MS42 Solving Structures Through Combination of Reciprocal and Direct Space Methods

MS42-01
Correlated disorder in thermoelectric materials
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Abstract
X-ray diffraction from powders and single crystals has for decades been the key analytical tool in materials science. Bragg intensities provide information about the average crystal structure, but often it is disorder and specific local structure that control key material properties. This is especially the case for thermoelectric materials where disorder for example strongly affects the thermal conductivity. For 1D data there has been an immense growth in combined analysis of Bragg and diffuse scattering using the Pair Distribution Function (PDF), and for example we frequently use 1D PDF analysis to study nanocrystal nucleation [1]. For single crystals, diffuse scattering studies have a long history with elaborate analysis in reciprocal space, whereas direct space analysis of the 3D-PDF is still in its infancy. We have used 3D-PDF analysis to study the crystal structures of high-performance thermoelectric materials Cu2Se [2], PbTe and PbS [3, 4], 19-e half-heusler Nb1-xCoSb [5, 6] and InTe [7], where the true local structure is essential for understanding the unique properties.

References
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