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MIPT
MOSCOW INSTITUTE OF PHYSICS AND TECHNOLOGY

IIEFM 2021

Polymorphic transformations and melting of ice XVII: Molecular dynamics modeling

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Moscow institute of physics and technologies

Elbrus 2021

JOURNAL OF ALLOYS AND COMPOUNDS

New phase in the water–hydrogen system

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nature communications

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New porous water ice metastable at atmospheric pressure obtained by emptying a hydrogen-filled ice

Leonardo del Rosso, Milva Celli & Lorenzo Ulivi

nature materials

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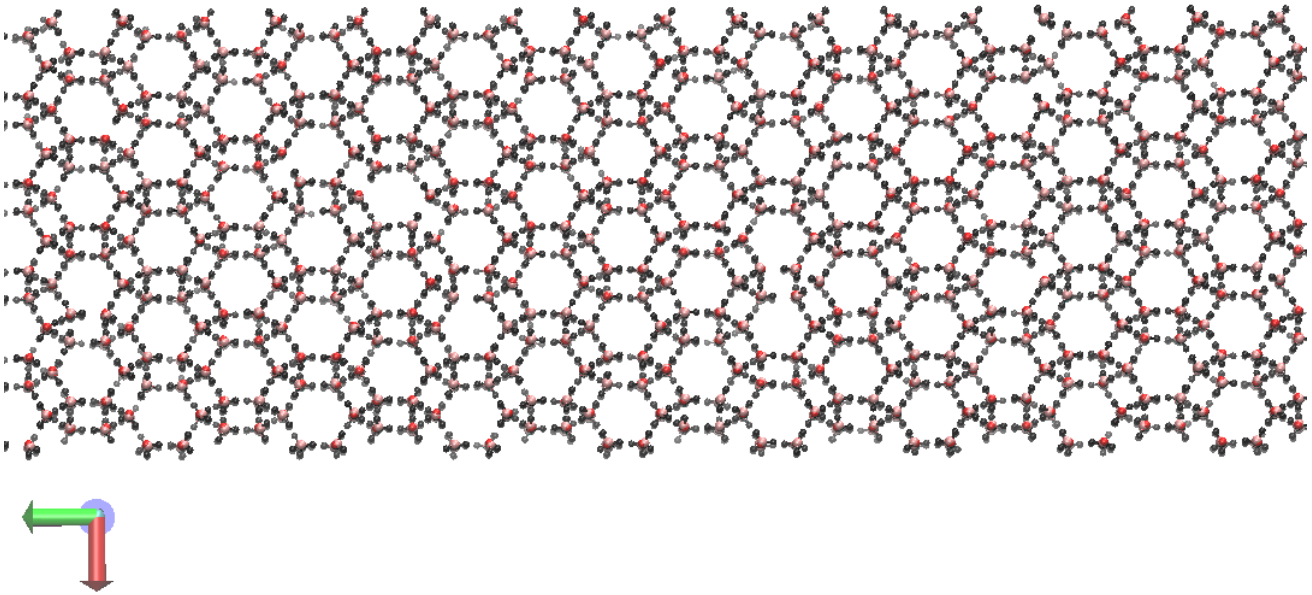
Cubic ice Ic without stacking defects obtained from ice XVII

Leonardo del Rosso, Milva Celli, Francesco Grazzi, Michele Catti, Thomas C. Hansen, A. Dominic Fortes & Lorenzo Ulivi

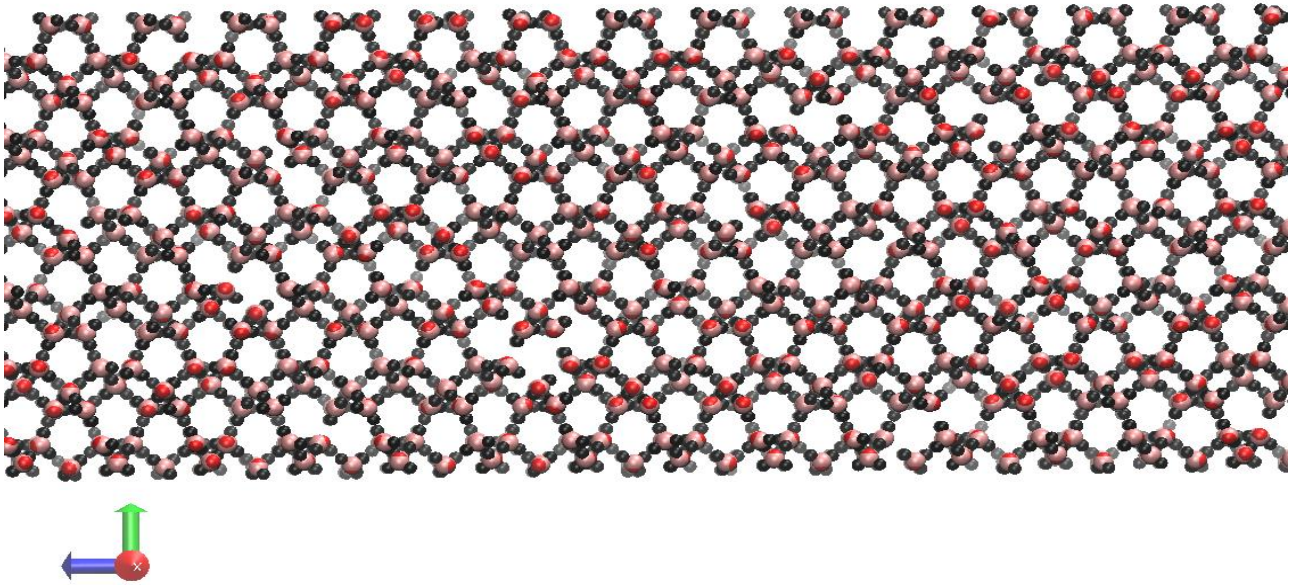
Motivation

Verification of the experimentally discovered transition of ice XVII into cubic ice and transition mechanism explanation

