Abstract No: STEM 14 Science, Technology, Engineering and Mathematics

Investigating temperature dependence of lithium-ion diffusion through the silicon (111) surface

Ranaweea R. M. L. H.[1], Samarakoon Y. M. I. B.[2], Amaraweera T. H. N. G.[1*], Wijayasinghe H. W. M. A. C.[2]

Demand for high energy density rechargeable lithium-ion batteries has drastically increased in the last few decades. Graphite is the most common anode material used for rechargeable lithium-ion batteries. But it possesses less specific energy density hence is difficult to apply for high energy applications. Therefore, many studies to find out high specific capacity anode materials. One of the important high specific capacity, novel anode materials is silicon and its oxidative derivatives. But less diffusivity of lithium ions is one of the major drawbacks of these materials. Since it is very difficult to get the atomic picture of the anode during the lithiation process using analytical methods, computational methods have also been employed. Therefore, this research aims to carry out molecular dynamics simulations on silicon to study the migration of the lithium ions through silicon structure. Silicon model with 111 plane was modeled. X, Y and Z axis lengths of the lattice were around 30 Å, 26 Å and 50 Å respectively. Inside this lattice 896 of silicon atoms and 16 lithium atoms were placed. Modified embedded atom method (MEAM) potential is used to simulate the system by using Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) source code. After model validation, optimum voltage of diffusion for lithium ions, their mean square displacement (MSD) and diffusion coefficient (DC) are calculated. The optimum diffusion voltage for lithium ions is 2.1 V A^{-1}. The DC of the lithium ions in silicon (111) surface at 300 K is 6.13×10^{-13} cm^2 s^{-1} which is very close to the experimental values obtained in previous studies. Then the model was subjected to different temperatures (250 K to 450 K) while lithium ions were diffusing through 111 surfaces. DC of lithium ions was calculated at 10 K temperature gaps. Although there is an increment of the DC for lithium atoms with respect to temperature increments, it is not a stereotypical increment. Additionally, it has shown 93.85 % increase in DC for lithium ions when it goes from 250 K to 450 K. This shows a drop in friction acts on lithium atoms from the silicon environment as temperature rises.

Keywords: Silicon, Lithium, Lithium-ion battery, LAMMPS, DC, MSD

[1] Department of Applied Earth Sciences, Uva Wellassa University of Sri Lanka
[2] National Center for Advanced Battery Research, National Institute of Fundamental Studies
* gayani@uwu.ac.lk