Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A Molecular Dynamics Simulation of the Density Fluctuation in the Diatomic Fluids around the Critical Points SHOHEI IKAWA, Shinshu Univ, TAKASHI TOKUMASU, Tohoku Univ, NOBUYUKI TSUBOI, Kyushu Institute of Technology, SHINICHI TSUDA, Shinshu Univ — In this study, we investigated the principle of corresponding state on the density fluctuation around the critical points of non-polar diatomic fluids. We performed the Molecular Dynamics (MD) simulation for the extraction of the fluctuation structure around the critical points of 2-Center-Lennard-Jones (2CLJ) fluids, which have anisotropy depending on the molecular elongations. We estimated the fluctuation structure by two methods. One is the evaluation of the dispersion of the number of molecules at a certain domain, and the other is the calculation of static structure factor. As a result, in 2CLJ fluids that have shorter molecular elongations comparatively, the principle of corresponding state is satisfied because of the small differences in the fluctuation structure extracted in the present two methods. In addition, paying attention to the time variation of the density fluctuation, we confirmed that the characteristic frequency of the fluctuation is clearly lower around the critical point compared with the other conditions. Hereafter, we are going to calculate a dynamic structure factor, further investigating the principle of corresponding state of density fluctuation.

Shohei Ikawa
Shinshu Univ

Date submitted: 09 Jan 2014 Electronic form version 1.4