$$\mathbf{a} = \frac{1}{V^*}(\mathbf{b}^* \times \mathbf{c}^*), \quad \mathbf{b} = \frac{1}{V^*}(\mathbf{c}^* \times \mathbf{a}^*), \quad \mathbf{c} = \frac{1}{V^*}(\mathbf{a}^* \times \mathbf{b}^*). \tag{1.1.15}$$

The relationship between the reciprocal and the real lattice parameters expressed geometrically rather than in the vector formalism used above is

$$\begin{aligned} a^* &= \frac{bc\sin\alpha}{V}, \\ b^* &= \frac{ac\sin\beta}{V}, \\ c^* &= \frac{ab\sin\gamma}{V}, \\ \cos\alpha^* &= \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}, \\ \cos\beta^* &= \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma}, \\ \cos\gamma^* &= \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}, \\ V &= abc\sqrt{1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma}. \end{aligned} \tag{1.1.16}$$

Equation (1.1.16) is the most general expression for non-orthogonal lattices. The expressions simplify considerably for higher-symmetry crystal systems.

We now re-derive Bragg's law using the vector notation introduced above (Fig. 1.1.6). The wave vectors of the incoming and outgoing beams are given by $\mathbf{s}_0$ and $\mathbf{s}$, respectively. They point in the direction of propagation of the wave and their length depends on λ. For elastic scattering (for which there is no change in wavelength on scattering), $\mathbf{s}_0$ and $\mathbf{s}$ have the same length.

We define the scattering vector as

$$\mathbf{h} = (\mathbf{s} - \mathbf{s}_0), \tag{1.1.17}$$

which for a specular reflection is always perpendicular to the scattering plane. The length of $\mathbf{h}$ is given by

$$\frac{h}{s} = 2\sin\theta. \tag{1.1.18}$$

Comparison with the formula for the Bragg equation (1.1.3),

$$\frac{n\lambda}{d} = 2\sin\theta, \tag{1.1.19}$$

gives

$$\frac{n\lambda}{d} = \frac{h}{s}. \tag{1.1.20}$$

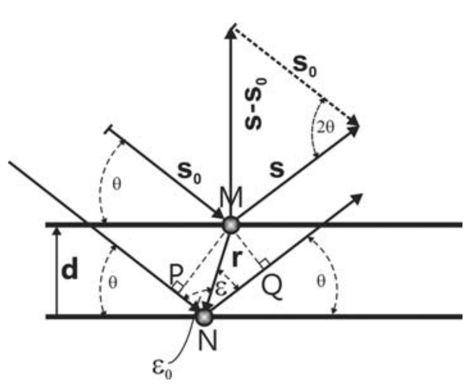

Figure 1.1.6
Illustration of the important wave and scattering vectors in the case of elastic Bragg scattering. [Reproduced from Dinnebier & Billinge (2008) with permission from the Royal Society of Chemistry.]

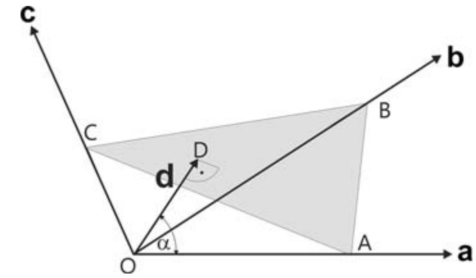

Figure 1.1.7
Geometrical description of a lattice plane in terms of real-space basis vectors. The arc and dot below the letter D indicate a right angle. [Reproduced from Dinnebier & Billinge (2008) with permission from the Royal Society of Chemistry.]

Setting the magnitude of $\mathbf{s}$ to $1/\lambda$, we get the Bragg equation in terms of the magnitude h of the scattering vector,

$$h = \frac{n}{d}. \tag{1.1.21}$$

This shows that diffraction occurs when the magnitude of the scattering vector is an integral number of reciprocal-lattice spacings $1/d$. We define a vector $\mathbf{d}^*$ perpendicular to the lattice planes with length $1/d$. Since $\mathbf{h}$ is perpendicular to the scattering plane, this leads to

$$\mathbf{h} = n\mathbf{d}^*. \tag{1.1.22}$$

Diffraction can occur at different scattering angles 2θ for the same crystallographic plane, giving the different orders n of diffraction. For simplicity, the number n will be incorporated in the indexing of the lattice planes, where

$$d^*_{nh,nk,nl} = nd^*_{hkl}, \tag{1.1.23}$$

e.g., $d^*_{222} = 2d^*_{111}$, and we get an alternative expression for Bragg's equation:

$$\mathbf{h} = \mathbf{d}^*_{hkl}. \tag{1.1.24}$$

The vector $\mathbf{d}^*_{hkl}$ points in a direction perpendicular to a real-space lattice plane. We would like to express this vector in terms of the reciprocal-space basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$.

First we define $\mathbf{d}_{hkl}$ in terms of the real-space basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. Referring to Fig. 1.1.7, we can define

$$\mathbf{OA} = \frac{1}{h}\mathbf{a}, \quad \mathbf{OB} = \frac{1}{k}\mathbf{b}, \quad \mathbf{OC} = \frac{1}{l}\mathbf{c} \tag{1.1.25}$$

with h, k and l being integers, as required by the periodicity of the lattice.

The plane-normal vector $\mathbf{d}_{hkl}$ originates on one plane and terminates on the next parallel plane. Therefore, $\mathbf{OA} \cdot \mathbf{d} = (\mathrm{OA})d\cos\alpha$. From Fig. 1.1.7 we see that, geometrically, $(\mathrm{OA})\cos\alpha = d$. Substituting, we get $\mathbf{OA} \cdot \mathbf{d} = d^2$. Combining this with equation (1.1.25) leads to

$$\frac{1}{h}\mathbf{a} \cdot \mathbf{d} = d^2 \tag{1.1.26}$$

and consequently

$$h = \mathbf{a} \cdot \frac{\mathbf{d}}{d^2}, \quad k = \mathbf{b} \cdot \frac{\mathbf{d}}{d^2}, \quad l = \mathbf{c} \cdot \frac{\mathbf{d}}{d^2}. \tag{1.1.27}$$

By definition, h, k and l are divided by their largest common integer to be Miller indices. The vector $\mathbf{d}^*_{hkl}$, from Bragg's equation (1.1.24), points in the plane-normal direction parallel to $\mathbf{d}$ but with length $1/d$. We can now write $\mathbf{d}^*_{hkl}$ in terms of the

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