vector **d**:

$$\mathbf{d}^*_{hkl} = \frac{\mathbf{d}}{d^2}, \qquad (1.1.28)$$

which gives

$$\mathbf{d}^*_{hkl} = \frac{\mathbf{d}_{hkl}}{d^2} = h\mathbf{a} + k\mathbf{b} + l\mathbf{c}, \qquad (1.1.29)$$

or written in terms of the reciprocal basis

$$\mathbf{d}^*_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*, \qquad (1.1.30)$$

which was obtained using

$$\begin{aligned}\mathbf{d}^*_{hkl}\cdot\mathbf{a}^* &= h\mathbf{a}\cdot\mathbf{a}^* + k\mathbf{b}\cdot\mathbf{a}^* + l\mathbf{c}\cdot\mathbf{a}^* = h,\\ \mathbf{d}^*_{hkl}\cdot\mathbf{b}^* &= h\mathbf{a}\cdot\mathbf{b}^* + k\mathbf{b}\cdot\mathbf{b}^* + l\mathbf{c}\cdot\mathbf{b}^* = k,\\ \mathbf{d}^*_{hkl}\cdot\mathbf{c}^* &= h\mathbf{a}\cdot\mathbf{c}^* + k\mathbf{b}\cdot\mathbf{c}^* + l\mathbf{c}\cdot\mathbf{c}^* = l. \qquad (1.1.31)\end{aligned}$$

Comparing equation (1.1.30) with equation (1.1.11) proves the identity of $\mathbf{d}^*_{hkl}$ and the reciprocal-lattice vector $\mathbf{h}_{hkl}$. Bragg's equation, (1.1.24), can be re-stated as

$$\mathbf{h} = \mathbf{h}_{hkl}. \qquad (1.1.32)$$

In other words, diffraction occurs whenever the scattering vector **h** equals a reciprocal-lattice vector $\mathbf{h}_{hkl}$. This powerful result is visualized in the useful Ewald construction, which is described in Section 1.1.2.4.

Useful equivalent variations of the Bragg equation are

$$|\mathbf{h}| = |\mathbf{s} - \mathbf{s}_0| = \frac{2\sin\theta}{\lambda} = \frac{1}{d} \qquad (1.1.33)$$

and

$$|\mathbf{Q}| = \frac{4\pi\sin\theta}{\lambda} = \frac{2\pi}{d}. \qquad (1.1.34)$$

The vector **Q** is the physicist's equivalent of the crystallographer's **h**. The physical meaning of **Q** is the momentum transfer on scattering and it differs from the scattering vector **h** by a factor of 2π.

1.1.2.3. *The Bragg equation from the Laue equation*

Another approach for describing scattering from a material was first described by Laue (von Laue, 1912). The Laue equation can be derived by evaluating the phase relation between two wavefronts after hitting two scatterers that are separated by the vector **r**. The path-length difference $\Delta = |\mathrm{CD}| - |\mathrm{BA}|$ between the two scattered waves introduces a phase shift between the two outgoing waves (Fig. 1.1.8). From Fig. 1.1.8 one immediately sees that the path-length difference is given by

$$\Delta = r\cos\varepsilon - r\cos\varepsilon_0. \qquad (1.1.35)$$

This path-length difference gives rise to a phase shift

$$\varphi = 2\pi\frac{\Delta}{\lambda} = 2\pi\left(\frac{r}{\lambda}\cos\varepsilon - \frac{r}{\lambda}\cos\varepsilon_0\right). \qquad (1.1.36)$$

The term in parentheses is

$$\mathbf{s}\cdot\mathbf{r} - \mathbf{s_0}\cdot\mathbf{r} = (\mathbf{s} - \mathbf{s_0})\cdot\mathbf{r} = \mathbf{h}\cdot\mathbf{r}. \qquad (1.1.37)$$

The amplitude of the scattered wave at a large distance away in the direction of the vector **s** is

$$A(\mathbf{h}) = \exp(2\pi i 0) + \exp(2\pi i\mathbf{h}\cdot\mathbf{r}) \qquad (1.1.38)$$

