

Database Considerations for Nano-crystalline, Semi-crystalline and Amorphous Materials

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Historically, the ICDD PDF databases have consisted of entries based on normal Bragg diffraction from crystalline materials having conventional Bravais lattice symmetry. However, it is well known that for many materials, e.g. clays, polymers, some pharmaceuticals, and so-called nano-crystalline materials, the X-ray powder diffraction pattern is not satisfactorily described by a simple list of d's and I's. The additional characteristics of these patterns provide additional information about the specimen being studied, information such as crystallinity, crystallite size, local structural order, defect population/type, strain effects, etc. Because these features provide valuable information, there is value in documenting and cataloging these additional pattern characteristics.

The ICDD has a significant number of experimentally collected powder diffraction patterns stored in electronic format. This presentation will discuss the challenges associated with assembling such data into a database, the importance of associated information (e.g., data collection parameters), and strategies for providing user access to these patterns.