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Advances in Materials Characterization and Analysis using the Powder Diffraction File

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Crystallographic databases play a vital role in materials research, influencing materials development and providing a reference for materials characterization. Material identification using Powder X-ray diffraction (PXRD) method is the most powerful technique in solid state characterization since the landmark 1936 publication of Hanawalt and Rinn [1]. The International Centre for Diffraction Data (ICDD) Powder Diffraction File (PDF®) [2] is a powerful database for materials characterization that has been used extensively by the scientific community. Starting with 1000 entries on printed cards in 1941, the database has grown to contain over 1 million unique material data sets. The Powder Diffraction File has a wealth of information that a materials scientist can take advantage of for materials identification, characterization, computation and design. The Powder Diffraction File in Relational Database (RDB) format contains extensive chemical, physical, bibliographic and crystallographic data including atomic coordinates enabling characterization and computational analysis.
Proper database structure, data validations and phase-type classifications are crucial in making any database useful and reliable. Various structural and chemical classifications implemented in the database will be presented in detail. These classifications are important in data mining studies and optimizing diffraction pattern search/match methods. While using a database, it is important to know the quality of the crystal structure, diffraction pattern data and any data field of interest found in the database. With the varying quality of published data in the literature, the PDF database editorial review processes require rigorous data evaluation methods to define data based on its quality.

This presentation will focus on exploring recent developments and applications of Powder Diffraction File in various aspects of materials characterization and analysis.

Reference

[1] J.D. Hanawalt and H.W. Rinn Ind. Eng. Chem. Anal. Ed. 8(4) (1936) 244–247.

[2] S. Gates-Rector and T. Blanton. Powd. Diffr. 34(4) (2019) 352-360.

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