

Title	Molecular dynamics study of poly (ethylene oxide) (PEO) containing LiI salt
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Purpose of this study	To get an insight into the transport mechanism of Li ion in PEO. Application: Li ion battery
System (Material)	PEO and LiI salt.
Program (including analysis)	COGNAC v1.3
Method & Some important input parameters	(Method) Molecular dynamics simulation modeled by united atom model with empirical potentials. To calculate coulomb interaction, charges are sited at non-bonding interaction sites as point charges. (Inputs) Degree of polymerization and number of molecule. Bonding interaction (bond, angle and torsion potentials were used) and non-bonding interaction (OPLS). Temperature was set at 363K.
Advance & Problem	(Advance) -It was observed that Li ⁺ in PEO melts has two characteristic modes of motion. -It was also observed that Li ⁺ and I ⁻ form ion cluster with increasing salt concentration consistently with experiments. (Problem) -Tremendous additional calculation is required for quantitative evaluation of diffusion coefficient deriving ionic conductivity.
References	[Manuscript] Progress of Theoretical Physics Supplement No. 138 (2000) (Accepted) [Presentation at conferences (Meetings)] The 5th International Conference on Computational Physics (ICCP5 (1999)) CMD18-European Physical Society (2000) Polymer Preprints Japan (2000)
KeyWords (in English)	MD, PEO, Li, LiI, conductivity, OPLS, ewald, united atom model

Results (Remarks)

Output:

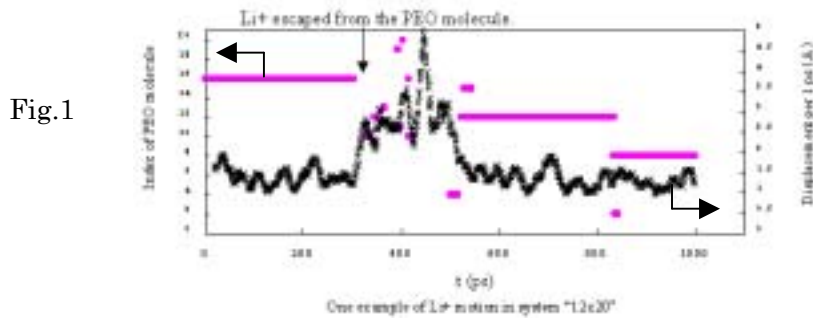


Fig.1)

One example of Li⁺ motion in the system. (Degree of polymerization : 12)
 The circles indicate the index number of PEO molecule with which this Li⁺ forms a complex, and the cross symbols indicate the displacement of the Li⁺ per 1 ps.

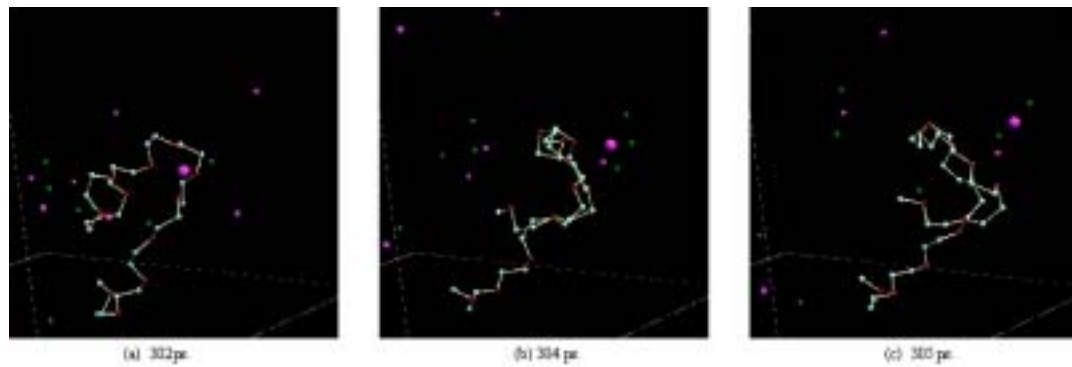


Fig.2

Fig.2)

The snapshots in each time step. The Li⁺ (referred at Fig.1) is drawn as large balls for visual.

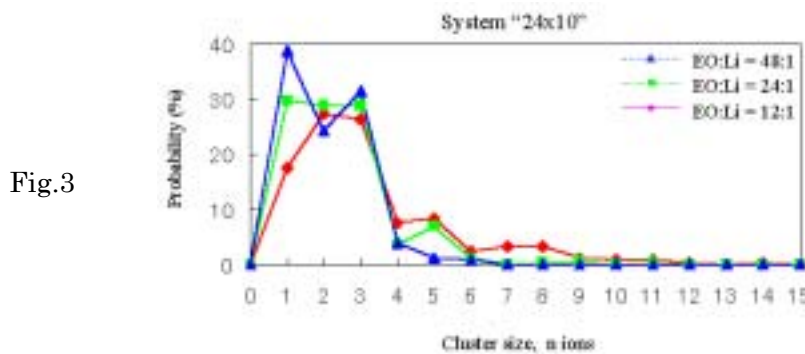


Fig.3

Fig.3)

Size distribution of the ionic cluster for various salt concentrations. The larger ion cluster (consists of Li⁺ and I⁻) was formed with increasing salt concentration (Degree of polymerization : 24).