[Ewald]
(Chapter 5.3.1 in *Elements*)

The Ewald Construction

It is convenient to represent the scattering in terms of the *Ewald construction*, shown in Figure 5.9 in *Elements*. For given $\vec{\mathbf{k}}_o$, draw a sphere of radius $\left|\vec{\mathbf{k}}_o\right|$, centered at the beginning of $\vec{\mathbf{k}}_o$. Place the origin (000) of the reciprocal lattice (RL) at the end of $\vec{\mathbf{k}}_o$.

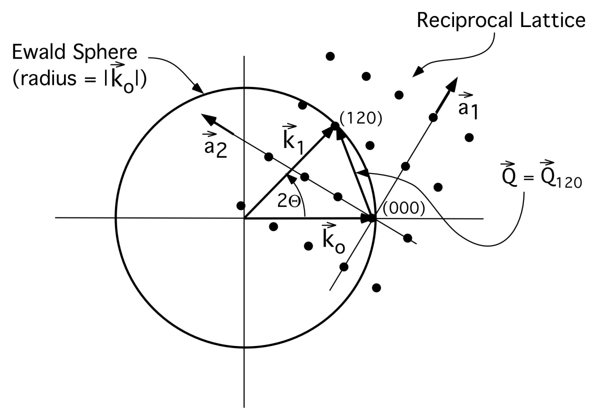

Figure 5-E1. The Ewald construction.

For illustrative purposes, the figure, rendered in two dimensions, shows a section of the RL in which the RL points are aligned in a plane containing $\vec{\mathbf{k}}_o$ and some direction $\hat{\vec{\mathbf{k}}}_1$. This is in general not so; the direction to the detector, $\hat{\vec{\mathbf{k}}}_1$, is arbitrary. The vector $\vec{\mathbf{k}}_1$, drawn from the origin of $\vec{\mathbf{k}}_o$, must lie on the Ewald sphere, which is the locus of elastic scattering. Scattering can take place only when the crystal orientation (and thus the RL orientation) is such that a RL point lies exactly at the point on the sphere where $\vec{\mathbf{k}}_1$ lies, as shown at $\vec{\mathbf{Q}}_{120}$ in the figure. Crystal structure determination requires measurements of reflected intensities (that is, structure factors) for a large number of reciprocal lattice points. See Chapter 9.

To determine the intensities of reflections at individual reciprocal lattice points requires either a two-dimensional position-sensitive detector with small pixels to separately register scattered neutrons according to their directions or using an old-fashioned method: scanning angles with a well-collimated detector to receive only one reflection at a time.

There are two ways to carry out measurements: monochromatic beam and white (broad wavelength band) beam. In the monochromatic case, only those reflections for which $\vec{\mathbf{Q}} \leq 2\left|\vec{\mathbf{k}}_o\right|$ can register in the detector, no matter what the direction $\vec{\mathbf{k}}_1$ of the detector. This can be seen by imagining the RL in Figure 5.9 to extend all the way across the Ewald sphere in three dimensions. In the white-beam case, irradiating the crystal with neutrons $k_{\mathbf{min}} \leq k_o \leq k_{\mathbf{max}}$ illuminates all the reflections between the two corresponding Ewald spheres, as in Figure 5RL.2.

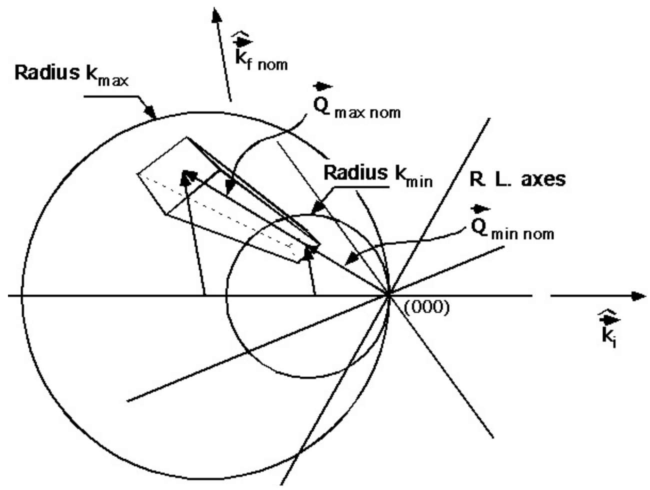

Figure 5-E2 Two Ewald spheres, the smaller one for the minimum incident wave vector, the larger one for the maximum incident wave vector, showing the region of Q-space intercepted by a large detector.

A large pixelated detector registers scattered neutrons in the reciprocal lattice volume between the Ewald spheres for the minimum and maximum incident-neutron wave vectors. The solid angle subtended by the detector from the sample defines the volume of **Q**-space examined. The detector is usually position-sensitive, for example, an Anger camera or a multiwire proportional counter, defining a large number of separate, adjacent, angularly resolved areas.

Because higher order reciprocal lattice vectors $\vec{\mathbf{Q}}_{nhnknl} = n\vec{\mathbf{Q}}_{hkl}$ and the corresponding scattered neutron wave vectors are parallel to the first-order ones, Laue spots can represent the sum of intensities for all illuminated orders, confusing their interpretation. Tailoring the wavelength band in the incident beam can minimize this problem and the potential problem of simultaneous reflection when more than one RL point lies on the Ewald sphere.

Because $\vec{\mathbf{Q}}_{hkl} = h\vec{\mathbf{a}}_1 + k\vec{\mathbf{a}}_2 + l\vec{\mathbf{a}}$, where hkl are integer Miller indices, the measured angular positions of a small number of reflections of low order, about 20, provide the reciprocal lattice basis vectors $\vec{\mathbf{a}}_1, \vec{\mathbf{a}}_2,$ and $\vec{\mathbf{a}}_3$ (nine quantities) in relation to reference axes fixed in the instrument, as well as, simultaneously, a few $(hkl)s$. All are integer sets, so that the problem represents a set of *Diophantine* equations (polynomial equations that have only integer solutions). The $\vec{\mathbf{a}}$ s are the basis vectors of the reciprocal lattice and constitute the *orientation matrix* for the crystal in the instrument. This process is usually automated, carried out by a computer in the process of data analysis. Wavelengths for each reflection follow in the course of analysis.