

Analysis of short range order in x-ray amorphous indomethacin using x-ray powder diffraction and pair-wise distribution functions.

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Previous work [1] has shown the loss of crystalline order in a polycrystalline sample of indomethacin (IMC) under grinding. The resulting powder patterns do not exhibit any well-defined crystalline diffraction indicating that the material has become x-ray amorphous. Using the pair wise distribution (PDF) transform on the x-ray amorphous patterns it is possible to characterize the local molecule-molecule order that still exists in the x-ray amorphous material. By matching the PDF from the x-ray amorphous material to the PDF derived from the known crystalline polymorphs of IMC it can be shown that the remaining local order matches the original crystalline polymorph. The possibility that the x-ray amorphous IMC produced through grinding is actually a nano-crystalline material and not a true amorphous material can be confirmed by using Rietveld modeling of the x-ray amorphous powder pattern.

[1] Zografi and Crowley