Contribution ID: **286** Type: **Oral Presentation**

Atomistic Simulation Study on Lithiated Manganese Dioxide Nanostructures

Wednesday, 13 July 2011 14:30 (15 minutes)

<p>Nanostructured materials are used to develop lithium-ion batteries with high energy, high-rate capability and excellent cycling stability due to their huge surface area, short distance for mass and charge transport and freedom for volume change. They are capable of reversibly accommodating large amount of Li, on intercalation mesoporous β-MnO₂ can accommodate Li/Mn = 0.92:1 with 81

Atomistic computer simulations offer a unique platform of exploring structural features at the nanoscale. Simulated amorphisation and recrystallisation technique, involving tens of thousands of atoms, has been successfully used to generate models of various nano-forms of the complex manganese dioxides, which include microstructural details. In the current study, we apply this method to study lithium insertion into the nanospheres, nanosheets, nanorods and nanoporous structures of the binary manganese dioxides. Different Li concentrations (up to Li:Mn = 0.73:1) were inserted into the different nanostructures. Molecular dynamics simulation under the NPT ensemble was performed, in order to allow the system to expand. The variation of mechanical properties and changes of microstructural features with low and high lithium concentration are investigated. The resulting microstructure provides valuable insights into the origins of electrochemical activity which could make it a suitable battery electrode.

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

No

Primary author: Mr KGATWANE, Kenneth (University of Limpopo)

Co-authors: Prof. SAYLE, Dean (Cranfield University); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Mr KGATWANE, Kenneth (University of Limpopo)

Session Classification: CMPMS2

Track Classification: Track A - Condensed Matter Physics and Material Science