1.91: Reciprocal Space

The basis vectors **a***, **b***, **c*** of the reciprocal space are related to the basis vectors **a**, **b**, **c** of the direct space (or crystal space) through either of the following two equivalent sets of relations:

(1)

a*. **a** = 1; **b***. **b** = 1; **c***. **c** = 1;

a*. **b** = 0; **a***. **c** = 0; **b***. **a** = 0; **b***. **c** = 0; **c***. **a** = 0; **c***. **b** = 0.

(2)

a* = (**b** × **c**)/ (**a**, **b**, **c**);

b* = (**c** × **a**)/ (**a**, **b**, **c**);

c* = (**b** × **c**)/ (**a**, **b**, **c**);

where (**b** × **c**) is the vector product of basis vectors **b** and **c** and (**a**, **b**, **c**) = *V* is the triple scalar product of basis vectors **a**, **b**and **c** and is equal to the volume *V* of the cell constructed on the vectors **a**, **b** and **c**.

The reciprocal and direct spaces are reciprocal of one another, that is the reciprocal space associated to the reciprocal space is the direct space. They are related by a Fourier transform and the reciprocal space is also called *Fourier space* or *phase space*.

The **vector product** of two direct space vectors, $\mathbf{r}_1 = u_1 \mathbf{a} + v_1 \mathbf{b} + w_1 \mathbf{c}$ and $\mathbf{r}_2 = u_2 \mathbf{a} + v_2 \mathbf{b} + w_2 \mathbf{c}$ is a reciprocal space vector,

$$\mathbf{r*} = \mathbf{r_1} \times \mathbf{r_2} = V (v_1 w_2 - v_2 w_1) \mathbf{a*} + V (w_1 u_2 - w_2 u_1) \mathbf{b*} + V (u_1 v_2 - u_2 v_1) \mathbf{c}.$$

Reciprocally, the vector product of two reciprocal vectors is a direct space vector.

As a consequence of the set of definitions (1), the **scalar product** of a direct space vector **r** = *u* **a** + *v* **b** + *w* **c** by a reciprocal space vector **r*** = *h* **a*** + *k* **b*** + *l* **c*** is simply:

r . **r*** = *uh* + *vk* +*wl*.

In a **change of coordinate system**, The coordinates of a vector in reciprocal space transform like the basis vectors in direct space and are called for that reason *covariant*. The vectors in reciprocal transform like the coordinates in direct space and are called *contravariant*.