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

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Correlated disorder is any type of deviation from the average crystal structure that is correlated over the range of a few unit cells only. As correlated disorder lies at the origin of the physical properties of a compound, many open questions in materials science are related to it. Unfortunately, the diffuse scattering analysis from single-crystal X-ray and neutron diffraction needs large crystals which are often not available. In the case of submicron sized crystals, pair distribution function analysis on powder samples could be applied. However, as an alternative we suggest to turn to single-crystal electron diffraction. While the quantitative analysis of diffuse X-ray and neutron scattering has already been done for different types of correlated disorder, we will present for the first time the quantitative analysis of diffuse electron scattering using an evolutionary algorithm in *DISCUS* [1].

In the electron diffraction patterns of $Li_{1.2}$ $Ni_{0.13}Mn_{0.54}Co_{0.13}O_2$ diffuse streaks are present, which are caused by stacking faults (i.e. variations in the stacking of subsequent Li-, O- and transition metal -layers). An evolutionary refinement algorithm in *DISCUS* was used to determine the stacking fault probability as well as the twin ratio in $Li_{1.2}Ni_{0.13}Mn_{0.54}Co_{0.13}O_2$ by a refinement of the intensity profile of the diffuse streaks. The refinement algorithm was first tested on simulated data, after which it was applied to experimental electron diffraction data obtained by three-dimensional electron diffraction (3D ED).

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

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