Contribution ID: **292** Type: **Oral Presentation**

The Mechanical Properties Study of Li1+XMn2O4, 0 ≤ X ≤ 1 Cathode Materials

Monday, 26 July 2021 16:00 (15 minutes)

One of the major limitations associated with spinel LiMn2O4 despite its superior properties such as high voltage, great cycling performance, being environmentally friendly and cost-effective is the impact of the stress it endures through strain during the process of cycling. For that reason, this study seeks to understand the implications that come with stress-strain and how it affects the mechanical properties of a battery material; and eventually come with a better nanoporous structure that can withstand these harsh conditions.
Herein, the amorphisation and recrystallisation technique were used to simulate the Li-Mn-O nanoporous structures of different lattice sizes at 75, 69 and 67 Å and varying lithium concentrations, (Li1+XMn2O4, 0 ≤ X ≤ 1) using the DL_POLY code. Recrystallisation of the nanoporous structures resulted in single and multiple grained materials with microstructures that shows a profusion of point defects. Furthermore, the microstructures capture the spinel layered composites which are also validated by the X-ray diffraction patterns of these structures. The stress and strain analysis shows that nanoporous 69 Å has the highest yield strength compared to its nanoporous counterparts. This, therefore, implies that nanoporous 69 Å is more robust and can be a better candidate to help restrict battery hazards in the future as far as fracture is concerned.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

Primary author: Ms BEAUTY, Shibiri (University of Limpopo)

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

Presenter: Ms BEAUTY, Shibiri (University of Limpopo)

Session Classification: Physics of Condensed Matter and Materials

Track Classification: Track A - Physics of Condensed Matter and Materials