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Quantitative analysis of diffuse electron scattering in the lithium-ion battery cathode material Li1.2Ni0.13Mn0.54Co0.13O2

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Materials with short-range order produce diffraction patterns that contain both Bragg reflections and 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 Li1.2Ni0.13Mn0.54Co0.13O2, 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 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.

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

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