3.18: Laue equations

The three Laue equations give the conditions to be satisfied by an incident wave to be diffracted by a crystal. Consider the three basis vectors, **OA** = **a**, **OB** = **b** , **OC** = **c** of the crystal and let $\vec{s}_o$ and $\vec{s}_h$ be unit vectors along the incident and reflected directions, respectively. The conditions that the waves scattered by *O* and *A*, *O* and *B*,*O* and *C*, respectively, be in phase are that

$$\vec{a} \cdot (\mathrm{s}_h - \vec{s}_o) = h\lambda$$

$$\vec{b} \cdot (\vec{s}_h - \vec{s}_o) = k\lambda$$

$$\vec{c} \cdot (\vec{s}_h - \vec{s}_o) = l\lambda$$

If these three conditions are simultaneously satisfied, the incoming wave is reflected on the set of lattice planes of Miller indices *h/n, k/n, l/n*. *h, k, l* are the indices of the reflection.

The three Laue equations can be generalized by saying that the diffraction condition is satisfied if the scalar product

$$\vec{r} \cdot (\vec{s}_h/\lambda - \vec{s}_o/\lambda)$$

is an integer for any vector

$$\vec{r} = u\vec{a} + v\vec{b} + w\vec{c}$$

where (u, v, w integers) of the direct lattice. This is the case if

$$(\mathbf{s_h}/\lambda - \mathbf{s_0}/\lambda) = h\,\mathbf{a^*} + k\,\mathbf{b^*} + l\,\mathbf{c^*},$$

where *h, k, l* are integers, namely if the diffraction vector **OH** = $\mathbf{s_h}$,/λ - $\mathbf{s_0}$/λ is a vector of the reciprocal lattice. This is the diffraction condition in reciprocal space.

History

The three Laue conditions for diffraction were first given in Laue, M. (1912). *Eine quantitative Prüfung der Theorie für die Interferenz-Erscheinungen bei Röntgenstrahlen*. *Sitzungsberichte der Kgl. Bayer. Akad. der Wiss* 363--373, reprinted in *Ann. Phys.* (1913), **41**, 989-1002 where he interpreted and indexed the first diffraction diagram (Friedrich, W., Knipping, P., and Laue, M. (1912). *Interferenz-Erscheinungen bei Röntgenstrahlen*, *Sitzungsberichte der Kgl. Bayer. Akad. der Wiss*, 303--322, reprinted in *Ann. Phys.*, (1913), **41**, 971-988, taken with zinc-blende, ZnS. For details, see P. P. Ewald, 1962, IUCr, 50 Years of X-ray Diffraction, Section 4, page 52.

Contributors

- Online Dictionary of Crystallography