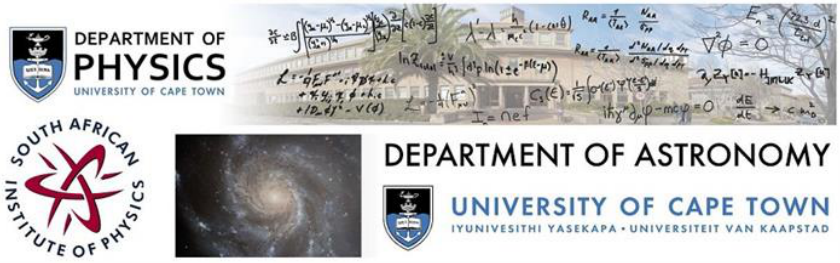

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Effect of pressure on the nanostructured of TiO2 during recrystallisation

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
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Titanium dioxide (TiO2) nanoparticles, nanowires, nanosheets and nanoporous are of great interest in many applications. This is due to inexpensive, safety and rate capability of the material. It has being considered as a replacement of graphite anode material in rechargeable lithium batteries. In this work we use molecular dynamics simulations to investigate the effect of pressure on nanostructures of TiO2 during recrystallisation, employing DL_POLY code. We have successfully recrystallised all four nanostructures from amorphous precursors. Configuration energies, calculated as a function of time, were used to monitor the recrystallisation. Calculated X-Ray Diffraction (XRD) spectra, using the model nanostructures, reveal that the nanostructures are polymorphic with TiO2 domains of both rutile and brookite in accord with experiment. At higher pressure the configuration energy depict that systems takes long to recrystallise and also indicate that the brookite phase is disappearing. Compression of 75 and 1000 KPa structures is equivalent to the insertion of lithium atoms generated by Matshaba. Bulk structure indicate channels where lithium atoms can move during charging or discharging.

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