Phase Modification Descriptor in the Powder Diffraction File™

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As the name suggests in phase identification using diffraction methods, the aim is to identify the phase not just the chemical composition. Historically, only Greek characters describing the phase modifications are stored in a separate field in Powder Diffraction File™. Other descriptors ('Form A' , 'High temperature phase' etc) were stored under comments making it difficult to search and display prominently. An editorial task was undertaken to tidy this up and to create a table with proper phase descriptors. Starting with release 2016, phase descriptors are displayed on the PDF card. Phase modification descriptor is a broader aspect than polymorphic designation as it also include polytypes and other structural variations. Entries with identical empirical formula (Inorganic) and different crystal structures, with missing phase modification descriptors, are explored to find a suitable descriptor, if exists. Once we have a phase modification descriptor, then we can extend the assignment to other entries with missing descriptor(s) based on their similarity in structure and composition. There are 36,487 entries with phase descriptors in the upcoming Release 2017. A special emphasis is given in assigning and reviewing phase descriptors of materials of high commercial interest such as alumina and cement phases. This presentation will describe the details involved in identifying and assigning various phase modification descriptors using some case studies.