6.3.3: Powder X-ray Diffraction

When an X-ray is shined on a crystal, it diffracts in a pattern characteristic of the structure. In powder X-ray diffraction, the diffraction pattern is obtained from a powder of the material, rather than an individual crystal. Powder diffraction is often easier and more convenient than single crystal diffraction since it does not require individual crystals be made. Powder X-ray diffraction (XRD) also obtains a diffraction pattern for the bulk material of a crystalline solid, rather than of a single crystal, which doesn't necessarily represent the overall material. A diffraction pattern plots intensity against the angle of the detector, 2θ.

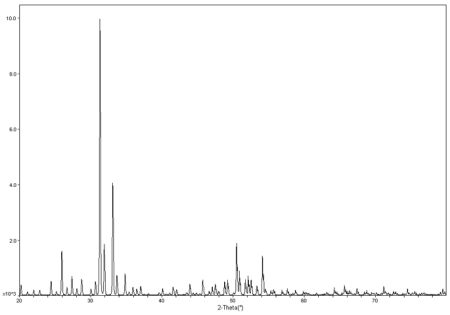
Introduction

Since most materials have unique diffraction patterns, compounds can be identified by using a database of diffraction patterns. The purity of a sample can also be determined from its diffraction pattern, as well as the composition of any impurities present. A diffraction pattern can also be used to determine and refine the lattice parameters of a crystal structure. A theoretical structure can also be refined using a method known as **Rietveld refinement**. The particle size of the powder can also be determined by using the Scherrer formula, which relates the particle size to the peak width. The Scherrer fomula is

$$t = \frac{0.9\lambda}{\sqrt{B_M^2 - B_s^2}\,\cos\theta} \tag{6.3.3.1}$$

with

- λ is the x-ray wavelength,
- B_M is the observed peak width,
- B_S is the peak width of a crystalline standard, and
- θ is the angle of diffraction.



To the left is an example XRD pattern for $Ba_{24}Ge_{100}$. The x axis is 2θ and the y axis is the intensity.

References

1. Dann, S.E. *Reactions and Characterization of SOLIDS.* Royal Society of Chemistry, USA (2002).
2. Skoog, D.A.; Holler, F.J.; Crouch, S.R. *Principles of Instrumental Analysis*. Sixth Edition, Thomson Brooks/Cole, USA (2007).

Contributors and Attributions

- Jason Grebenkemper