Characterization of the correlated disorder in $Ge_2Bi_4Te_7$

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3DED (three-dimensional electron diffraction) is currently already routinely used for the characterization of the average structure from Bragg reflections, and recently its use for quantifying correlated disorder from electron diffuse scattering is also taken off [1,2,3].

In this work, we used a combination of 3DED, HAADF-STEM and STEM-EDX to quantify the correlated disorder in $Ge_4Bi_2Te_7$. $Ge_4Bi_2Te_7$ is reported to contain vacancy-layers along $<11\bar{1}>_{Fm3m}$ and $<1\bar{1}\bar{1}>_{Fm3m}$ with a higher Bi-concentration neighbouring these layers, which leads to the occurrence of streaks of diffuse scattering [4, 5].

Using the combination of advanced TEM techniques, we have not only confirmed the defects previously found by single crystal X-ray Diffraction but also observed and characterized a plethora of other forms of correlated disorder not reported before in literature for this material, including domains with locally different structure and composition, interstitial atoms and local periodicity between Ge and Bi. This diversity in correlated disorder results in 3D diffuse scattering and superstructure reflections that previously passed unnoticed to other techniques.

This work illustrates the large potential of TEM in characterizing correlated disorder from the analysis of diffuse scattering.

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