Two orientations of ice XVII that calculations were carried ou



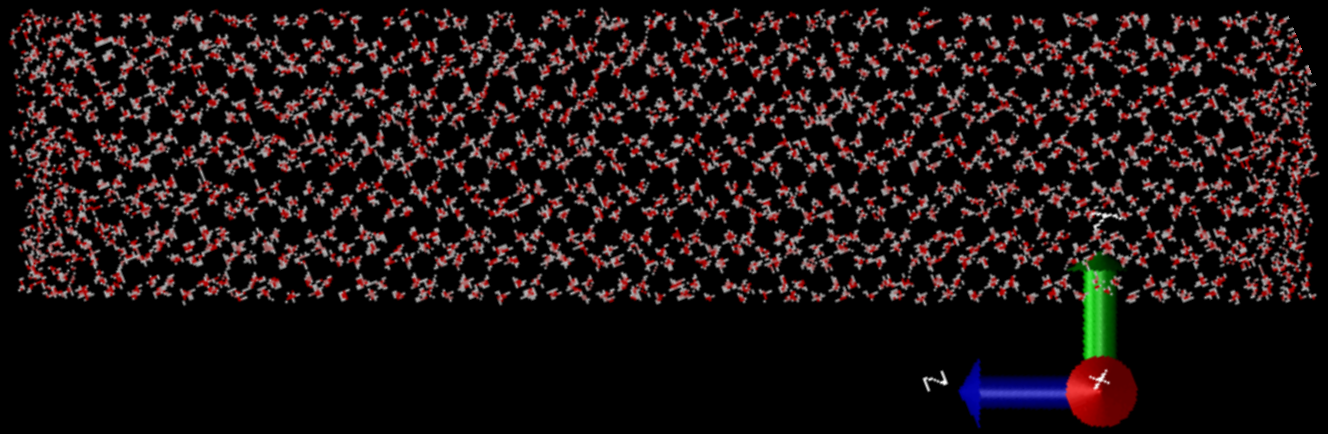
Y - Orientation



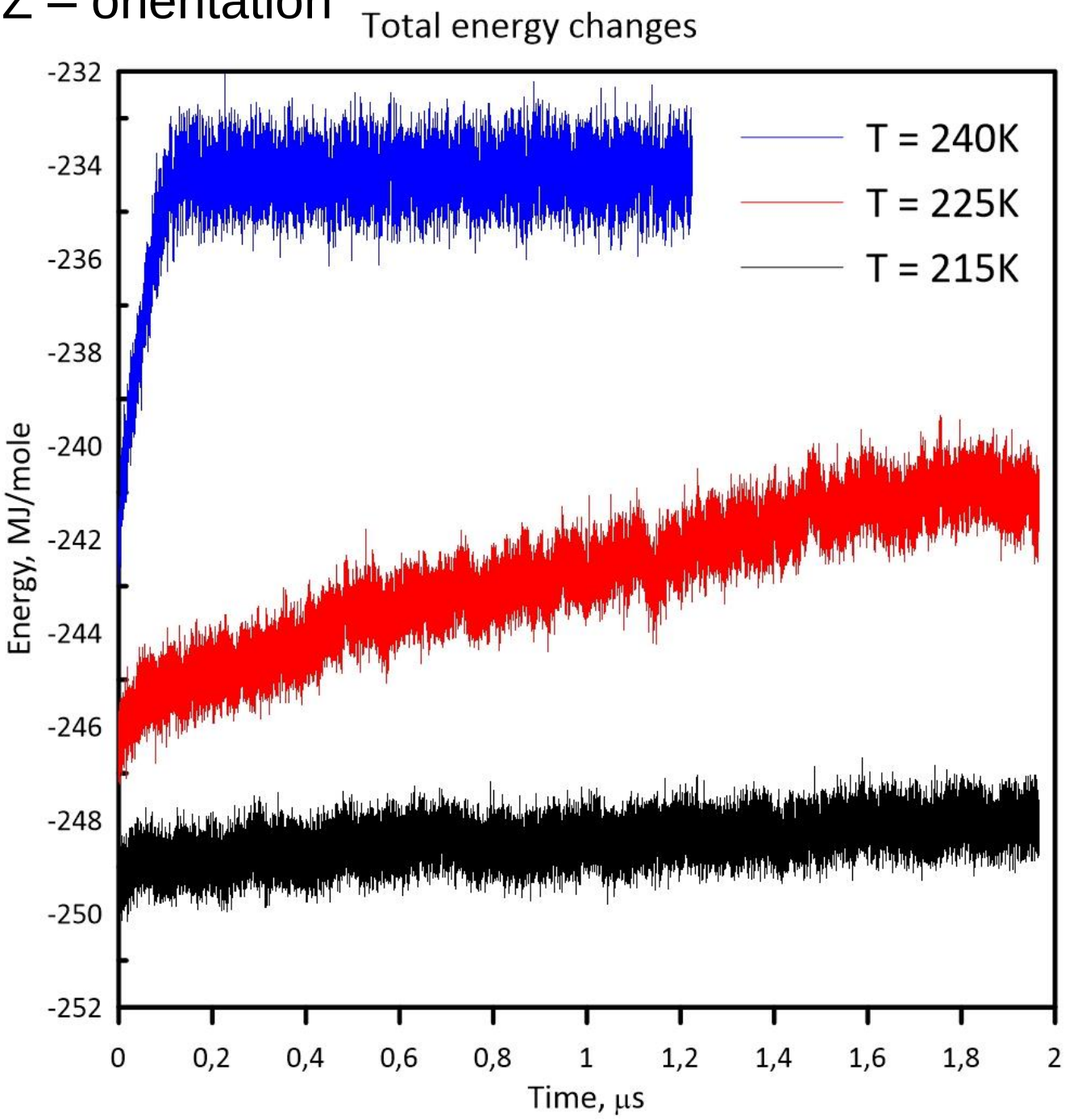
Z - Orientation

Z – Orientation

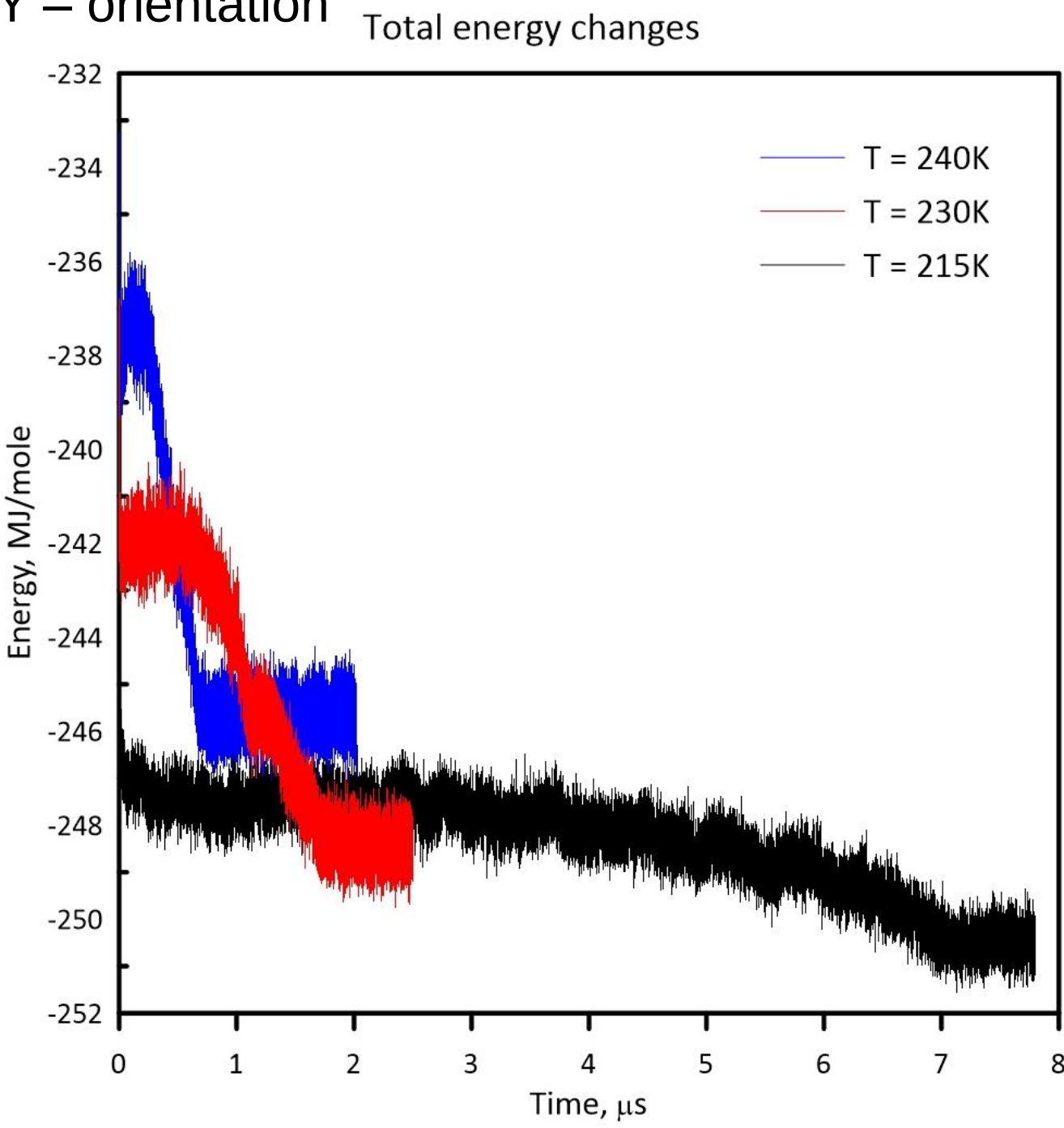
240K



NVT ensembles for Z – orientation

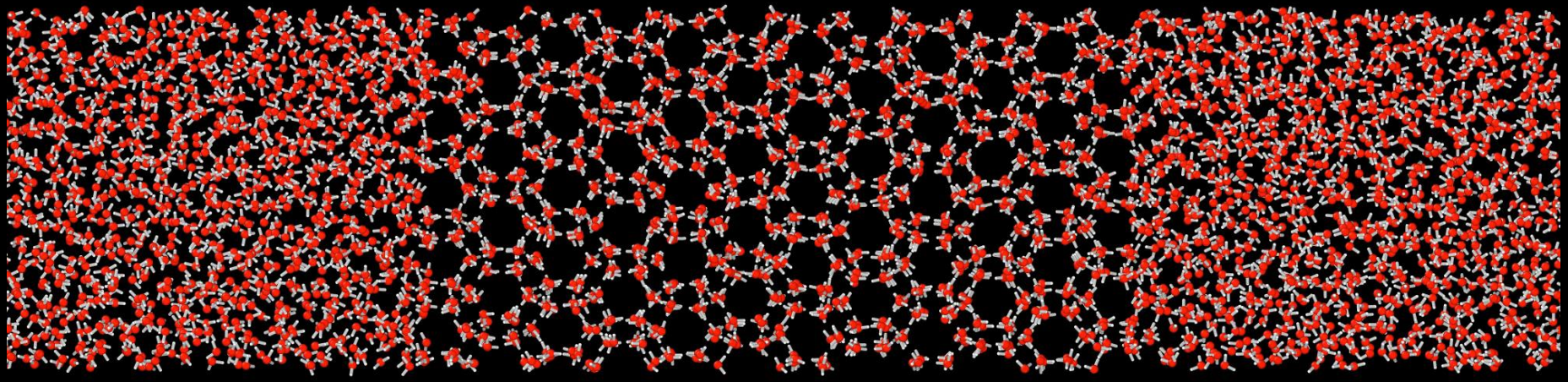


NVT ensembles for Y – orientation



