

DIFFRACTION, NON-CRYSTALLINITY, AND THE PDF DATABASE

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Classic X-ray diffraction and the PDF database have focused primarily on the coherent diffraction of X-rays by a crystalline lattice of atomic and molecular species. As early as 1938, Hanawalt, Frevel, and Rinn¹ developed a systematic method for the identification of crystalline materials based on the discrete peaks of their X-ray diffraction patterns. However, for materials with little or no crystallinity, few, if any, clearly identifiable Bragg peaks are present, and the ability to identify the material is compromised. Nevertheless, the X-ray powder diffraction/scattering patterns for these materials reveal information characteristic of their structural state, be it amorphous, nanocrystalline, or semicrystalline. As today's pharmaceutical industries are exploiting these less-crystalline states of matter to improve physical properties (bioavailability, compressibility, reactivity, binding capacity), the need for understanding, identifying, and characterizing these materials is more important than ever. In this presentation, the identification and characterization of these types of materials, using X-ray powder diffraction/scattering data coupled with the PDF database, will be described.

¹J.D. Hanawalt, H.W. Rinn, and L.K. Frevel, "Chemical Analysis by X-ray Diffraction", *Ind. & Eng. Chem.* 10, 457 (1938).