on. The intensity of the reflected lines decreases with increase in the value of n or θ. The highest possible order is determined by the condition that $\sin\theta$ cannot exceed unity. Also, since $\sin\theta \leq 1$, λ must be $\leq d$ for Bragg reflection to occur. Taking $d \approx 10^{-10}$ m, we obtain $\lambda \leq 10^{-10}$ m or 1Å. X-rays having wavelength in this range are, therefore, preferred for analysis of crystal structures.

2.2.2 The Von Laue Treatment : Laue's Equations

Von Laue treated the phenomenon of diffraction in a more general way by considering the scattering of x-rays from individual atoms in the crystal followed by their recombination to obtain the directions of diffraction maxima. It will be shown below that diffraction maxima appear in some specific directions which obey certain conditions known as the *Laue's equations*. It also proves the validity of Bragg's treatment and the Bragg's law can be derived from the Laue's equations.

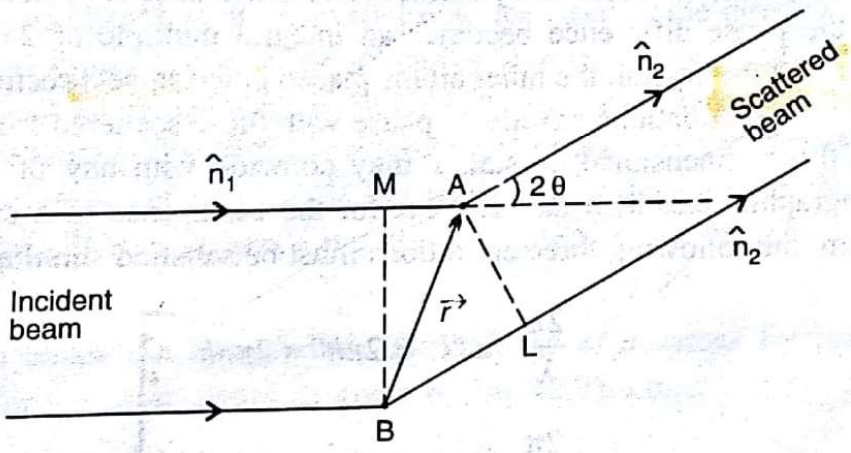

Fig. 2.3. *Scattering of x-rays from two identical scattering centres separated by a distance* **r**.

Consider the scattering of an incident beam from two identical scattering centres A and B placed at a distance r from each other in a crystal as shown in Fig. 2.3. Let $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$ be the unit vectors in the directions of the incident and scattered beams respectively and let the angle between $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$ be 2θ. Draw BM and AL perpendiculars to the directions of the incident and scattered beams respectively. Then the path difference between the rays scattered from A and B is given by

$$\text{Path difference} = AM - BL = \mathbf{r}.\hat{\mathbf{n}}_1 - \mathbf{r}.\hat{\mathbf{n}}_2 = \mathbf{r}.\,(\hat{\mathbf{n}}_1 - \hat{\mathbf{n}}_2) = \mathbf{r}.\mathbf{N}$$

where $\mathbf{N} = \hat{\mathbf{n}}_1 - \hat{\mathbf{n}}_2$. As will be seen later, the vector **N** happens to be a normal to the reflecting plane. It is a plane which may be assumed to be reflecting the incident ray into the direction of the scattered ray following the ordinary laws of reflection. This is one of the planes which forms the basis of Bragg's treatment. From Fig. 2.4, we find

$|\mathbf{N}| = 2 \sin\theta$

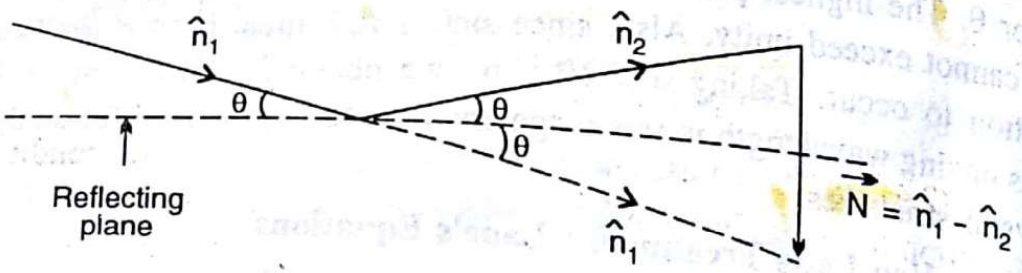

Fig. 2.4. *Geometrical relationship of incident beam, scattered beam, reflecting plane and the normal.*

