THE ANALYSIS OF NANOMATERIALS, AMORPHOUS MATERIALS AND SEMICRYSTALLINE MATERIALS

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There is an increasing prevalence of non-crystalline or partially crystalline materials used in solid state pharmaceutical formulation applications. Examples include micronized and nanosized active pharmaceutical ingredients (API's), excipients such as starch and cellulose, and polymers used for encapsulation and/or drug release. These materials present unique challenges in their analysis and characterization by diffraction methods because of the absence of sharp well defined diffraction peaks and profiles that are characteristic of crystalline materials.

Methods are being developed that are generically grouped under the title of "Total Pattern Analyses" whereby the entire digital profile of a diffraction pattern is used to study degrees of order, domains sizes, and contributions from scatter and background in order to extract information about all the materials present in the solid state independent of their crystallinity. Several speakers in prior PPXRD meetings such as Bates, Gilmore, Becker, Faber and Degan have talked about tools being developed that utilize full digital patterns for material investigations.

The scientific staff at the International Centre for Diffraction Data has been studying how to evolve the Powder Diffraction File so that we can facilitate the study and analysis of non-crystalline materials, nanomaterials and the amorphous state. Work has been done using full digital pattern simulations to approximate various domain sizes.[1] This has been previously applied to the study of polymorphism and crystallinity in cellulose. [2]. Polymers are being input as full digital experimental patterns that include both crystalline and amorphous components. New editorial systems are under development so that we can classify, index and standardize amorphous materials and nanomaterials. The presentation will review these developments and demonstrate applications to pharmaceutical analyses.

[1] P. Scardi, M. Leoni and J. Faber, "Diffraction Line Profile from a Disperse System: A Simple Alternative to Voightian Profiles", Powder Diffraction, Vol. 21, No. 4, p 270 (2006).

[2] T. G. Fawcett, S. N. Kabekkodu, J. Kaduk and E. Bucher, "Reexamining Structure and Crystallinity in Cellulose", Abstract available at www.icdd.com/ppxrd/06