Australian Synchrotron
USER MEETING 2014
20 – 21 November
National Centre for Synchrotron Science

Contribution ID : **152** Type : **Poster**

A combined experimental and computational approach to understanding and developing solid-state ionic conductors

Thursday, 20 November 2014 17:30 (90)

Materials that exhibit significant mobility of different types of charge carriers have potential applications as fuel-cell membranes, electrodes, batteries and sensors. A thorough understanding of the fundamental atomic-scale mechanisms of the conduction processes in these materials is necessary to identify ways in which their local chemistry and structure can be modified to lower activation barriers and optimize pathways for conduction.

Inelastic neutron scattering experiments will be performed to probe structural fluctuations that may trigger or facilitate the diffusion process. Together with ab initio molecular dynamics (MD) calculations these results will then be used to develop and rigorously verify classical force fields for empirical calculations to extend the simulations to timescales required to observe actual conduction processes. The results will suggest ways in which the local chemistry and structure of materials can be modified to lower activation barriers and optimize the pathways for ionic conduction.

Good oxide-ionic conductivity, simple chemical composition and the scope for chemical and structural modification make apatite-type Nd9.33Si6O26 a good initial target system. Nd9.33Si6O26 crystallizes in the hexagonal apatite structure P63/m and has 6.7% Nd vacancies located at the 4f site only. A thorough analysis of different arrangements of Nd vacancy positions has been performed to obtain a suitable input model for ab initio MD calculations. Possible arrangements have been classified by the corresponding sum of distances between the vacancies to quantify the degree of distribution and investigate the influence of different vacancy distributions on subsequent calculations.

Keywords or phrases (comma separated)

Summary

Primary author(s) : Ms WIND, Julia (University of Sydney)

Co-author(s) : Prof. LING, Chris (University of Sydney)

Presenter(s) : Ms WIND, Julia (University of Sydney)

Session Classification : Welcome Function, Poster Session, Exhibition

Track Classification : Advanced Materials