# Calculation of the elastic properties of amorphous ice: Molecular dynamic simulation

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

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] garkul.aa@phystech.edu

In contrast to ordinary first-order transitions, the kinetics of crystalline-to-amorphous and amorphous-amorphous transformations is much less understood. Lattice instability is supposed to be the mechanism triggering solid-state amorphization (SSA). Cooperative vibration soft modes may be responsible for coordination changes in amorphous phases the displacive mechanism. For a microscopic understanding of how such transformations take place in crystalline and amorphous ices, the molecular dynamics (MD) method is an effective theoretical tool. In this work, the model of ice TIP4P ICE is considered, amorphous ice of high (HDA) and low (LDA) density is obtained. The transformation of one amorphous form into another is considered. Calculation of elastic properties of amorphous ice has been carried out, the result is compared with experiment [1]. System modeling and calculations are implemented using the LAMMPS package.

[1] Gromnitskaya E L, Stal'gorova O V, Brazhkin V V and Lyapin A G 2001 *Phys. Rev. B* **64**