Answer on Question #51234, Physics, Solid State Physics

A crystal has a cubic unit cell of 4.2 Å. Using a wavelength of 1.54 Å at what angle θ would you expect to measure the (111) peak?

Solution:

 $1/d^2 = h^2/a^2 + k^2/b^2 + l^2/c^2$ so for the (111) of a cubic cell $d_{111} = a/\sqrt{3}$. Applying the Bragg condition for diffraction: $\lambda = 2d_{hkl} \sin \theta_{hkl}$.

Therefore:

$$\theta = \arcsin\left(\frac{\lambda}{2d_{hkl}}\right) = \arcsin\left(\frac{1.54 \cdot 10^{-10}}{2 \cdot 4.2 \cdot 10^{-10}}\right) = 18.5^{\circ}$$

Answer: Thus $\theta = 18.5^{\circ}$ and the peak is measured at $2\theta = 37^{\circ}$