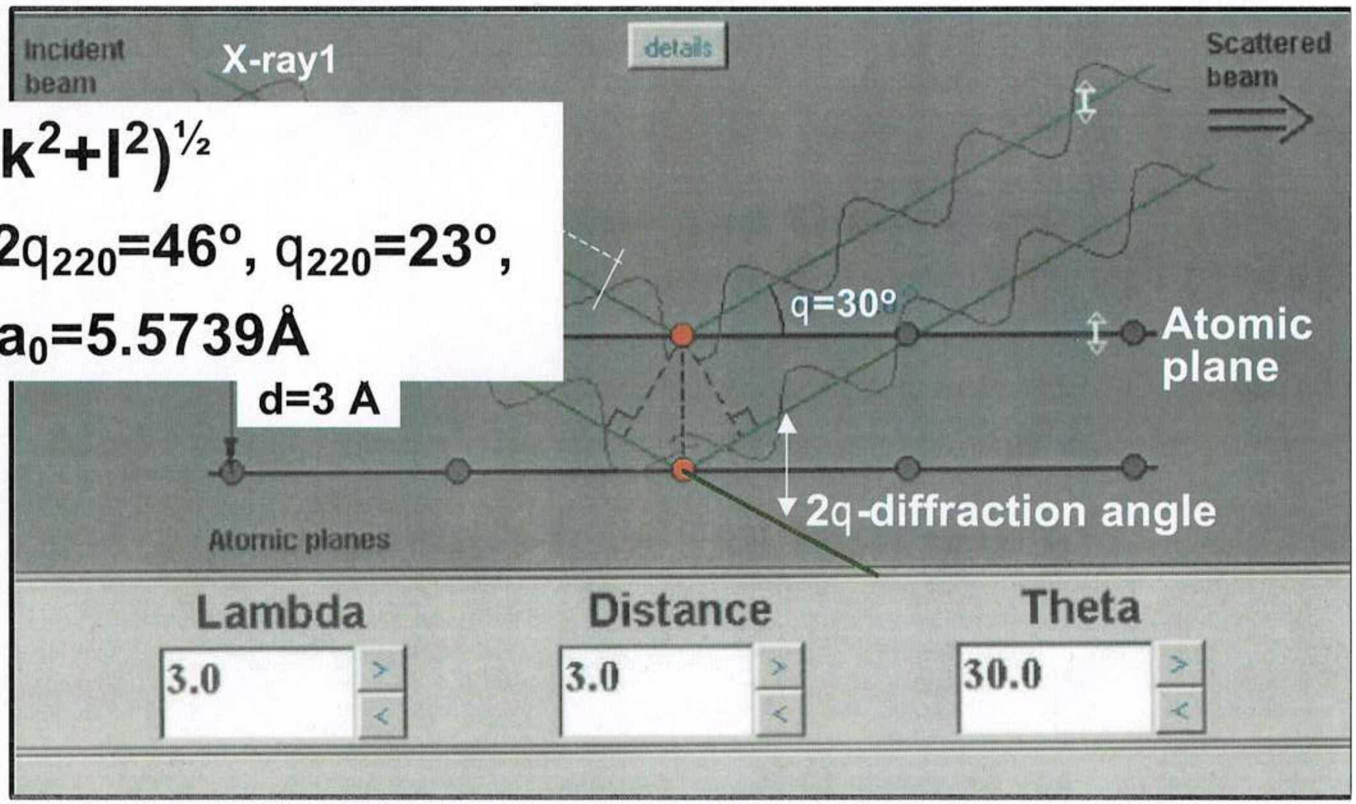
$$n\,l = 2d\sin q$$ n-integer

Diffraction occurs only when Bragg's Law is satisfied Condition for constructive interference (X-rays 1 & 2) from planes with spacing d