When we generalize the idea laid out above to n scatterers, we get

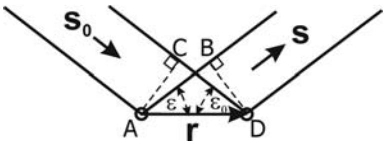

Figure 1.1.8
Scattering from an object consisting of two scatterers separated by **r**.

$$A(\mathbf{h}) = \sum_{j=1}^{n}\exp\big(2\pi i\mathbf{h}\cdot\mathbf{r}_j\big). \qquad (1.1.39)$$

For simplicity, consider the case of an infinite one-dimensional crystal of scatterers that are equally spaced by distance a_i. In this case, $r_j = aj$ and

$$A(h) = \sum_{j=-\infty}^{\infty}\exp(2\pi i h a j). \qquad (1.1.40)$$

Using the definition for a periodic delta function,

$$\lim_{n\to\infty}\sum_{j=-n}^{n}\exp(2\pi i h a j) = \sum_{k=-\infty}^{\infty}\delta(k - ha) \qquad (1.1.41)$$

and

$$A(h) = \sum_{k=-\infty}^{\infty}\delta(k - ha), \qquad (1.1.42)$$

which is a periodic array of delta functions at positions $h = k/a$. This means that sharp peaks of intensity will only appear when this expression holds, which are the reciprocal-lattice points. This is the same result as given by the Bragg equation (1.1.3) in one dimension. Extending to three dimensions, equations (1.1.40) and (1.1.42) become

$$\begin{aligned}A(\mathbf{h}) = &\sum_{j=-\infty}^{\infty}\exp\big(2\pi i(\mathbf{h}\cdot\hat{\mathbf{a}})aj\big)\sum_{k=-\infty}^{\infty}\exp\big(2\pi i(\mathbf{h}\cdot\hat{\mathbf{b}})bk\big)\\ &\times\sum_{l=-\infty}^{\infty}\exp\big(2\pi i(\mathbf{h}\cdot\hat{\mathbf{c}})cl\big), \qquad (1.1.43)\end{aligned}$$

where $\hat{\mathbf{a}} = \mathbf{a}/a$, and

$$A(\mathbf{h}) = \sum_{\mu,\nu,\eta=-\infty}^{\infty}\delta[\mu - (\mathbf{h}\cdot\hat{\mathbf{a}})a]\delta[\nu - (\mathbf{h}\cdot\hat{\mathbf{b}})b]\delta[\eta - (\mathbf{h}\cdot\hat{\mathbf{c}})c]. \qquad (1.1.44)$$

Equation (1.1.44) has the same meaning in three dimensions, where intensity appears only when all three delta functions are non-zero. This occurs for the conditions

$$\mathbf{h}\cdot\hat{\mathbf{a}} = \frac{\mu}{a},\ \ \mathbf{h}\cdot\hat{\mathbf{b}} = \frac{\nu}{b}\ \text{and}\ \mathbf{h}\cdot\hat{\mathbf{c}} = \frac{\eta}{c}, \qquad (1.1.45)$$

where μ, ν and η are integers. From this follows

$$\mathbf{h}\cdot\mathbf{a} = \mu,\ \ \mathbf{h}\cdot\mathbf{b} = \nu\ \text{and}\ \mathbf{h}\cdot\mathbf{c} = \eta. \qquad (1.1.46)$$

These conditions are met when

$$\mathbf{h} = \mu\mathbf{a}^* + \nu\mathbf{b}^* + \eta\mathbf{c}^* = \mathbf{d}^*_{\mu\nu\eta}. \qquad (1.1.47)$$

This is exactly Bragg's equation in the form given in equation (1.1.30).

For practical purposes including the indexing of powder patterns and refinement of a structural model, given a set of lattice parameters a, b, c, α, β, γ, the positions for all possible reflections hkl can be calculated according to