Table 2.1.1
Types of beam-path components available in laboratory X-ray powder diffraction

The column numbering corresponds to the positions indicated in Fig. 2.1.2 at which individual components can be mounted.

Position 1	Positions 2 and 4	Position 3		Position 5
X-ray sources	X-ray optics	Goniometer base	Specimen stages	Detectors
Fixed target Moving target (rotating anodes, liquid-metal jets)	Absorptive (apertures, metal filters) Diffractive (monochromators, analysers) Reflective (multilayer mirrors, capillary optics)	Vertical [ω–θ (θ–θ), ω–2θ (θ–2θ)] Horizontal [ω–θ (θ–θ), ω–2θ (θ–2θ)]	Fixed, rotating Specimen changer Eulerian cradles Kappa stages Tilt/fixed χ stages *XYZ* stages Flow-through cells Non-ambient (low temperature, high temperature, humidity, high pressure)	Scintillation Gas ionization (metal wire, micro-gap) Semiconductor (SiLi, strip/pixel, CCD/CMOS)

sible angular range may be limited for large components owing to collision issues, while heavy loads on vertical goniometers may impede alignment and lead to early wear and tear. Restrictions will be discussed in Sections 2.1.5 to 2.1.7 for the individual components.

These days, the exchange of lighter components, such as most X-ray optics, specimen stages and detectors, does not require any tools at all (such as when a snap-lock mechanism is employed) or more than a few screws for fixing. Alignment is normally not required when components are factory pre-aligned and handled with care, and when mounts are manufactured with good quality. Intrinsic changes of the beam direction (*e.g.* focusing crystal monochromators or X-ray mirrors) or beam offsets (*e.g.* two-bounce channel-cut monochromators) need compensating translation and/or rotation of the components involved.

The exchange of large, heavy components, or complicated rebuildings such as the conversion of a goniometer (vertical ↔ horizontal, θ–θ ↔ θ–2θ *etc.*), may be still possible for technically skilled users. However, special tools may be necessary, requiring shipment of the component(s), or even the instrument, back into the factory. In addition, X-ray, machine and electrical safety directives by the local authorities have to be obeyed, and conversions may require updating approval to use the instrument. In such cases it may be more economic to operate two dedicated instruments instead.

The instrument control software plays a particularly important role in the context of instrument configuration and automated instrument conversion. In modern instruments, each beam-path component is equipped with an identification chip or hole masks read out by light barriers, which uniquely identify the respective component and link it with all its individual stored or coded properties. This information may range from part numbers, usage history or alignment information such as beam offsets, through to a virtually unlimited wealth of any physical data required to configure and operate that particular component. This ‘component recognition’ feature provides for completely new and important capabilities of laboratory powder diffractometers, the most important of which are:

(*a*) Any beam-path components, and each change of status, can be automatically detected, validated and configured, allowing true ‘plug & play’ operation.
(*b*) Real-time conflict detection: detection of incompatible, incorrectly mounted or missing instrument components. This feature can also help the user in choosing compatible instrument components, as already discussed above.
(*c*) Automatic, motorized adjustments of beam direction or beam-offset changes, based on the information stored in the related components’ ID chips, as individually determined at the factory *via* pre-alignment.
(*d*) Every instrument detail can be saved together with the measurement data, providing for a complete and accurate documentation of the experiment. In principle, every measurement can be exactly reproduced even years later.
(*e*) Measurement instructions can include instrument information. For example, manufacturers or users can configure the measurement software to propose instrument configurations deemed best for particular applications. A user with appropriate rights can choose to enforce a certain instrument configuration so that measurements will not start unless the instrument has detected the required configuration.

Both the platform concept and the huge advances in instrumentation and instrument control software have dramatically changed the laboratory X-ray instrumentation landscape in the past few years. The ease with which an instrument configuration can be changed is not only useful for less-skilled users. Probably even more importantly, it allows the use of the same instrument, in different configurations, for different X-ray application areas. It can generally be said that laboratory X-ray instrumentation has overcome the (mostly historical) dividing lines between different applications, which were mostly between single-crystal diffraction, powder diffraction and thin-film analysis. As far as differences still remain, these are usually solely the consequence of dedicated instrument components for meeting specific application requirements, resulting in specialized measurement and data-evaluation software, which is rarely included with each instrument.

2.1.4.3. *Range of applications*

It is the flexibility of today’s X-ray diffractometers that leads to their usefulness for a wide range of X-ray scattering techniques beyond traditional X-ray powder ‘Bragg diffraction’. Table 2.1.2 provides an overview.

X-ray scattering techniques represent the vast majority of techniques that X-ray diffractometers are used for. Properly configured, however, the same instrument can also be used to collect X-ray absorption (X-ray radiography) or X-ray emission (X-ray fluorescence) data, even if the achievable data quality cannot compete with dedicated instruments.

For X-ray radiography, an instrument will be configured in transmission geometry with the X-rays projected towards a

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