Using the standard trigonometric results

$$\cos(\alpha+\theta)=\cos\alpha\cos\theta-\sin\alpha\sin\theta,$$
$$\cos(\alpha-\theta)=\cos\alpha\cos\theta+\sin\alpha\sin\theta, \quad (1.1.5)$$

equation (1.1.4) becomes

$$n\lambda=\mathrm{MN}(2\sin\alpha\sin\theta) \quad (1.1.6)$$

with

$$d=\mathrm{MN}\sin\alpha, \quad (1.1.7)$$

which may be substituted to yield the Bragg equation:

$$n\lambda=2d\sin\theta. \quad (1.1.8)$$

The Bragg equation holds for any radiation or particle that is used to probe the structure of the sample: X-rays, neutrons or electrons. Another equivalent, and highly useful, form of the Bragg equation for the particular case of X-rays is

$$Ed=\frac{6.199}{\sin\theta}\ \text{with}\ \lambda=\frac{12.398}{E}, \quad (1.1.9)$$

where the energy E of the X-rays is in keV and λ is in ångströms.

The Bragg law results in narrow beams of high intensity that emerge from the crystal in specific directions given by the Bragg equation, resulting in sharp spots on the detector, and there is a one-to-one correspondence between these Bragg spots (often referred to as Bragg reflections) and each set of crystallographic planes. Each Bragg spot is therefore labelled with the same set of Miller indices, *hkl*, as the set of planes that gave rise to it.

It is possible to construct a 'reciprocal space' where the axes of the space are in units of inverse length. The reference coordinate frame of the reciprocal space is defined by a set of basis vectors whose directions are perpendicular to the plane normals of the (100), (010) and (100) planes of the crystal. Thus, a *point* in this reciprocal space corresponds to a *direction* in direct space and every allowed reflection according to the Bragg law is represented by a point in reciprocal space. The set of points arising from the Bragg law forms a lattice in reciprocal space, which is called the 'reciprocal lattice', and each single crystal has its own reciprocal lattice. [See *International Tables for Crystallography* Volume B (Shmueli, 2008) for more details.]

To derive the Bragg equation, we used an assumption of specular reflection, which is borne out by experiment: for a crystalline material, destructive interference eliminates scattered intensity in all directions except where equation (1.1.3) holds. Strictly this holds only for crystals that are infinite in extent and which the incident X-ray beam can penetrate without loss of intensity. This does not sound like a particularly good approximation, but in practice it holds rather well. Even a fairly low energy X-ray beam that only penetrates, say, a micrometre into the material will still probe ~10 000 atomic layers. The condition is not strictly obeyed in the presence of defects and disorder in the material. In such materials the Bragg peaks are modified in their position, their width and their shape, and there is also an additional component of the diffracted intensity that may be observed in all directions, away from reciprocal-lattice points, known as diffuse scattering.

1.1.2.2. *The Bragg equation from the reciprocal lattice*

Here we develop in more detail the mathematics of the reciprocal lattice. The reciprocal lattice has been adopted by crystallographers as a simple and convenient representation of the physics of diffraction by a crystal. It is an extremely useful tool

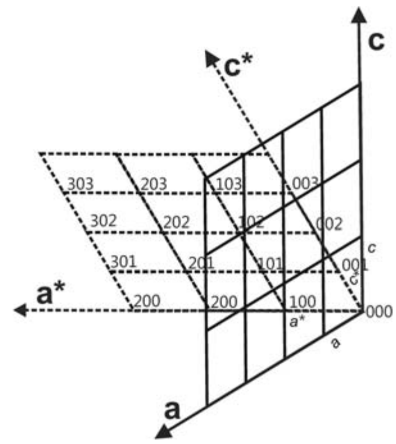

Figure 1.1.5
A two-dimensional monoclinic lattice and its corresponding reciprocal lattice. [Adapted from Dinnebier & Billinge (2008) with permission from the Royal Society of Chemistry.]

for describing all kinds of diffraction phenomena occurring in powder diffraction.

Consider a 'normal' crystal lattice with lattice vectors **a**, **b** and **c**, which have lengths a, b and c, respectively, and angles α between **b** and **c**, β between **a** and **c** and γ between **a** and **b**. The unit-cell volume is given by V. A second lattice with lattice parameters a^*, b^*, c^*, α^*, β^*, γ^* and unit-cell volume V^* with the same origin exists such that

$$\mathbf{a}\cdot\mathbf{b}^*=\mathbf{a}\cdot\mathbf{c}^*=\mathbf{b}\cdot\mathbf{c}^*=\mathbf{a}^*\cdot\mathbf{b}=\mathbf{a}^*\cdot\mathbf{c}=\mathbf{b}^*\cdot\mathbf{c}=0,$$
$$\mathbf{a}\cdot\mathbf{a}^*=\mathbf{b}\cdot\mathbf{b}^*=\mathbf{c}\cdot\mathbf{c}^*=1. \quad (1.1.10)$$

This is known as the reciprocal lattice[1] (Fig. 1.1.5), which exists in so-called reciprocal space. As mentioned above, we will see that it turns out that the points in the reciprocal lattice are related to the vectors defining the crystallographic plane normals. There is one point in the reciprocal lattice for each set of crystallographic planes, (hkl), separated by distance d_{hkl}, as discussed below. For now, just consider h, k and l to be integers that index a point in the reciprocal lattice. A reciprocal-lattice vector $\mathbf{h}_{hkl}$ is the vector from the origin of reciprocal space to the reciprocal-lattice point for the plane (hkl),

$$\mathbf{h}_{hkl}=h\mathbf{a}^*+k\mathbf{b}^*+l\mathbf{c}^*,\quad h,k,l\in\mathbb{Z}. \quad (1.1.11)$$

where $\mathbb{Z}$ is the set of all integers.

The length of the reciprocal basis vector $\mathbf{a}^*$ is defined according to

$$\mathbf{a}^*=x(\mathbf{b}\times\mathbf{c}), \quad (1.1.12)$$

where the scale factor x can easily be deduced, using equations (1.1.12) and (1.1.10), as

$$\mathbf{a}^*\cdot\mathbf{a}=x(\mathbf{b}\times\mathbf{c}\cdot\mathbf{a})=xV\Rightarrow x=\frac{1}{V}, \quad (1.1.13)$$

leading to

$$\mathbf{a}^*=\frac{1}{V}(\mathbf{b}\times\mathbf{c}),\quad \mathbf{b}^*=\frac{1}{V}(\mathbf{c}\times\mathbf{a}),\quad \mathbf{c}^*=\frac{1}{V}(\mathbf{a}\times\mathbf{b}) \quad (1.1.14)$$

and, *vice versa*,

[1] The reciprocal lattice is a commonly used construct in solid-state physics, but with a different normalization: $\mathbf{a}\cdot\mathbf{a}^*=2\pi$.

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