Class 7

Recag = Ni-Po, simple cubic
- 1 atom per cell
- 6 neighbors (nearest)
  \[ 2r = a \]

\[ \begin{align*}
\text{Ni, Fe, body-centered cubic} \\
&2 \text{ atoms per cell} \\
&8 \text{ neighbors} \\
&\sqrt{2} \text{ a}
\end{align*} \]

\[ \begin{align*}
\text{Au, face-centered cubic} \\
&4 \text{ atoms per cell} \\
&12 \text{ neighbors} \\
&\sqrt{2} \text{ a}
\end{align*} \]
X-ray diffraction. How do we understand the structure of matter?

1895: Wilhelm Conrad Röntgen discovers X-rays.

Soon thereafter, people figure out that typical X-ray wavelengths ($\lambda \approx 1.4 \times 10^{-8} \text{ cm} = 10^{-10} \text{ m}$) are similar to spacings between atoms in crystals (which they could find from density measurements).
Max von Laue in 1912 showed that crystals diffract X-rays (Nobel in 1914).

Young W. L. Bragg in 1912 saw the von Laue paper & came up with the famous law \[ 2d \sin \theta = n \lambda \]

His father W. H. Bragg verified the formula experimentally & they shared the Nobel in 1915 (W. L. Bragg was 25!).
The Bragg Law

Ray 2 has a longer path than ray 1 by $\sqrt{rxy + y^2} = dsin\theta$ (the path difference)

by $rxy = dsin\theta$ & $y^2 = dsin\theta$
The path difference in
\[ d \sin \theta + d \sin \theta = 2d \sin \theta \]
From wave theory, constructive interference occurs when the path difference is an integral multiple of the wavelength
\[ 2d \sin \theta = n \lambda \]
the \( x \)-ray wavelength
\[ n \text{ integer} \]
\[ 2d_1 \sin \theta_1 = n \lambda \text{ etc.} \]
A knowledge of all d-spacings allows the structure to be known.
Cubic close-packing
ABCABCABC
stacking

Hexagonal close-packing
<ABABABAB->
stacking

These holes always exist
Cubic-close packing is the same as face-centered cubic.
Some other structures

Diamond

NaCl (rock salt)

4 tetrahedral neighbors

6 Na neighbors

7 Na neighbors

6 Cl neighbors

Z = 0.75

Z = 0.5

Z = 0.25

Z = 0

Z = 1
$Cs \rightarrow Cl$

$z = \frac{1}{2}$

$z = 0 = 1$

$8 \text{ neighbors}$

$Cs \text{ from } Cl$

$Cl \text{ from } Cs$