Table 2.1.3
Characteristic wavelengths and absorption edges of metal filters in common use

These data are taken from *International Tables for Crystallography* Vol. C (2004). Metal filters are discussed in Section 2.1.6.3.1.2.

Anode material	$K\alpha_2$	$K\alpha_1$	$K\beta_3$	$K\beta_1$	Metal filter	K absorption edge (Å)
Cr	2.2936510 (30)	2.2897260 (30)	2.0848810 (40)	2.0848810 (40)	V	2.269211 (21)
Co	1.7928350 (10)	1.7889960 (10)	1.6208260 (30)	1.6208260 (30)	Fe	1.7436170 (49)
Cu	1.54442740 (50)	1.54059290 (50)	1.3922340 (60)	1.3922340 (60)	Ni	1.4881401 (36)
Ga†	1.3440260 (40)	1.3401270 (96)	1.208390 (75)	1.207930 (34)		
Mo	0.713607 (12)	0.70931715 (41)	0.632887 (13)	0.632303 (13)	Zr Nb	0.6889591 (31) 0.6531341 (14)
Ag	0.5638131 (26)	0.55942178 (76)	0.4976977 (60)	0.4970817 (60)	Rh Pd	0.5339086 (69) 0.5091212 (42)

† Currently used with dedicated Montel optics only.

with a beam of low divergence and to match the incident beam size to the size of the specimen or the region of interest.

The illumination of larger specimen areas is particularly important for any applications involving polycrystalline specimens, where focusing of the diffracted beam has an advantage over parallel-beam optics in terms of higher beam flux and divergence in that the angular resolution in the diffraction pattern increases. Using an X-ray beam with too small a cross section and/or divergence will result in a smaller or even too small number of diffracting crystallites. This will generally lead to a loss in the diffracted intensity, and may additionally lead to an inhomogeneous intensity distribution in space, leading to random and uncorrectable intensity errors (known as 'particle statistics error', 'spottiness error' or 'granularity error'), and needs to be avoided by all means.

The combination of an appropriate X-ray source with appropriate X-ray optics thus depends on the properties of the specimen and the requirements of the application, and contributes most to the attainable data quality. This is in full agreement with the statement made earlier that there are only a few instrument configurations that will be ideal for any two application areas, or every conceivable sample within a single application area. While changes of most X-ray optics are extremely easy these days, changing between different types of X-ray sources may require significant effort. The choice of the most appropriate X-ray source therefore requires, at the time of instrument acquisition, careful consideration of the types of specimen in relation to the analyses to be conducted.

2.1.6.2. *X-ray sources*

In this section the general concepts of the commonest types of X-ray sources will be described. The physics of X-ray generation and the properties of X-rays have been extensively covered in the literature. More detailed information can be found in, for example, *International Tables for Crystallography* Vol. C (2004) as well as in the textbooks by Pecharsky & Zavalij (2009), Clearfield *et al.* (2008), Jenkins & Snyder (1996), and Klug & Alexander (1974).

2.1.6.2.1. *Generation of X-rays and the X-ray spectrum*

In laboratory X-ray sources, X-rays are produced by a multi-keV electron beam impinging on a metallic target. The X-ray spectrum that is obtained is characterized by a broad band of continuous radiation, accompanied by a number of discrete spectral lines characteristic of the target material. The continuous part of the spectrum ('*Bremsstrahlung*') is generated by the rapid deceleration of the electrons within the target, ranging from lowest energies as a result of gradual deceleration through to a cutoff wavelength whose energy corresponds to the initial kinetic energy of the electron, as a result of instantaneous deceleration. The discrete spectral lines ('characteristic radiation') are the result of electrons knocking out core electrons from the target material. This results in emission of 'fluorescent' X-rays when the perturbed atom relaxes to its ground state by filling up the energy levels of the electrons that have been knocked-out by means of electron transitions from higher electron shells. The energy of the fluorescent radiation is characteristic of the atomic energy levels of the target material. The most commonly used characteristic radiation is that of $K\alpha$, representing the transition of a $2p$ electron (L shell) filling a hole in a $1s$ (K) shell.

The target materials that are commonly in use strongly depend on the application and the type of X-ray source used. The most commonly used target materials range from Cr through to Co, Cu, Mo and Ag. With the recent introduction of liquid-metal targets, see Section 2.1.6.2.2.2(*b*), Ga will find increasing use in applications requiring the smallest spot sizes and highest brilliance. A list of characteristic wavelengths and absorption edges of commonly used metal ($K\beta$) filters is given in Table 2.1.3.

Today's laboratory X-ray sources can be classified as shown in Table 2.1.1, and are described in Section 2.1.6.2.2. For performance considerations see Section 2.1.6.2.3.

2.1.6.2.2. *Types of X-ray sources*

The performance of X-ray sources is usually characterized *via* brilliance as a measure for the quality of the emitted X-rays. The brilliance of an X-ray source is determined by several factors such as electron power density and the take-off angle.

The electron power density is the most important factor. Only a small fraction of <1% of the applied electron energy is converted into X-rays, so most of the incident energy is dissipated within the target as heat. The maximum power density and thus brightness of the X-ray source is limited by the melting or evaporation temperature of solid or liquid metal targets, respectively, and the efficiency with which the heat is removed from the area on which the electrons impact.

The take-off angle describes the angle under which the focal spot is viewed, and typically ranges from 3° to 7°, but may be up to 45°, depending on the type of X-ray source. The actual take-off angle that is chosen represents a compromise. On the one hand, it should be as small as possible to minimize the effectively seen