Molecular Dynamic Simulation studies of Manganese Lithium Borate-Based Glasses

Pattarapong Nijapai[a], Saroj Rujirawat[a], Rattikorn Yimnirun[b], Pinit Kidhunthod[c]
a School of Physics, Institute of Science, and NANOTEC-SUT COE on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima, 30000, Thailand
b School of Energy Science and Engineering,Vidyasirimedhi Instituteof Science and Technology, Rayong 21210, Thailand
c Synchrotron Light Research Institute (Public Organization), 111 University Avenue, Muang District, Nakhon Ratchasima 30000, Thailand
d5910069@g.sut.ac.th

The structure of manganese lithium borate-based glass was studied by using molecular dynamic (MD) simulation. In this work, a glass system of $0.2MnO_2 - 0.8(Li_2\text{-}2B_2O_3)$ was introduced. DL_POLY MD package[1] based on Buckingham potential parameter[2,3,4] was employed to calculate structure of this glasses. The ten pair radial distribution functions of this glass were obtained from the MD simulation. To understanding this glass structure, MD-EXAFS result which came from FEFF8.2 package[5] was compare with EXAFS spectrum at Mn K–edge of this glass. Consequently, a good agreement between calculated and measured EXAFS data was obtained leading to a fully address of local structures of this glassy materials with a mean Mn-O coordination network of 3.01(2).

Keywords: Manganese Lithium Borate Glass, Molecular Dynamics Simulation, EXAFS.

[1] W Smith, TR Forester,Journal of molecular graphics, 14, 3, 136-141 (1996)
[2] T.S.Bush, J.D.Gale, C.R.A.Catlow and P.D. Battle, J. Mater Chem., 4, 831-837 (1994)
[3] E.Kashchieva, B.Shivachev and Y.Dimitriev, J. Non-Crystalline Solids., 351, 1158-1161 (2005)
[4] Jolley, K., Smith, R. and Joseph, K., Nuclear Instruments and Methods in Physics Research, Section B, 352, 140-144 (2015)
[5] J.J. Rehr, J.J. Kas, F.D. Vila, M.P. Prange, K. Jorissen, Phys. Chem. Chem. Phys., 12, 5503-5513 (2010).