MS43-P05 | The inversion model and its limitations for spinel $ZnAl_2O_4$: a multi technique study.

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Point defects in spinel compounds have a significant influence on the physical properties, and they are therefore highly useful for modifying the properties of the materials. While simplified models may reasonably describe experimental data, the inability to model the full complexity of the defects can lead to erroneous structural trends. With a commonplace assumption that inversion of the cations are the only contributing defect, most research in this area relies on a single characterization technique. Taking a multi-technique approach shows why a single technique approach is insufficient for accurately modeling the contribution from point defects in spinel compounds. By using ZnAl₂O₄ as a benchmark material, our multi-technique structural investigation clearly shows that the current cation inversion model is inaccurate, and instead the nature of the ZnAl₂O₄ spinel structure include several synthesis dependent point defects. Based on a comprehensive parameter-study of ZnAl₂O₄, which was synthesized using four different techniques, and combined with various post treatments, we suggest a way forward for systematically incorporating defects in the spinel structure.