Molecular dynamics analysis of amorphous ice transformations: nucleation mechanisms

Garkul A A[1,2,@] **and Stegailov V V**[1,2,3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] garkul.aa@phystech.edu

Water exhibits many anomalous properties, including the presence of several amorphous states. The most common of these are low-density (LDA) and high-density (HDA) amorphous ice.
Unlike conventional first-order phase transitions, the kinetics of amorphous-amorphous transitions has been much less studied. In this work, we make an attempt to build a microscopic picture of the experimentally studied [1] transformations between LDA and HDA induced by pressure or heating using the molecular dynamics method with the TIP4P/Ice water model [2]. We study carefully the change in structure during transformations based on the radial distribution function. The system size effects are considered as well. The comparison with the experimental data enriches our understanding of the transitions observed. Our modelling gives new information on the nucleation mechanisms during transformations between LDA and HDA and, thus, helps answering the question about first-order nature of this transition.

[1] Gromnitskaya E, Stal'gorova O, Brazhkin V and Lyapin A 2001 *Physical Review B* **64** 094205
[2] Abascal J, Sanz E, García Fernández R and Vega C 2005 *The Journal of chemical physics* **122** 234511