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Atomistic Simulation Studies of Layered Li_2MnO_3 Nanospherical Cathode Materials

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Li-excess Mn-based materials are potential candidates for the next generation of cathode materials owing to their high discharge capacity (>200 mAh/g). This drives the interest for the intercalation/deintercalation processes using host electrodes with dimensions at the nanoscale, as this is sufficiently quick to deliver the power required from Li-ion batteries. The favorable material Li_2MnO_3 is known to be electrochemically inactive in the parent bulk form, and can be rendered Li-active by leaching Li from the structure. However the structural configuration and nucleation process of Li_2MnO_3 have not been documented, particularly during the cycling process. The current study employs the molecular dynamics (MD) DL_POLY code to generate the nanoparticles using amorphization and recrystallization (A&R) technique under microcanonical and canonical ensembles (NVE and NVT), respectively. Nanoparticles were deintercalated to delineate the charging process and investigate new possible Li-Mn-O intermediate phases that may emanate in the $\text{Li}_2\text{MnO}_3 \rightarrow \text{LiMnO}_2$ tie-line. The microstructural snapshots depict the formation of intermediate structures due to Li extraction and O loss. Furthermore, XRDs for intermediate structures shows the emergence of new peaks together with the main characteristics' peaks of the Li_2MnO_3 . Here it is shown that structural complexity evolves during synthesis – specifically, during the nucleation and crystallization process with microstructural features such as grain-boundaries (Li_2MnO_3 , $\text{Li}_{1.5}\text{MnO}_{2.5}$ and LiMnO_2), dislocations and intrinsic point defects (Li_2MnO_3). Findings of this work demonstrate how the deintercalation results affect the structural transition of the Li_2MnO_3 cathode material, and shed valuable details about the intermediate structural transformations that transpire during cycling.

Apply to be considered for a student award (Yes / No)?

Yes

Level for award (Hons, MSc, PhD, N/A)?

Hons

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