Contribution ID: **114** Type: **Poster**

Investigating the Mechanical Properties of Lithiated Li1+XMn2O4, (0 ≤ x ≤ 1) Nanoporous Composites

The demand for batteries with higher energy density and storage capacity has been increasing over the past three decades. As such spinel LiMn2O4 have been found to be one of the promising and paramount cathode materials due to its inexpensiveness, environmental friendliness and structural stability when compared to its counterparts, such as LiCoO2. However, this material suffers from high voltage fade due to the Jahn-Teller distortion. This is caused by volume expansion in bulk materials; resulting in a material that has reduced symmetry and energy, consequently causing fractures to the material. Nanoporous materials for rechargeable Li-ion batteries have been considered to be a solution for Li-ion batteries due to their large exposed surface areas within the pore. This rare features enhance ionic diffusion and consequently improves electrochemical performance and mechanical stability. Furthermore, they also have the ability to expand freely upon lithiation without compromising the structural integrity of the electrode material.
Herein, molecular dynamics simulations employing the DL_POLY code have been used in a quest to investigate the mechanical properties of lithiated Li-Mn-O nanoporous materials of different cell dimensions (75 Å, 69 Å and 67 Å) and lithium concentration (Li1+xMn2O4, 0 ≤ x ≤ 1). When the lithium concentration is increased, all the structures experience volume expansion and nanoporous 67 Å shows more resilience to fracture compared to nanoporous 69 and 75 Å, due to its high yield strength. However, at Li1.75Mn2O4 concentration, nanoporous 69 Å depicts a higher yield strength. This is also validated by cleaner XRDs at this concentration compared to the other nanoporous structures. This implies that the cavity to wall ratio of nanoporous 69 Å results in an electrode material that is more resilient and not prone to fracture.

Supported Student

Primary author: Ms SHIBIRI, Beauty (University of Limpopo)

Co-authors: Dr LEDWABA, Raesibe Sylvia (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Ms SHIBIRI, Beauty (University of Limpopo)

Session Classification: SIG Poster

Track Classification: SIG Seminar: Chemistry, Material Science and Health Science