Atomistic Simulation Studies on Volume Expansion of Lithiated nano-MnO_2

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Manganese dioxide is an important material for electrochemical applications; including serving as a cathode material in Li-ion batteries and recently usage in lithium air batteries [1]. Atomistic simulation methods offer a unique platform of exploring structural features at the nanoscale. A crystallised nanosphere of MnO_2 consisting of 25000 atoms, and grown by amorphisation recrystallisaiton method [2], was lithiated by inserting 0 to 6000 Li ions. The volume change with Li content was investigated by performing molecular dynamics simulation under the NVT ensemble. This allowed the connolly volume to change whilst the lattice box is kept fixed. Elastic expansion of the nanosphere occurs below 33% lithium ion concentration while plastic deformation is noted above 33% lithium content; where the nanosphere breaks down and amorphises. The variation of mechanical properties and changes of microstructural features with low and high lithium concentration are analysed. The resulting microstructures provide valuable insights into the origins of electrochemical activity which accounts for its suitability as a battery electrode.

References

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