

STRUCTURE SOLUTION AND REFINEMENT APPROACHES FOR OXIDE CERAMICS

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Between extensive new materials development and routine use of in-situ analysis, we encounter many new phases, some of which are stable under ambient conditions and others that are not. The talk will highlight several interesting examples where charge flipping or simulated annealing was of great value in providing at least partial structures from powder diffraction data. Subsequent Rietveld analysis can highlight not only the overall average structures but interesting structural features including static disorder. The use of lab, synchrotron, and neutron powder diffraction will be considered, including some measurements at high temperature. In particular, we will demonstrate the ability to use even poor quality data to successfully solve or partially solve a structure.