Laue simulation report

This chapter focuses on 1D lattices. The Bragg condition quantifies the existence of a constructive interference between the X-rays scattered by two atoms in a lattice with lattice constant $a$.

$$2a \sin \theta = n\lambda$$

However, it is not enough to imagine atoms as point particles. The kinematic theory of x-ray diffraction states that the amplitude for the diffraction of an x-ray beam with initial wave vector $k$ to a final state with wave vector $k'$ is proportional to the Fourier transform of the electron density.

$$A(k \leftrightarrow k') \propto \int \rho(r) \exp(i\Delta k \cdot r) dr$$

If $\rho(r)$ is periodic, the diffraction intensity is non-zero only for a discrete set of values $\Delta k = G$, where $G$ is a vector of the reciprocal lattice. In 1D the reciprocal lattice has lattice constant $2\pi/a$. The permissible given $\Delta k$ values are given by the Laue condition:

$$\Delta k = \frac{2\pi n}{a}$$

Ex. 1. Select PRESET 1 of “laue” to see the electron density of a mono-atomic crystal on the left and the corresponding diffraction pattern on the right. The interatomic spacing is $a = 4 \text{Å}$. Write down the position of a few peaks. Verify that the peaks occur at the values of $\Delta k$ appropriate to the parameters in the panel display.

Ex. 2. Increase the lattice constant by a factor of 2. What is the effect on the diffraction pattern?
The diffraction plots show a decreasing intensity with increasing $\Delta k$ because the interference is different for different parts of the finite-sized atom. If the X-ray wavelength is large compared with the atomic size, waves scattered from different parts of the atom interfere constructively and the scattered amplitude is proportional with the number of electrons. The $\Delta k$-dependence of the scattered amplitude is described by the atomic form factor

$$f(\Delta k) = \int \rho(x) \exp(i\Delta k x) \, dx$$

Ex. 3. Use PRESET 2 to obtain the diffraction pattern of a single atom for with the atom shape is a Gaussian,

$$\rho(x) = \frac{Z}{\sigma \sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

Vary the size of the atom to find the relation between the atom size and the width in $\Delta k$ of the atomic form factor.

We can combine the Bragg condition and the atomic form factor to describe the intensity of the wave scattered from a crystal.

1. The intensity $I(\Delta k)$ is non-zero only when $\Delta k$ is a multiple of $2\pi/a$.
2. The intensity of the peak at $\Delta k=2\pi/a$ is proportional to the square of the atomic form factor evaluated at this $\Delta k$.

Ex. 4. Verify the two statements above. Load PRESET 2, CALCULATE, and COPY DIFFRACTION. Now select the MONATOMIC CRYSTAL from the MATERIAL menu, calculate again, and then STEAL DATA to compare the envelope of the crystal diffraction pattern with the single-atom diffraction. Are the values of $\Delta k$ at the peaks in the diffraction graph correct? Does the atomic diffraction pattern match the envelope of the peaks?
If there is more than one atom in the unit cell of the crystal, the atomic form factor needs to be replaced by the structure factor $S(\Delta k) = \sum_j \exp(i\Delta k x_j) f_j(\Delta k)$, where the sum is over the different atoms in the unit cell.

Let us assume we have a pair of identical atoms at distance $d$ in the unit cell. Then

$S(\Delta k) = f(\Delta k) + \exp(i\Delta k d) f(\Delta k)$

Ex. 5.
In some cases, even though the Bragg condition is satisfied, the scattering from two atoms interferes destructively to give zero intensity. Determine analytically the condition for these extinctions.

Ex. 6. STEAL DATA to compare the diffraction pattern of the DIATOMIC CRYSTAL with that of the ATOM PAIR. Change the position of the second atom to other values of $d/a = 1/2n$, with $n$ an integer, and verify that “laue” is correctly calculating the diffraction pattern.

Ex. 7. What is the diffraction pattern for a large ($>>1$) ratio of ATOMIC NUMBERS $Z_A/Z_B$? Or for a small ratio? Do you obtain any extinctions when the atomic numbers are different?