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Atomistic simulation and Li ion diffusion studies of bulk LixTiO2 nanostructures as anode electrode material for lithium ion batteries.

A molecular dynamics (MD) simulation was employed using the DL_POLY 2.20 code to investigate the effects of Li concentration, temperature and diffusion behaviour of Li ions in TiO2 bulk nanostructures. The TiO2 bulk with different concentrations of Li were recrystallised, cooled then heated at increased temperatures. Recrystallization was confirmed by configurational energy time graph and the cooling process was confirmed by the radial distribution function. The X-ray diffraction patterns and microstructural details were used to predict various polymorphs in LixTiO2 bulk nanostructures which were similar to bulk γ-MnO2 [1]. Diffusion coefficient with its Arrhenius plot have resulted in a nonlinear plot. The maximum diffusion coefficients and activation energies for Li ion in bulk TiO2 were calculated to be 10¬¬-16m2s-1 and 0.32eV respectively which are thus comparable to bulk β-MnO2 [2].
[1] Rapela R. at al., Phys. Chem. Phys., 2011,13, 1307-1313.
[2] Thi X.T. Sayle et al., J. Mater. Chem. A, 2016, 4, 6456.

Summary

Bulk, simulation, recrystallization and microstructures

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