

MS42-P02 | EXTRACTING COHERENT INFORMATION ABOUT PHASE TRANSFORMATIONS IN A FUNCTIONAL MATERIAL STUDIED BY X-RAY POWDER DIFFRACTION

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Structural phase transformations of polymorphic materials are mostly studied using an X-ray diffraction method. Numerous reports exist where the polymorphic products of a phase transformation have been identified using this technique. What is somewhat more challenging is collecting structural snapshots of a polymorphic transformation as it progresses and extracting coherent information from data that has not benefitted from a lengthy data collection. This type of analysis relies on rapid data collection and the ability to easily process numerous datasets.

In this work we describe a system where temperature- and pressure-induced phase transformations are studied by powder diffraction data collected on a laboratory diffractometer. The phase transformations influence the ability of the material's gas storage ability. The rapid and automated processing of data to extract salient features is demonstrated. In particular, relative phase abundances and structural information from each polymorph is determined. The structural characterization technique and data processing tools described here is of general relevance to crystalline functional materials.