Structure factor of the fcc lattice:

When the atoms of the fcc basis are identical and are located at $\vec{r}_1 = 0$, $\vec{r}_2 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3)$, $\vec{r}_3 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$, $\vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2)$, the structure form factor (scattering amplitude) is:

$$S_G(hk\ell) = f[1 + e^{-i\pi(k+\ell)} + e^{-i\pi(h+\ell)} + e^{-i\pi(h+k)}].$$

- Either $S_G = 0$ and this occurs when two of the exponentials equal -1 and the third equal +1. This requires that either two indices are even integers and one odd, or two indices are odd and one even.
- Or $S_G = 4f$ and this occurs when either all indices are even integers, or all are odd integers.

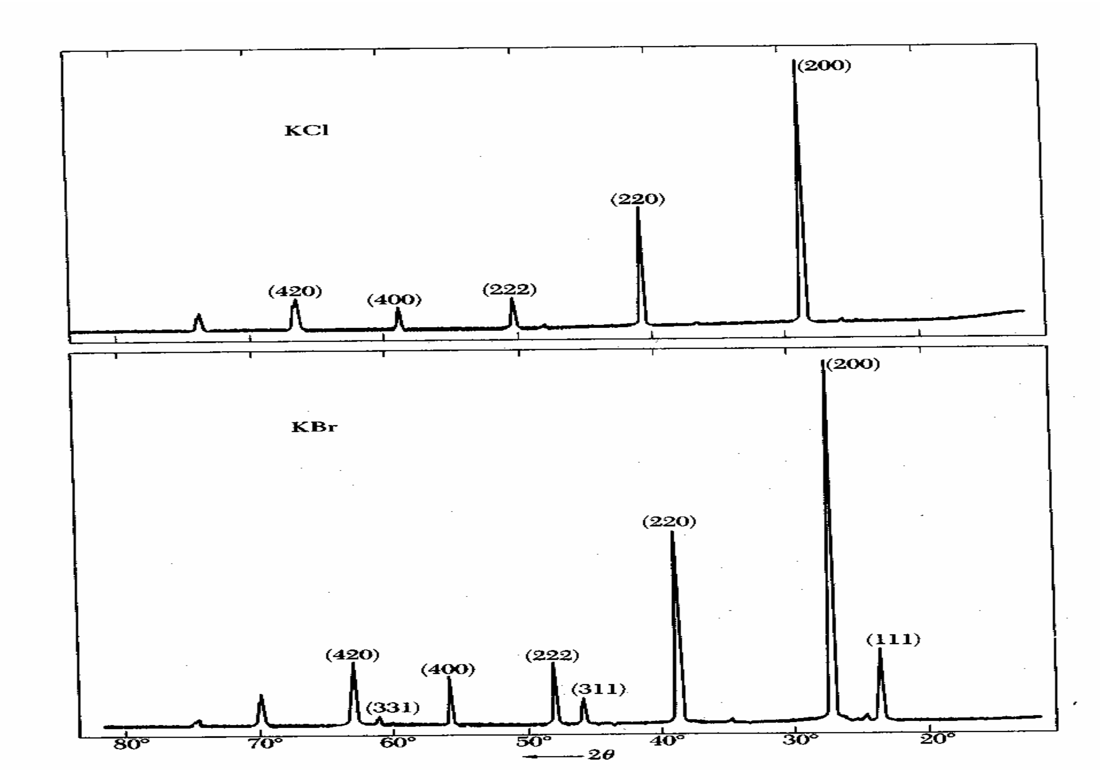

Figure 40: The x-ray diffraction from KCl and KBr powders.

Note: The KCl crystal structure which crystallizes like fcc lattice with a basis consisting of K^+ ion at 0 and Cl^- at the center of conventional cell $\frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$, looks to x-rays as if it were a monatomic simple cubic lattice of lattice constant $a/2$. This is because the number of electrons of K^+ ion and Cl^- are equal and thus the scattering amplitudes $f(K^+)$ and $f(Cl^-)$ are almost the same. (See figure 40).

Exercise:

The neutron diffraction pattern for powdered diamond is shown in figure 41. Find:

a) The structure factor of the basis of the conventional cell of diamond.

b) Show that the allowed reflections of the diamond structure satisfy $h + k + \ell = 4n$, where all indices are even and n is an integer, or else all indices are odd.

c) The zeros of structure factor.

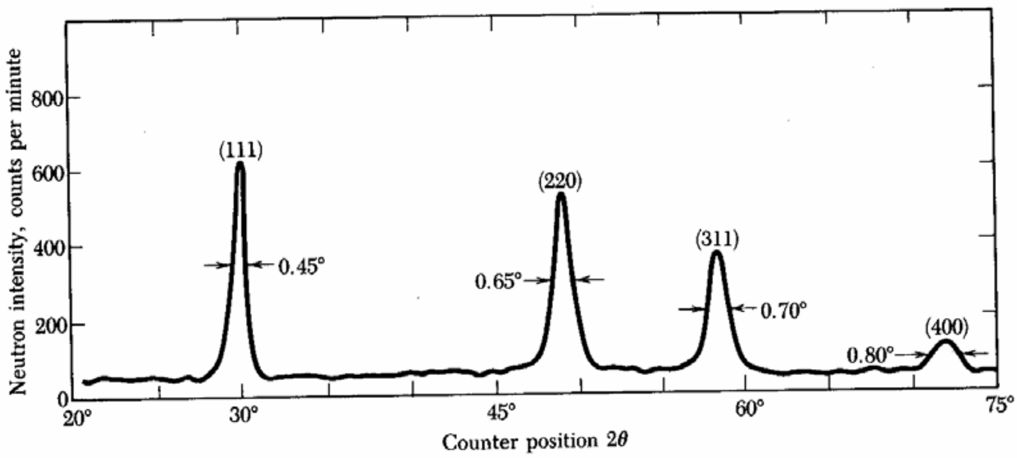

Figure 41:Neutron diffraction pattern for powdered diamond.