MS17-2-2 Quantitative analysis of diffuse electron scattering in the lithium-ion battery cathode material $Li_{1.2}Ni_{0.13}Mn_{0.54}Co_{0.13}O_2$
#MS17-2-2

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Abstract
Materials with short-range order produce diffraction patterns that contain both Bragg reflections and diffuse scattering. The average crystal structure can be determined from analysis of the Bragg reflections. To obtain information about the short-range order, it is necessary to analyse the diffuse scattering.
Our study shows, for the first time, a refinement of short-range order parameters from the diffuse scattering in single-crystal electron diffraction data. The approach was demonstrated on the lithium-ion battery cathode material $Li_{1.2}Ni_{0.13}Mn_{0.54}Co_{0.13}O_2$, for which the crystals are too small to be investigated with single-crystal X-ray or single-crystal neutron diffraction. Both the amount of stacking faults and the percentage of the different twins in the crystal were refined from the intensity distribution of the diffuse streaks using a differential evolutionary algorithm in DISCUS [1].
The approach was applied on reciprocal space sections reconstructed from three-dimensional electron diffraction (3D ED) data (Figure 1) since they exhibited less dynamical effects compared to in-zone precession electron diffraction (PED) patterns. The effect of dynamical scattering and thermal diffuse scattering on the intensity distribution of the diffuse streaks will also be discussed.

References
[1] Proffen, T., & Neder, R. B. (1997). J. Appl. Crystallogr. 30, 171-175.

Figure caption: [-210] reciprocal space section (a) reconstructed from three-dimensional electron diffraction (3D ED) data, (b) calculated for the refined short-range order parameters.