Y – Orientation

230K



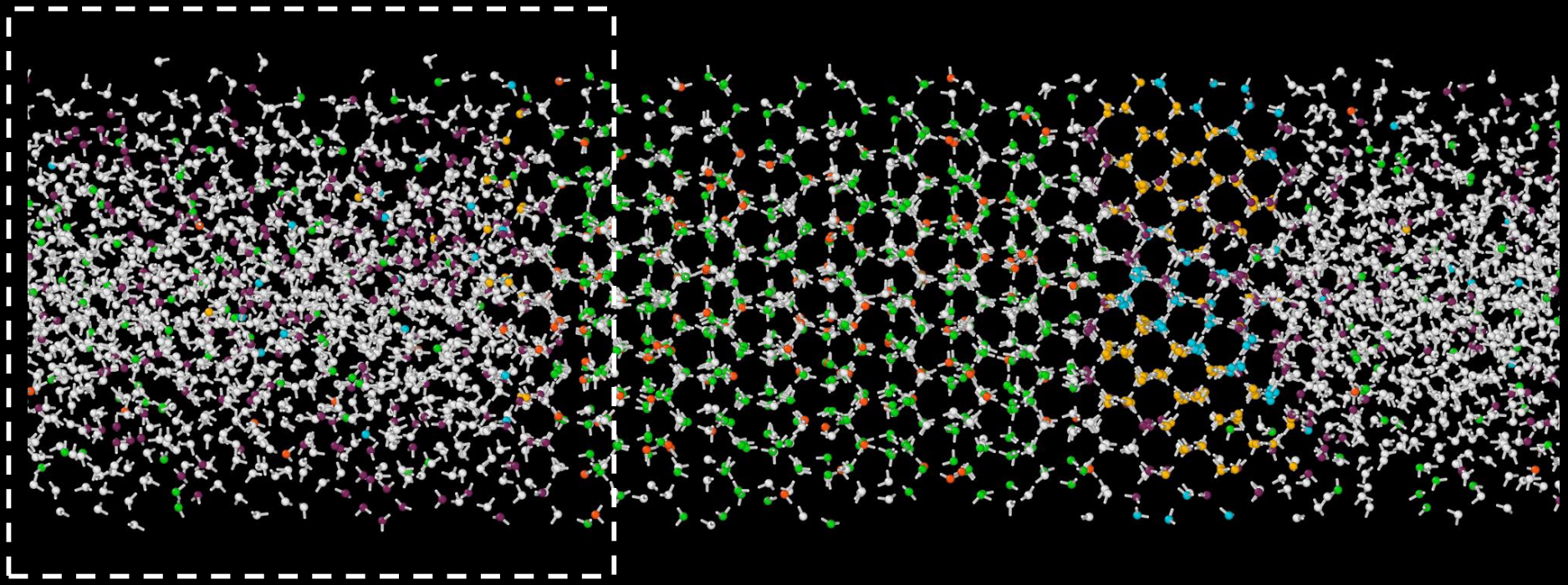
Y – Orientation

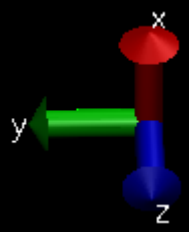
230K

● – Ice Ic

● – Ice Ih

● – Ice XVII

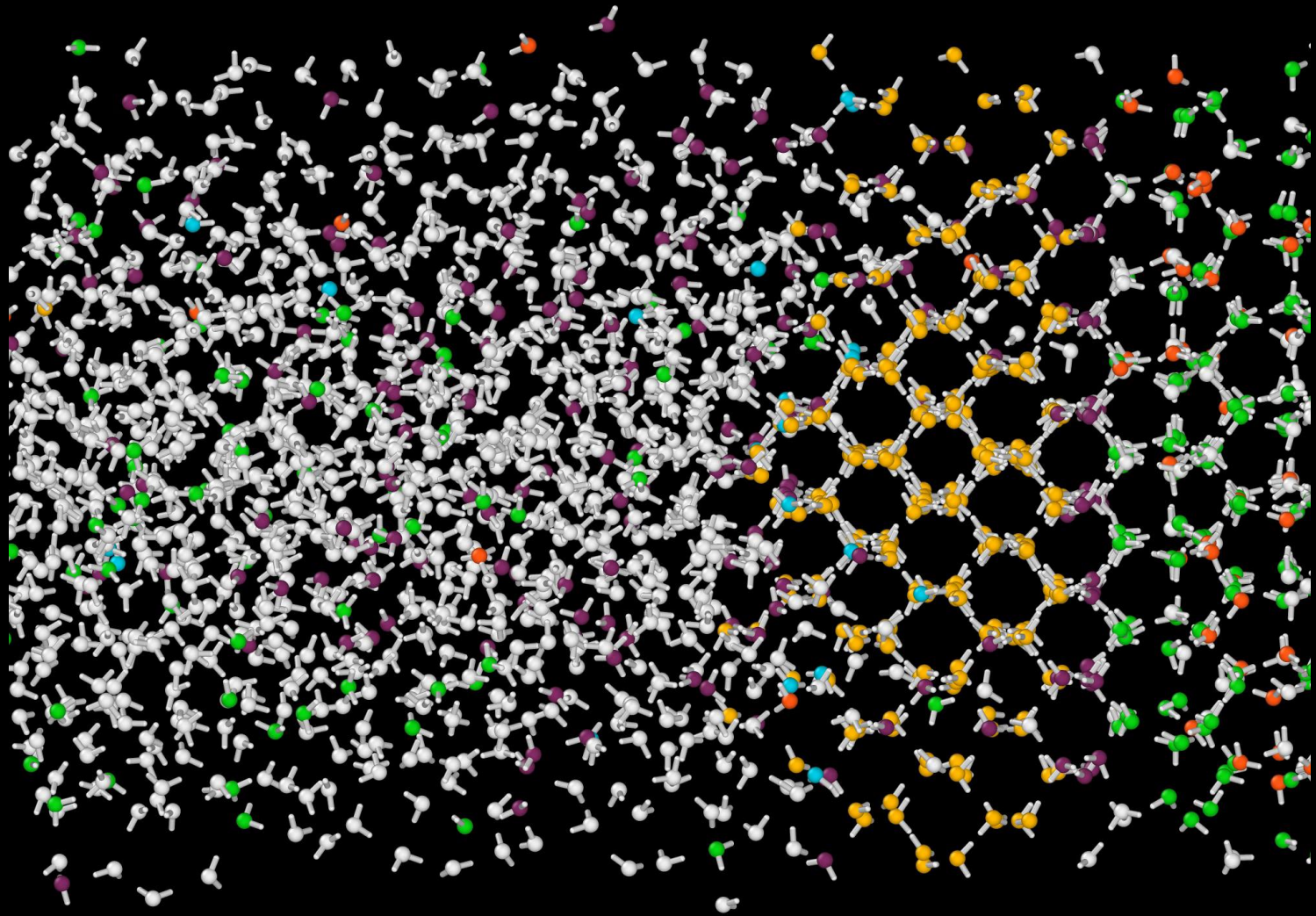




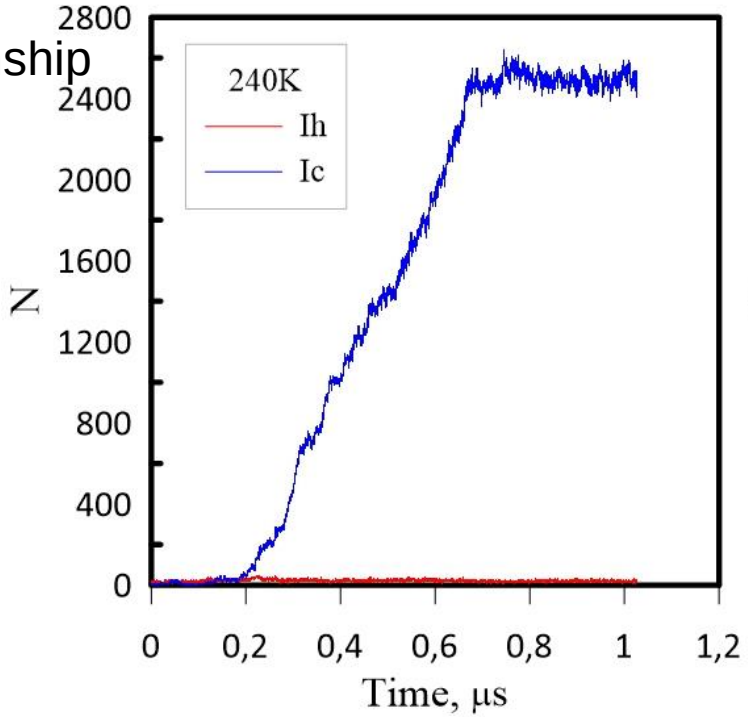
Chill+ algorithm

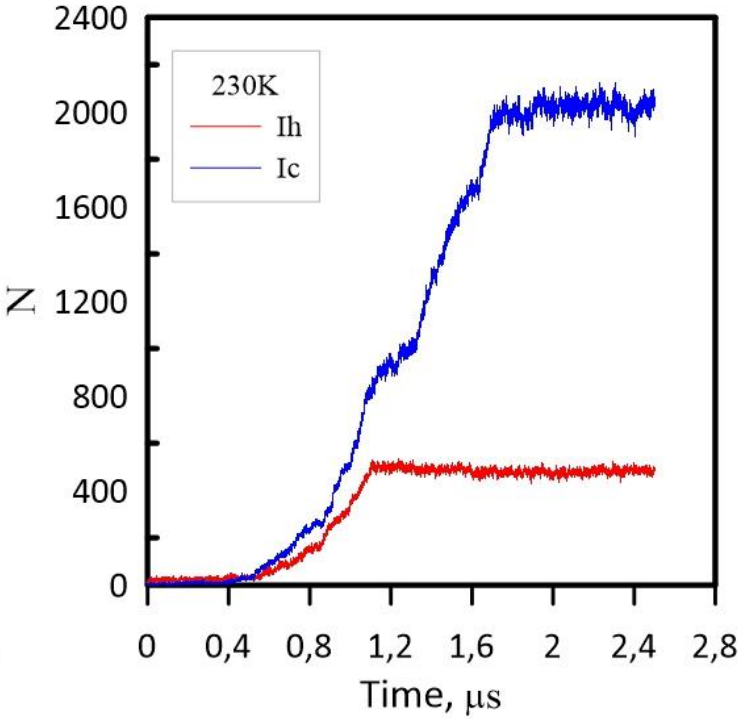
Y – Orientation

230K

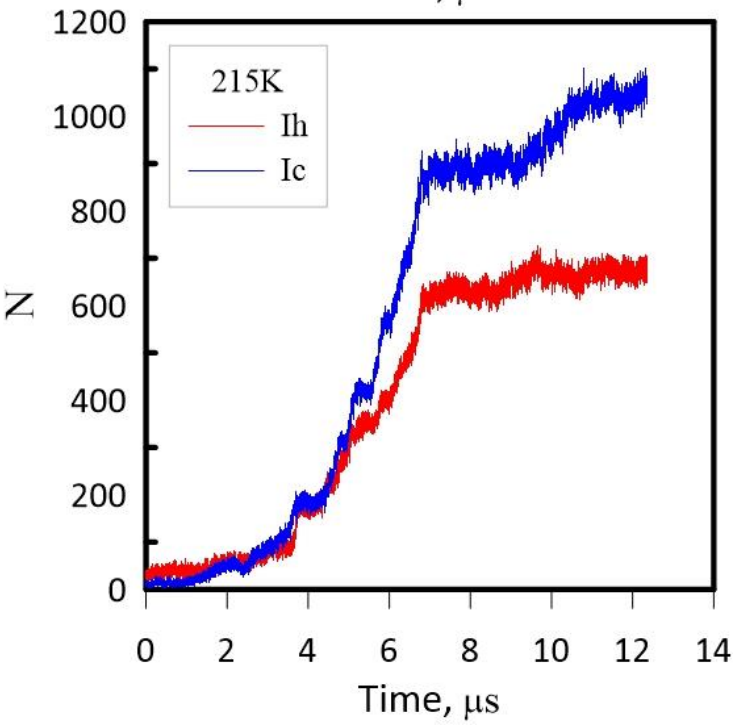


