Design for a Hyper Li-ion Transport Channel with Polyelectrolyte and Ionic Liquid through Molecular Dynamics Simulation

김슬우, 조준범, 권상우, 이민환, 이원보†
서울대학교
(wblee@snu.ac.kr†)

Polyelectrolyte-Li^+ battery has been used widely for their thermal and mechanical stability. Still, the low conductivity at ambient temperatures makes it hard to use practically. In this respect, 'ionic liquids' (ILs) have replaced conventional salts or any additives (nanoparticles or organic solvents) to modificate the poor performance. Here, we used PEO polymer chains as polyelectrolyte and N-methyl-N-butylpyrrolidinium bis(trifluoromethanesulfonyl) imide ($PYR_{14}TFSI$) as ionic liquid. Our motivation is a micro-scale cylindrical channel could accelerate the transport of Li-ion along the axial direction. To elucidate the phenomena on atomic scale, molecular dynamics (MD) simulation was employed. In present study, we compared three configurational systems; a bulk, a channel simply filled with polyelectrolyte and ILs, and a channel with branching PEO and filled with ILs. Also, we investigated the optimal diameter of the channel for rapid transport. It came out that branching PEO chain affects topology of the polymer chains and it consequently influence on the transport mechanism of Li-ion.