Table 2.3.6
Suitability of problems to high-resolution or high-intensity diffractometers

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Problem	High resolution	High intensity (medium resolution)
Solve a complex crystal or magnetic structure	Essential, especially in the presence of pseudo-symmetry	Not usually suitable†‡
Refine a complex crystal or magnetic structure	Essential. Will benefit from a high Q-range if available	Not usually suitable†‡
Solve or refine small inorganic structures	Beneficial, but not usually essential unless pseudosymmetry is present	Usually adequate
Quantitative phase analysis	Only required when peaks from the different phases are heavily overlapped	Usually adequate. Allows phase quantities to be tracked in fine environmental variable steps (T, P, E, H *etc.*) during *in situ* experiments
Phase transitions	Depends on the nature of the transition and complexity of the structures. Essential for transitions involving subtle unit-cell distortions and pseudosymmetry	Often adequate for small inorganic structure transitions and order–disorder transitions. Allows fine steps in an environmental variable (T, P, E, H *etc.*)
Line-broadening analysis	Essential for complex line broadening such as from a combination of strain and particle size, dislocations, stacking faults *etc.*	Adequate for tracking changes in severe line broadening as a function of an environmental variable (T, P *etc.*) especially if the pure instrumental peak shape is well characterized
Rapid kinetic studies	Not appropriate	Essential

† In some cases the symmetry and lattice parameters are such that the diffraction peaks are well spaced and not severely overlapped even at modest resolution. ‡ May be necessary to supplement high-resolution data to observe weak superlattice reflections in the presence of very subtle or incomplete order–disorder transitions.

Table 2.3.7
Guidance on choice of wavelength/detector bank

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Problem	Choice	Reasons
Solve complex or low-symmetry structures	Longer wavelength	Increase d-spacing resolution to allow correct symmetry and space group to be assigned
Refine a large or complex crystal structure	Shorter wavelength	Ensure that the number of peaks greatly exceeds the number of parameters. Improve determination of site occupancies and displacement parameters
Solve or refine magnetic structures	Longer wavelength	Ensure that large d-spacing peaks are observed. Spread the magnetic form factor over the entire diffraction pattern
Quantitative phase analysis	Usually shorter wavelength	Improve the accuracy of the determination. Longer wavelengths only required if peak overlap is severe
Phase transitions	Shorter wavelength	Ensures adequate data for order–disorder or other unit-cell-enlarging transitions
	Longer wavelength	Subtle unit-cell distortion or pseudosymmetric structures

In the general case, there is competition between the resolution and the intensity of diffractometers, although some of the modern TOF diffractometers (*e.g.* POLARIS, GEM, POWGEN, NOMAD and iMATERIA) simultaneously record patterns of moderate resolution and intensity, and high-intensity patterns at low resolution, in different detector banks. For the purposes of this chapter, high resolution is defined as a minimum diffraction peak width at half maximum height corresponding to $\Delta d/d \leq 10^{-3}$. This is the resolution typically required to observe lattice-parameter differences [*e.g.* $(a - b)/a$] of as little as 4×10^{-5} or so in the absence of sample-related peak broadening. Such a diffractometer is typically of the order of 10 to 1000 times slower than corresponding high-intensity diffractometers at the same neutron source. The decision to opt for a high-resolution diffractometer or a high-intensity diffractometer will depend critically on the nature of the problem under study. This situation was considered in Kisi & Howard (2008) and their conclusions are reproduced in Table 2.3.6.

It might be expected that the total information content in a diffraction pattern correlates with the d-spacing range covered and therefore this should be maximized. However, this expectation overlooks the different purposes for which powder-diffraction patterns are used. A greater density of diffraction peaks (*e.g.* in a CW pattern recorded using a short neutron wavelength) makes the detailed refinement of complex crystal structures more precise; however, it makes the determination of unit cell and systematic absences *more* difficult as well as reducing access to information contained within the peak shapes concerning the sample microstructure. Table 2.3.7 summarizes these effects. It should be noted that in this context parallels exist between a short-wavelength CW diffraction pattern and a low-angle-detector-bank TOF pattern; and between a longer-