Poster Presentation

CC.P17

Data Validation and Structural Classifications in Powder Diffraction File

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The new Powder Diffraction File™, housing more than 760,000 diffraction patterns and 200,000 crystal structures, has a wealth of information that a materials scientist can take advantage of in various ways, from materials identification, characterization to design. Various structural and chemical classifications implemented in the database will be presented in detail. These classifications are important in data mining studies and optimizing pattern search/match methods. While using any database in materials characterization, it is important to know the quality of the crystal structure or diffraction pattern found in the database. With varying quality of published data in the literature, database editorial review processes had to adopt rigorous data evaluation methods to classify data based on its quality. Every entry in the Powder Diffraction File™ has a quality mark and editorial comments describing the error and the correction. Results of the analysis of the quality of the crystal structures (~500,000) published over the years will be discussed along with the most common errors found. The recent developments in Powder Diffraction File will be presented.

Keywords: Data Validation, Powder Diffraction