Contribution ID: **297** Type: **Oral Presentation**

Armorphization and Recrystallization of spinel LiMn₂O₄ nano-architectures

Wednesday, 1 July 2015 09:40 (20 minutes)

Abstract content
   (Max 300 words)
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Spinel LiMn₂O₄ 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. LiMn₂O₄ indicated a diffusion rate that increased rapidly above 1500K, just before melting (˜1700 K) and reached its maximum diffusion at 2.756x10E-7 cm2.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. Recrystalization 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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Session Classification: DPCMM

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