RELAXATION AND TRANSPORT PROPERTIES OF LIQUID N-TRIACONTANE

Kondratyuk N.D.,[*1] ***Norman G.E.***[2]

[1]*MIPT, Dolgoprudny, Russia,* [2]*JIHT RAS, Moscow, Russia*
[*]*kondratyuk@phystech.edu*

Molecular modelling is used to calculate transport properties and to study relaxation of liquid n-triacontane ($C_{30}H_{62}$). The problem is important in connection with the behavior of liquid isolators in a pre-breakdown state [1].

Two all-atom models are used: DREIDING and AA-OPLS, as well as the united-atom model TraPPE, in which three hydrogen atoms in CH_3 and two in CH_2 merge with the carbon atom; the group formed is considered as an effective point particle. Shear viscosity is calculated using the Green-Kubo formalism. In the work [2], authors use 10 quasi-independent MD runs to get statistics for the viscosity calculation. We collect statistics from a single equilibrium MD trajectory by dividing it into a number of statistically independent parts. Diffusion coefficients are calculated via the Einshtein-Smoluchowski equation. MD simulations are carried out using software package LAMMPS.

The Green-Kubo method uses the stress autocorrelation function. The functions calculated appear to oscillate in the case of n-triacontane unlike for the atomic systems. Stress autocorrelation function is calculated for the liquid argon and methane (the simplest alkane) to prove this fact. Viscosity values for the both systems are obtained with a good accuracy. DREIDING potential gives correct value of the viscosity for the liquid n-triacontane, but the pressure turns out to be very high for the normal density. The value of pressure is consistent with the density in AA-OPLS model due to the Coulumb interactions and to the more complex form of the torsion interaction. The force fields are compared using the following criteria: required time for one MD step, compliance of the main physical and transport properties with experimental values. The problem of the system equilibration is considered.

The TRAPPE potential is used to model the n-triacontane liquid with an initial directional orientation. The time of relaxation to the disordered system, when all the molecules orientations are randomized, are obtained. The influence of the molecules orientations on the shear viscosity value and the shear viscosity relaxation are treated.

The work is partially supported by the RFBR grant 14-08-31550 mol_a.

1. Apfelbaum M. S., Apfelbaum E. M. // J. Electrostatics. 2001. V. 50. P. 129
2. Payal R., et al. // Mol. Sim. 2012. V. 38. P. 1234