Quantitative relationship between cubic and hexagonal ices

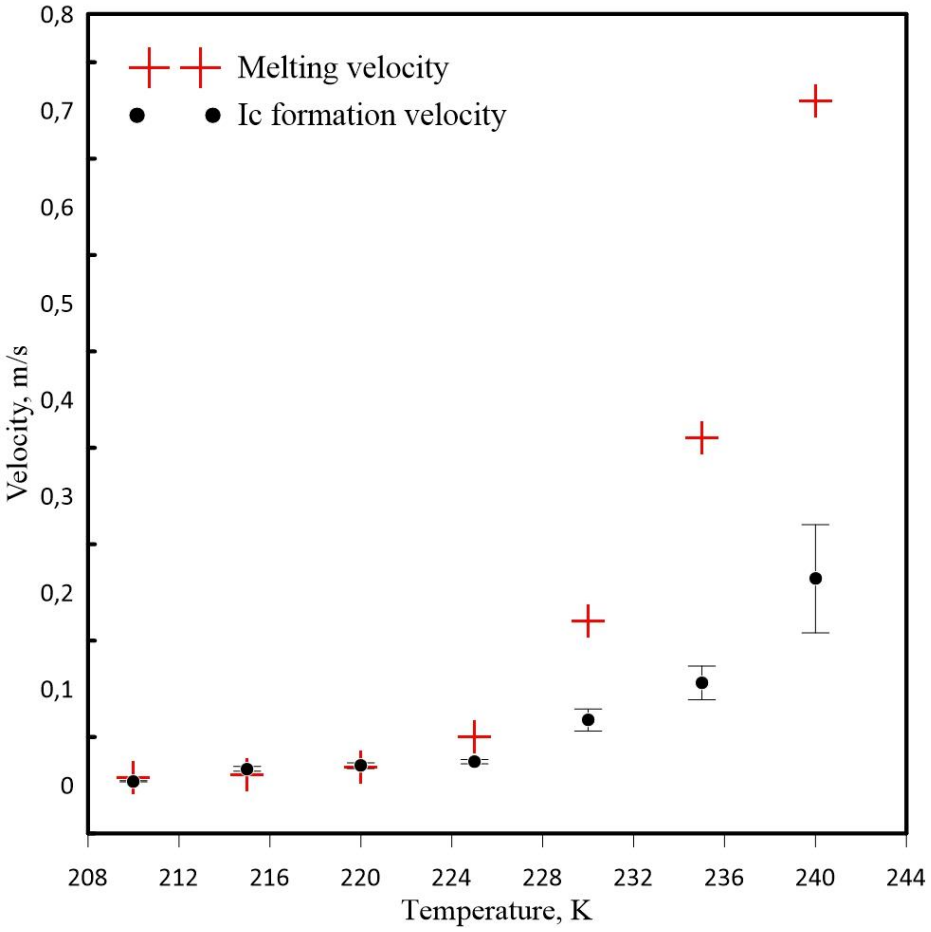


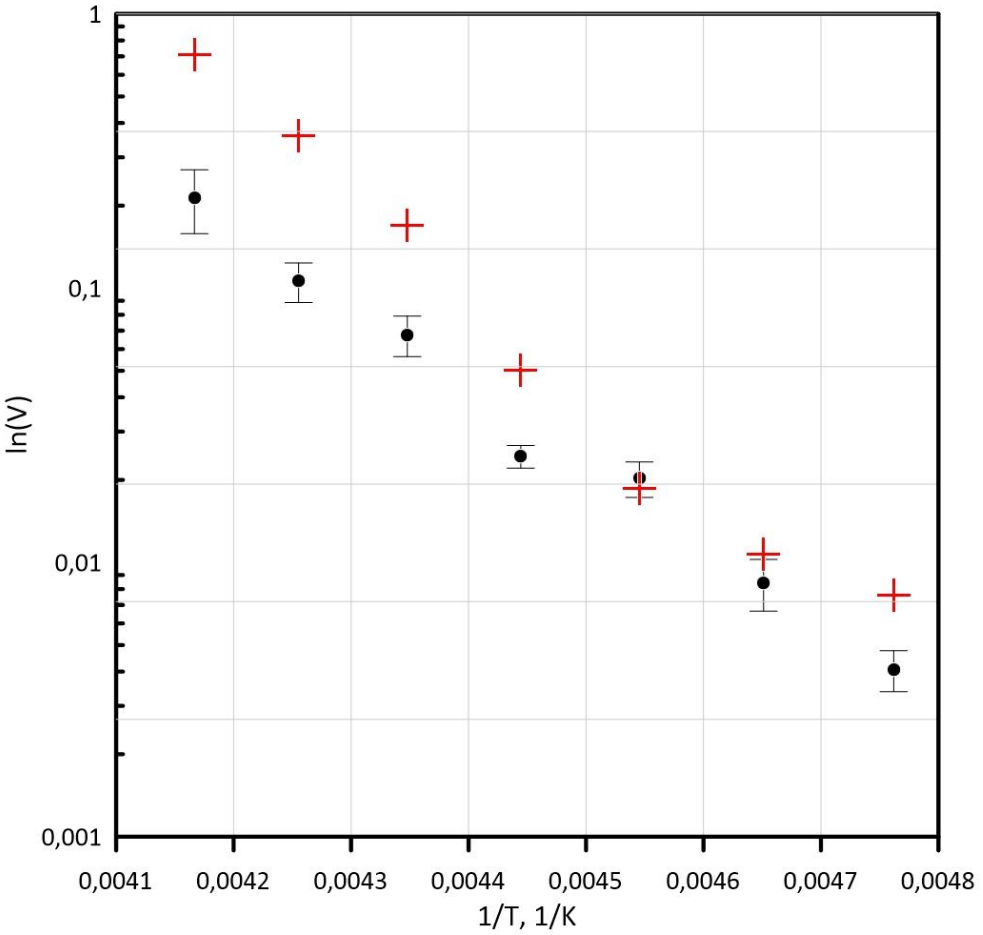


ments on HRPD and D20, respectively. The high degree of structural purity of ice Ic, with no detectable sign of stacking disorder, is demonstrated by the absence of any hexagonal ice Ih reflections or