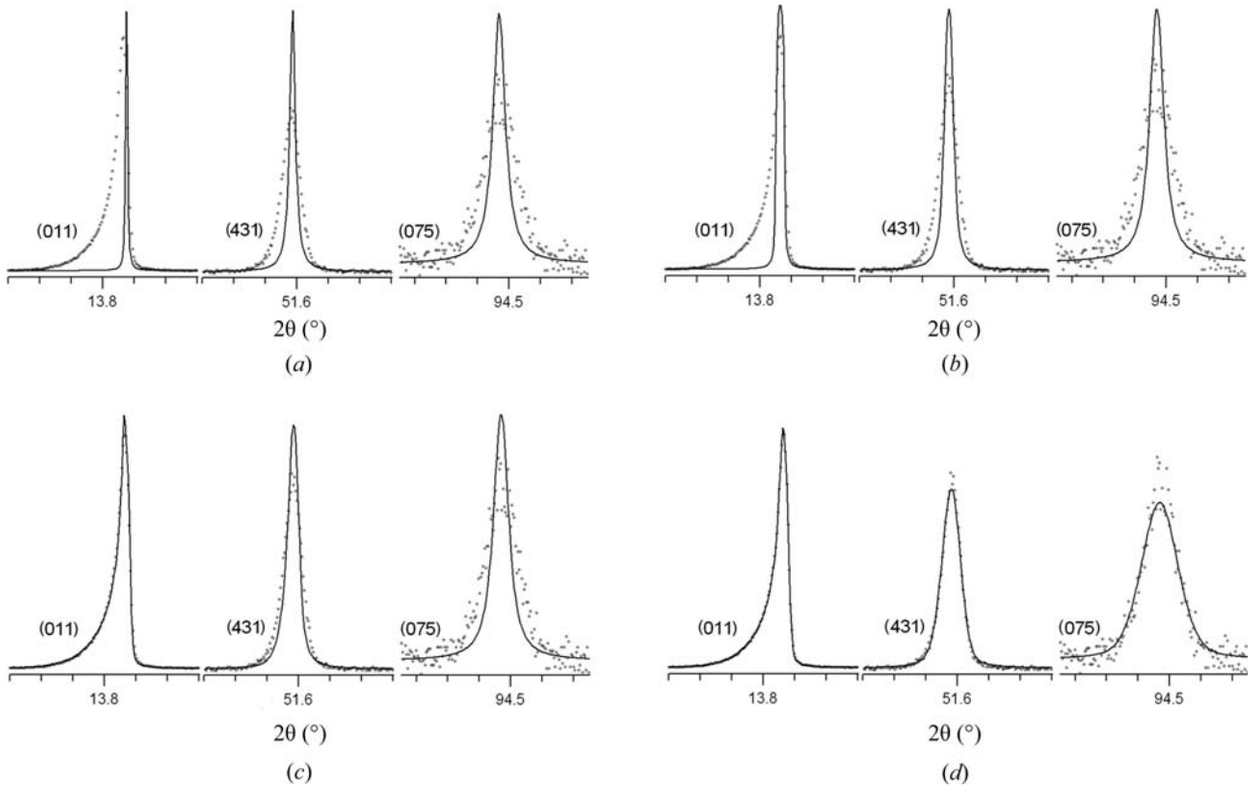

Figure 1.1.19
Peak fits of three selected reflections for an LaB_6 standard measured with Mo $K\alpha_1$ radiation ($\lambda = 0.7093$ Å) from a Ge(220) monochromator in Debye–Scherrer geometry using the fundamental-parameter approach. (*a*) A pure Lorentzian emission profile with a half width of 0.2695 mÅ is applied, refining the peak position and intensity only; (*b*) additionally, a hat shape function of the receiving slit in the equatorial plane with a width of 0.1 mm has been convoluted into the profile; (*c*) additionally, an axial convolution with filament-, sample- and receiving-slit lengths of 8 mm each and a secondary Soller slit with an opening angle of 2.5° has been convoluted into the profile; (*d*) additionally a small contribution of Gaussian broadening coming from the position-sensitive detector is convoluted into the profile. [From Mittemeijer & Welzel (2012). Copyright Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.]

These functions can be convoluted sequentially as needed, first with the delta-function Bragg peak, and subsequently with the existing profile from the previous convolutions, each time resulting in a new profile that can become quite complex (Fig. 1.1.19). It is often the case that for a particular resolution effect the angular dependence of the profile function is known from the geometry of the measurement, and the convolution function for each peak is determined with only a very small number of parameters.

1.1.4.1. *Sample contributions to the peak profile*

Features of the sample that affect the peak profile include crystallite domain size and shape, dislocations, disclinations, twin and stacking faults, antiphase domains, microstrains, grain surface relaxations, and compositional fluctuations. Here we reproduce some basic results as examples; they also illustrate some fundamental aspects of diffraction from real crystals.

1.1.4.1.1. *Crystallite size*

The starting point for the analysis of finite size effects is the Laue equation, equation (1.1.39), which is reproduced here for a one-dimensional crystal:

$$A(h) = \sum_{j=0}^{n} \exp(2\pi i a j h). \tag{1.1.65}$$

When we were deriving the Bragg equation from the Laue equation we assumed an infinite crystal, and the sum taken to infinity resulted in delta functions at the reciprocal-lattice points. Now we want to consider a finite crystal with n unit cells. There is an analytic form for this sum which, using Euler's identity, is given by

$$\begin{aligned} A(h) &= \frac{\exp\left(2\pi i(n+1)ah\right) - 1}{\exp(2\pi i a h) - 1} \\ &= \frac{\exp\left(i\pi(n+1)ah\right)}{\exp(i\pi a h)} \frac{\exp\left(i\pi(n+1)ah\right) - \exp\left(-i\pi(n+1)ah\right)}{\exp(i\pi a h) - \exp(-i\pi a h)} \\ &= \exp(i\pi n a h) \frac{\sin\left(\pi(n+1)ah\right)}{\sin(\pi a h)}. \end{aligned} \tag{1.1.66}$$

The intensity is obtained by taking the modulus squared of this complex function, resulting in

$$I(h) = \frac{\sin^2\left(\pi(n+1)ah\right)}{\sin^2(\pi a h)}. \tag{1.1.67}$$

This function has sharp maxima when $h = \nu(1/a)$, where ν is an integer. This large central maximum falls off with a width proportional to $1/n^2$ with oscillating tails of intensity where the frequency of the oscillations increases with increasing n. This is illustrated in Fig. 1.1.20 for two different values of n but the same value of a.

In general, the Fourier transforms of periodic patterns become sharper with increasing number of unit cells. The expression $\sin(\pi(n+1)ah)/\sin(\pi a h)$ is also called the geometric factor of the structure amplitude.

This size broadening is often modelled in practice by using an equation due to Scherrer. We now reproduce the simple deri-