

1.1. SUMMARY OF GENERAL FORMULAE

Finally, the angle ω between a first direction $[uvw]$ of the direct lattice and a second direction $[hkl]$ of the reciprocal lattice may also be derived from the scalar product of the corresponding vectors \mathbf{t} and \mathbf{r}^* .

$$\cos \omega = \frac{\mathbf{t} \cdot \mathbf{r}^*}{tr^*} = \frac{uh + vk + wl}{tr^*}. \quad (1.1.3.8)$$

1.1.4. The Miller formulae

Consider four faces of a crystal that belong to the same zone in consecutive order: $(h_1k_1l_1)$, $(h_2k_2l_2)$, $(h_3k_3l_3)$, and $(h_4k_4l_4)$. The angles between the i th and the j th face normals are designated φ_{ij} . Then the Miller formulae relate the indices of these faces to the angles φ_{ij} :

$$\frac{\sin \varphi_{12} \sin \varphi_{43}}{\sin \varphi_{13} \sin \varphi_{42}} = \frac{u_{12}u_{43}}{u_{13}u_{42}} = \frac{v_{12}v_{43}}{v_{13}v_{42}} = \frac{w_{12}w_{43}}{w_{13}w_{42}} \quad (1.1.4.1)$$

with

$$u_{ij} = \left| \frac{k_i l_i}{k_j l_j} \right|, \quad v_{ij} = \left| \frac{l_i h_i}{l_j h_j} \right|, \quad w_{ij} = \left| \frac{h_i k_i}{h_j k_j} \right|.$$

If all angles between the face normals and also the indices for three of the faces are known, the indices of the fourth face may be calculated. Equation (1.1.4.1) cannot be used if two of the faces are parallel.

From the definition of u_{ij} , v_{ij} , and w_{ij} , it follows that all fractions in (1.1.4.1) are rational:

$$\frac{\sin \varphi_{12} \sin \varphi_{43}}{\sin \varphi_{13} \sin \varphi_{42}} = \frac{p}{q} \quad \text{with } p, q \text{ integers.}$$

Therefore, (1.1.4.1) may be rearranged to

$$p \cot \varphi_{12} - q \cot \varphi_{13} = (p - q) \cot \varphi_{14}. \quad (1.1.4.2)$$

This equation allows the determination of one angle if two of the angles and the indices of all four faces are known.