$a_0 = d_{hkl} / (h^2+k^2+l^2)^{1/2}$

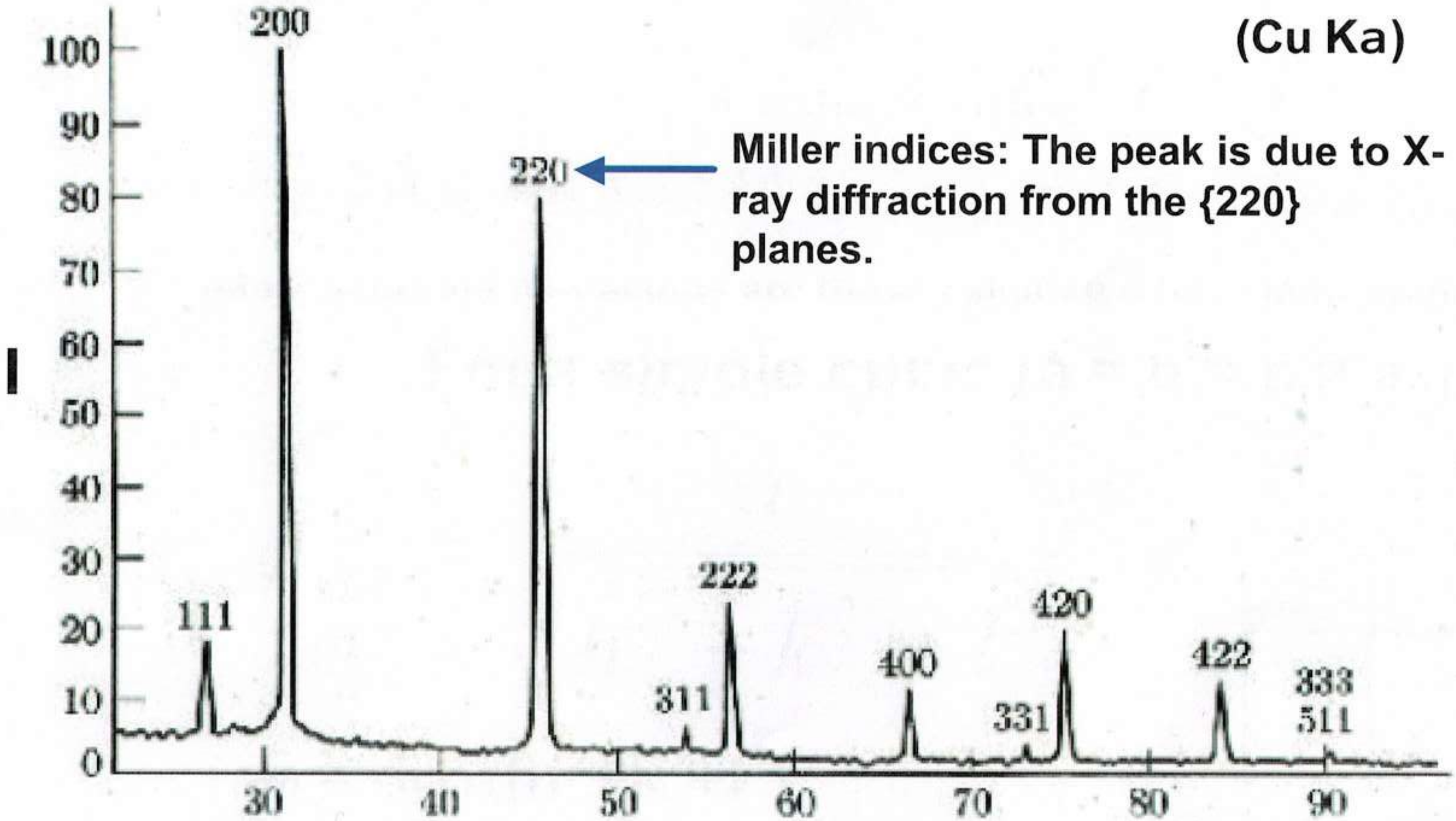
e.g., for NaCl, $2q_{220}=46°$, $q_{220}=23°$,

$d_{220} = 1.9707Å$, $a_0=5.5739Å$



http://www.eserc.stonybrook.edu/ProjectJava/Bragg/

XRD Pattern of NaCl Powder



Diffraction angle 2q (degrees)

Significance of Peak Shape in XRD

1. Peak position
2. Peak width
3. Peak intensity