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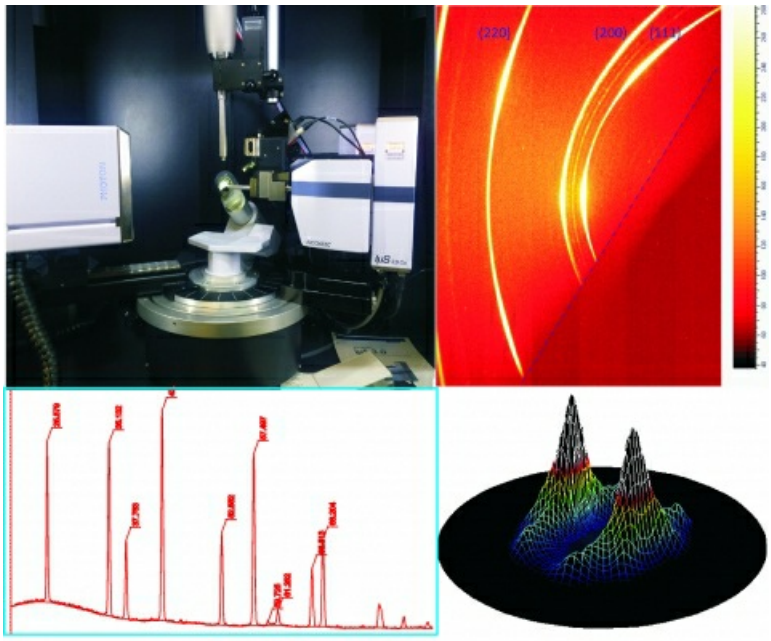
Powder X-ray diffraction applications with single crystal diffractometers

Bob He[1], Bruce Noll[2], Charles Campana[2]
[1]*Bruker AXS, Hercules, United States,* [2]*Bruker AXS, Madison, United States*
E-mail: bob.he@bruker.com

Data collection strategy and evaluation for powder X-ray diffraction (PXRD) applications with single crystal diffractometers are introduced in this presentation. A two-dimensional diffraction pattern contains abundant information about the atomic arrangement, microstructure and defects of a solid or liquid material. Single crystal and random powder represents two extreme cases of the diffraction samples. The Laue equations are suitable to interpret the diffraction pattern from single crystal. The Bragg law is more conveniently used for the diffraction pattern from a random powder. For the most other samples, the diffraction vector approach can be effectively used to interpret and evaluate the 2D diffraction data.
The 2D X-ray diffractometers, dedicated for PXRD, are typically designed to handle various sample types and applications, which may include sample stages for single or multiple samples, sample position and environment stages, X-ray optics and configurations for different applications. A single crystal diffractometer is dedicated to handle single crystal samples, which are typically much smaller than powder (polycrystalline) samples. The software for single crystal diffraction is significantly different from the software for PXRD. However, most single crystal diffractometers have the basic components and functions for PXRD, although with some limitations in configuration and sample handling. With proper sample preparation, data collection strategy and data evaluation software, a single crystal diffractometer can be used for many PXRD applications. Experimental examples are given for several typical PXRD applications, including phase identification, stress, texture, and crystal size. The software packages for each application are also recommended.
He, B. B. (2009). Two-dimensional X-ray Diffraction, John Wiley & Sons.



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