diffuse scattering between the Bragg peaks in the whole diffraction pattern, and by the good quality of the fit, which is characterized by a weighted profile agreement index, R_w, of 4.1% for the D20 data and 4.4% for the data taken on HRPD. Indeed, very weak reflections, such as (311) and (400), are also observed (see Supplementary Fig. 2), with an intensity matching that expected for a pure cubic crystal. The presence of any fraction of possible amorphous ice



Velocities of melting ice XVII and cubic ice formation





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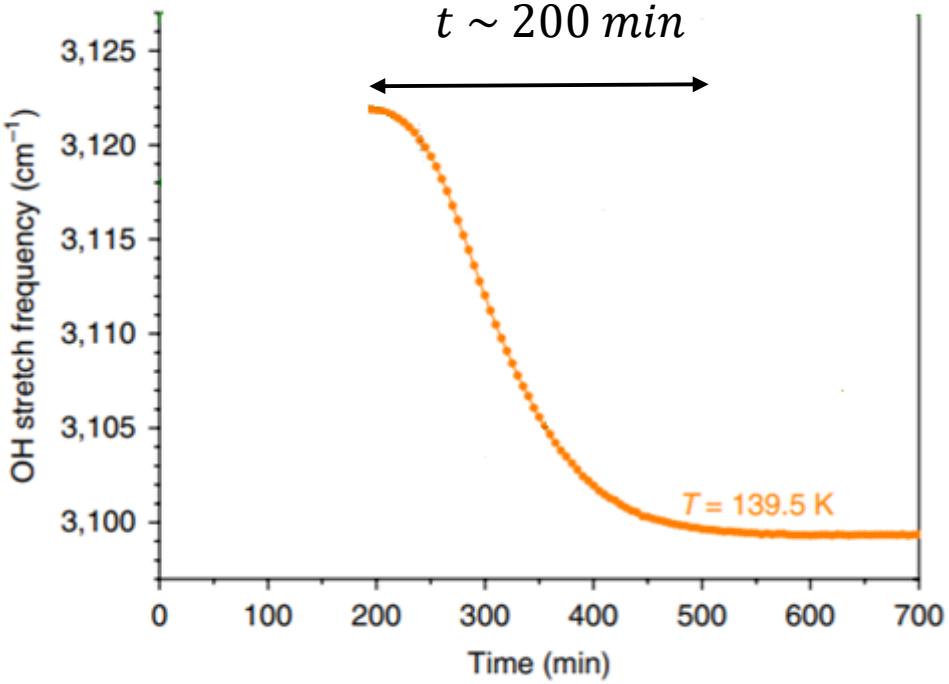
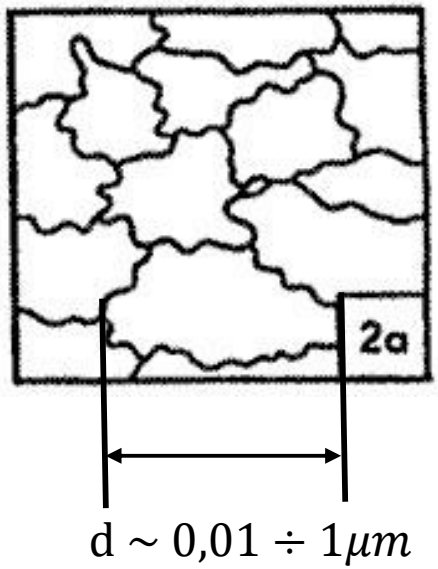
Cubic ice Ic without stacking defects obtained from ice XVII

