Contribution ID: **433** Type: **Poster Presentation**

Atomistic Insights into Amorphisation and Recrystallisation of Nano-Spherical LiNiO₂: Phase Retention and Microstructural Evolution.

LiNiO₂ (LNO) has emerged as a promising high-capacity cathode material for lithium-ion batteries (LIBs), offering a theoretical capacity of 270 mAh/g. However, its commercialisation is hindered by structural instability and rapid voltage degradation during cycling, primarily resulting from mechanical stress induced by phase transitions and volume changes. These effects lead to particle cracking and performance decay. Nanostructuring has been proposed as a potential solution to mitigate these issues by stabilising phase transitions and enhancing mechanical integrity. In this study, a simulated synthesis approach was employed to generate nano-spherical LiNiO₂ models and track the evolution of their microstructure during crystal growth. The synthesis involves simulated amorphisation, then proceeds to recrystallisation under a canonical ensemble with constant temperature and volume, and ends with gradual simulated annealing of the recrystallised structure. Through systematic trial and error, the optimal temperatures were identified as 1400 K for amorphisation and 1200 K for recrystallisation. The formation of LiNiO₂ was confirmed through simulated X-ray diffraction (XRD) patterns and atomic snapshots. However, the XRD analysis also revealed impurity peaks corresponding to spinel NiO phases. Post-cooling structural analysis confirmed phase retention, with both XRD and radial distribution function (RDF) analyses providing insights into the structural evolution of the material. These findings contribute to the optimisation of thermal processing conditions, paving the way for more structurally stable and high-performance LiNiO₂ cathodes in lithium-ion batteries.

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials