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Armorphization and Recrystallization of spinel LiMn_2O_4 nano-architectures

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Abstract content (Max 300 words) Formatting & Special chars

Spinel LiMn_2O_4 has attracted attention as a potential cathode material for use in advanced lithium ion batteries. The current study focused on the effects of high temperatures on the spinel system: the 3D framework sustainability, structural transformation and impacts of melting temperature on the lithium ion diffusion. Furthermore, understanding these materials will facilitate in the implementation of armorphization and recrystallization technique for spinel nano-architectures. Molecular dynamics simulations were carried out at various temperatures. The melting points and transformations are clearly visible on the RDF plots and structural snapshots of the supercells at different temperatures. LiMn_2O_4 indicated a diffusion rate that increased rapidly above 1500K, just before melting (~1700 K) and reached its maximum diffusion at $2.756 \times 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$ before it decreased. Simulated armorphization and recrystallization was carried out on the system. The nanoparticle started armorphizing into a nanosphere around 150 ps during the simulation and nucleated after 1500ps with the assistance of a crystalline seed in the centre of the armorphised nanoparticle. Recrystallization was complete after 6 ns, the latent heat of crystallization is therefore reflected in the energy difference between the first (0–1.5 ns) and second (6 ns –15ns) energy trace.

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yes

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

M.Sc.

Main supervisor (name and email) and his / her institution

Prof. Phuti Ngoepe

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