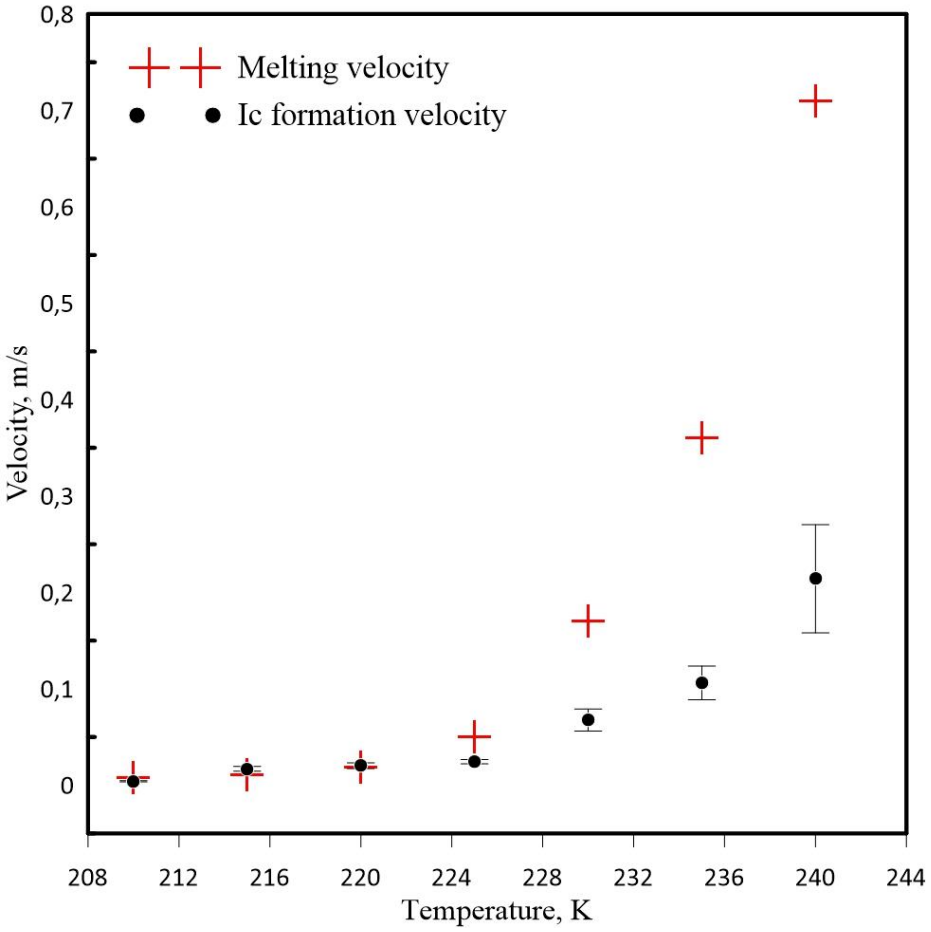
Leonardo del Rosso, Milva Celli, Francesco Grazzi, Michele Catti, Thomas C. Hansen, A. Dominic Fortes & Lorenzo Ulivi