The phase difference between the rays scattered from A and B is

$$\phi = \frac{2\pi}{\lambda} (\mathbf{r}.\mathbf{N}) \tag{2.2}$$

The radiations scattered by atoms A and B will interfere constructively only if the phase difference becomes an integral multiple of 2π. Due to periodicity of the crystal, the other atoms placed in the same direction would also scatter the radiations exactly in phase with those scattered from A and B. In a three-dimensional crystal, **r** may coincide with any of the three crystallographic axes **a**, **b** and **c**. Thus for the occurrence of a diffraction maximum, the following three conditions must be satisfied simultaneously :

$$\left.\begin{aligned} \frac{2\pi}{\lambda} (\mathbf{a}.\mathbf{N}) &= 2\pi h' = 2\pi n h \\ \frac{2\pi}{\lambda} (\mathbf{b}.\mathbf{N}) &= 2\pi k' = 2\pi n k \\ \frac{2\pi}{\lambda} (\mathbf{c}.\mathbf{N}) &= 2\pi l' = 2\pi n l \end{aligned}\right\} \tag{2.3}$$

where h', k' and l' represent any three integers. While obtaining Eqs. (2.3), it is assumed that atoms A and B are the nearest neighbours and, so, the magnitudes a, b and c represent the interatomic distances along their respective crystallographic directions. The integers h', k' and l' and h, k, l differ only by a common factor n which may be equal to or greater than unity. Thus the integers h, k and l cannot have a common factor other than unity and resemble the Miller indices of a plane which happens to be the reflecting plane. Let α, β and γ be the angles between the scattering normal **N** and the crystallographic axes **a**, **b** and **c** respectively. Then,

$\mathbf{a}.\mathbf{N} = aN \cos\alpha = 2\, a \sin\theta \cos\alpha$, and so on.

Therefore, Eqs. (2.3) become

$$\left.\begin{aligned} \mathbf{a}.\mathbf{N} &= 2a \sin\theta \cos\alpha = h'\lambda = nh\lambda \\ \mathbf{b}.\mathbf{N} &= 2b \sin\theta \cos\beta = k'\lambda = nk\lambda \\ \mathbf{c}.\mathbf{N} &= 2c \sin\theta \cos\gamma = l'\lambda = nl\lambda \end{aligned}\right\} \quad (2.4)$$

Equations (2.4) are known as *Laue's equations* and represent the conditions for diffraction to occur. In an orthogonal coordinate system, α, β and γ also satisfy the condition

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1 \quad (2.5)$$

where $\cos\alpha$, $\cos\beta$ and $\cos\gamma$ represent the direction cosines of the scattering normal. The Eqs. (2.4) and (2.5) yield the values of α, β, γ and θ for which diffraction takes place provided h, k, l and n are known. Thus, for a given reflecting plane, Eqs. (2.4) serve to determine unique values of θ and **N** which define a scattering direction.

From Eqs. (2.4), we also find that, for fixed θ, the direction cosines $\cos\alpha$, $\cos\beta$ and $\cos\gamma$ of the scattering normal are proportional to h/a, k/b and l/c. Also, as described in Sec. 1.9, the direction cosines of the normal to any arbitrary plane (hkl) are proportional to h/a, k/b and l/c. This leads to the conclusion that the scattering normal **N** is the same as the normal to the plane (hkl) and hence the arbitrary plane (hkl) happens to be the reflecting plane.

To obtain the Bragg's law, consider the expressions for interplanar spacing for the (hkl) planes as given by Eq. (1.7), i.e.,

$$d = \frac{a}{h}\cos\alpha = \frac{b}{k}\cos\beta = \frac{c}{l}\cos\gamma$$

In combination with Eqs. (2.4), these yield

$$2d \sin\theta = n\lambda$$

which is the Bragg's law. Here n represents the order of reflection and, as described above, is the greatest common factor among the integers h', k' and l' in Eqs. (2.4). Thus one may have the planes (hkl) and consider different orders of reflection from these; alternatively, one may have the planes $(nh\ nk\ nl)$ or $(h'k'l')$ and always consider the first order reflection. The latter practice is normally adopted during the process of structure determination by x-ray diffraction. It is obvious that the nth order reflection from the planes (hkl) would overlap with the first order reflection from the planes $(nh\ nk\ nl)$ or $(h'k'l')$. Thus, putting n equal to 1, one can get rid of the factor n in the Bragg's equation provided the reflections from all the planes, real or imaginary, having Miller indices with or without a common factor be considered.