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Atomistic Simulation Studies of Nanostructured TiO_2[1]

PHUTI NGOEPE, MALILI MATSHABA, University of Limpopo, DEAN SAYLE, Cranfield University — TiO_2 has been confirmed as a safe anode material in lithium ion batteries due to its higher Li-insertion potential, ($\sim$1.5V) in comparison with commercialised carbon anode materials. Recently in order to attain high rate capabilities of TiO_2 anode, for application in lithium ion batteries with both high power and high energy density, intensive attention has been paid to various TiO_2 nanostructures, such as nanoparticles, nanowires and mesoporous structures. In the current study, amorphisation recrystallization method is used to produce nano- porous, sheets and bulk structures for TiO_2 which have been extensively studied experimentally. Simulated X-ray diffraction patterns are produced from such structures and compared with the experimental XRDs. The simulated microstructures are analysed and compared with available high resolution transmission experimental results. Lithiation of TiO_2 nanostructures is considered and discussed in the context of current investigations and concentration profiles of different ions are shown in the structures. Semi-empirical models based on DFT tightbinding methods, are introduced for TiO_2 and lithiated its forms.

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