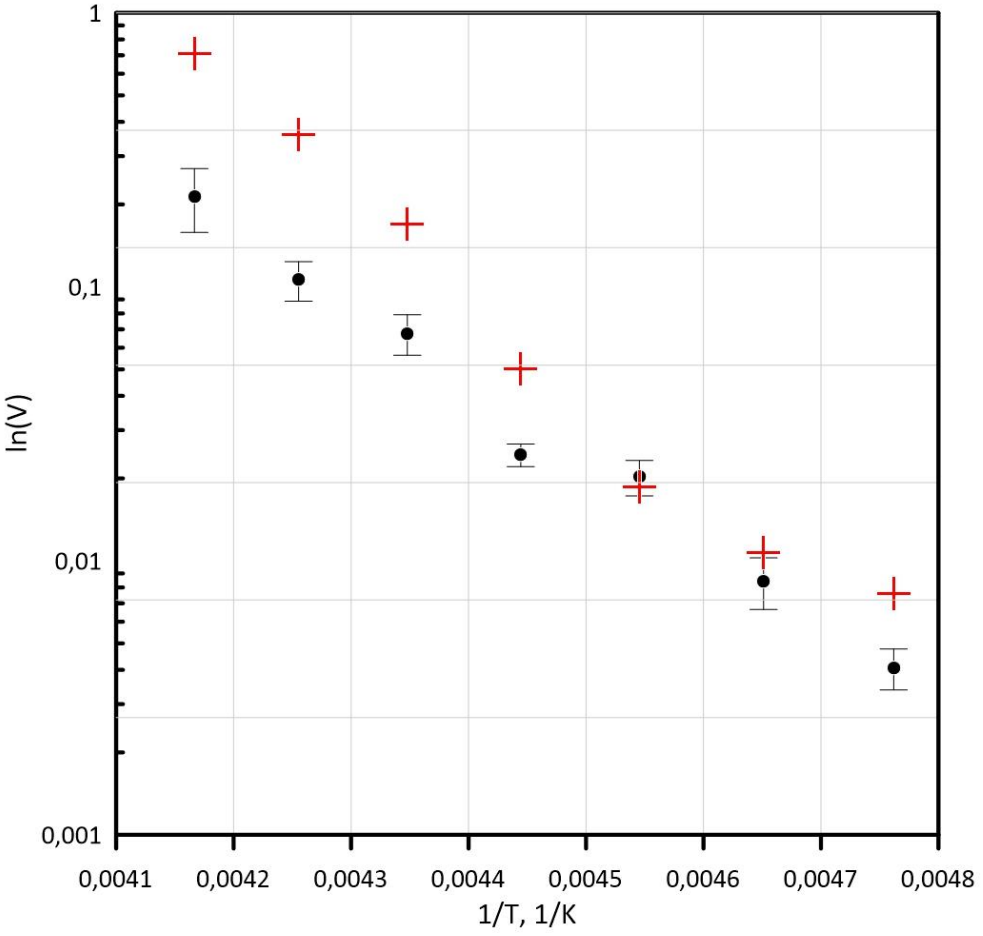




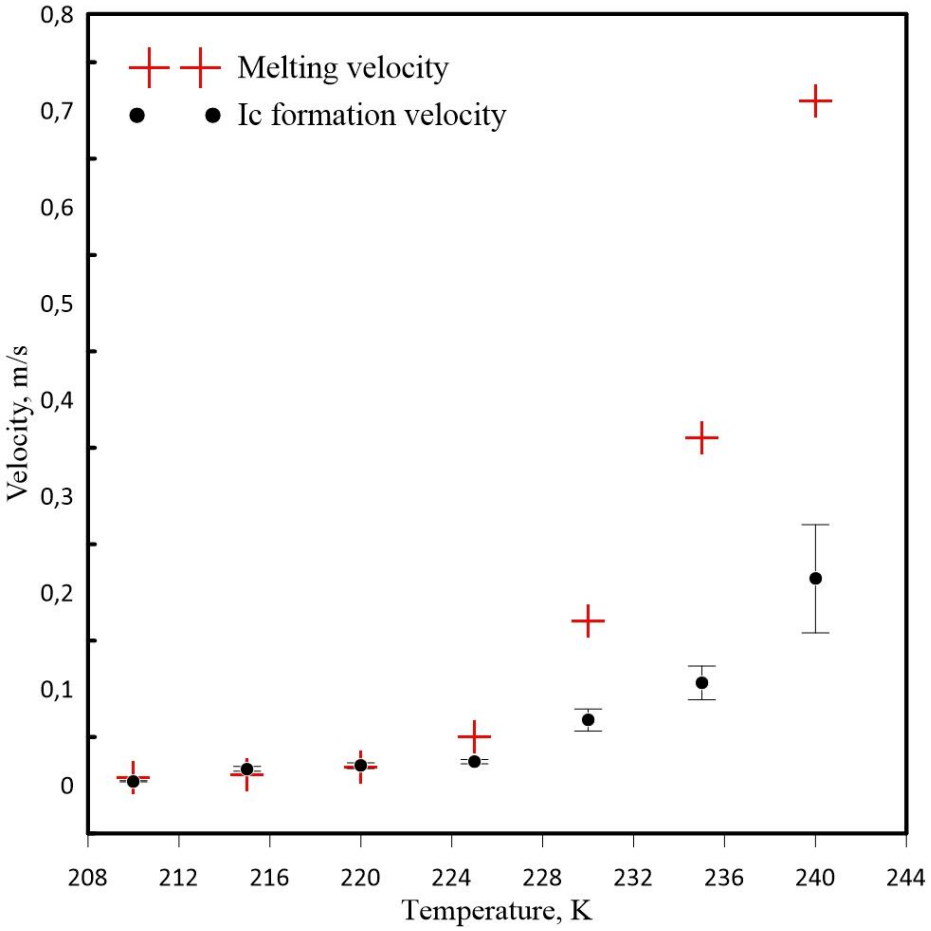
$V \sim 10^{-12} \div 10^{-10}\ m/s$

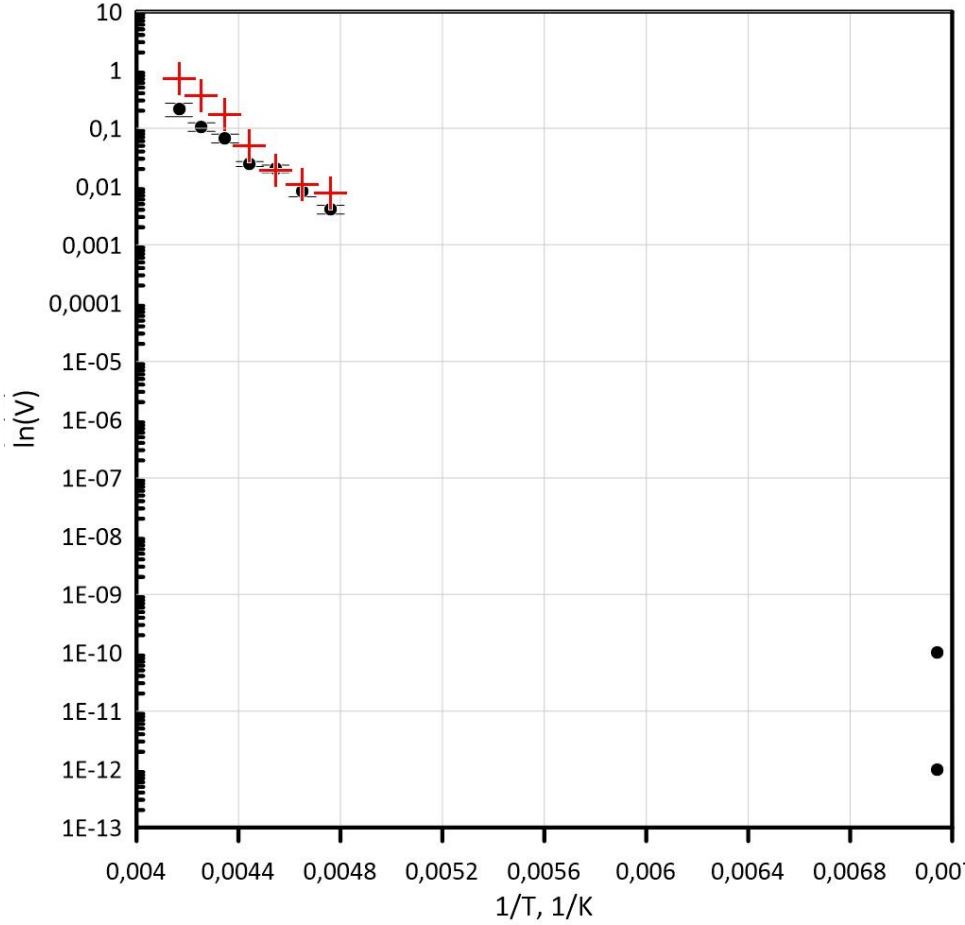
Velocities of melting ice XVII and cubic ice formation



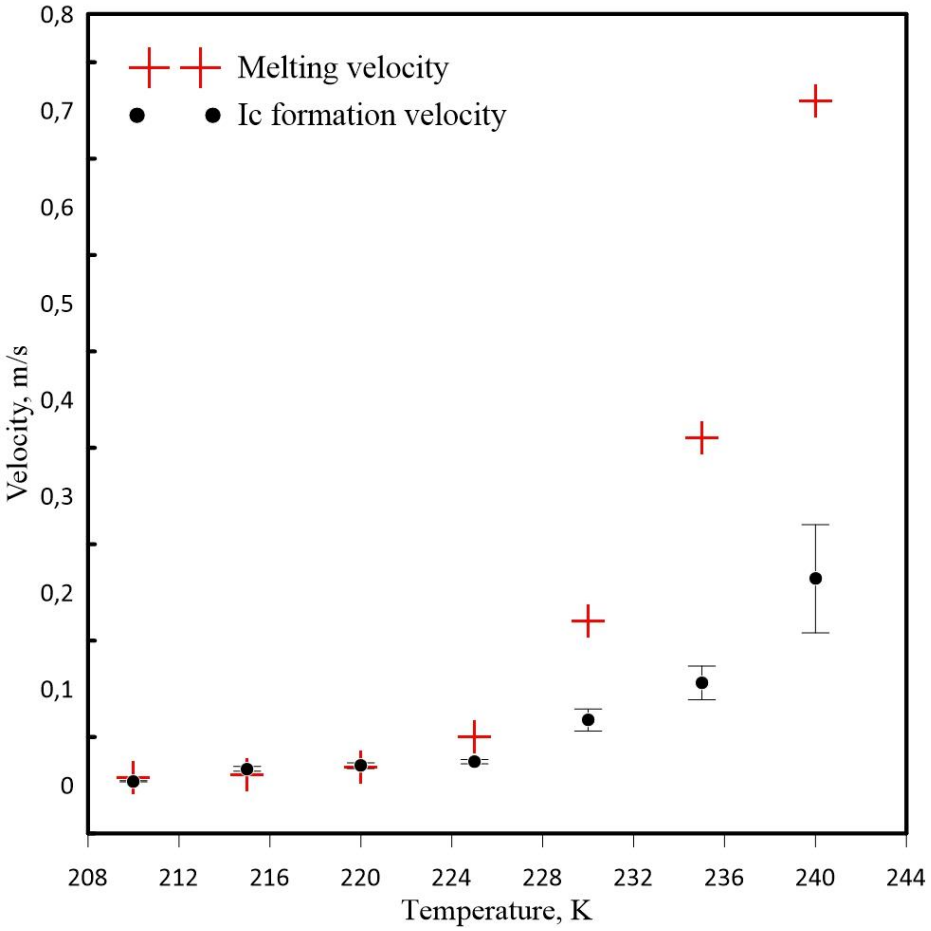


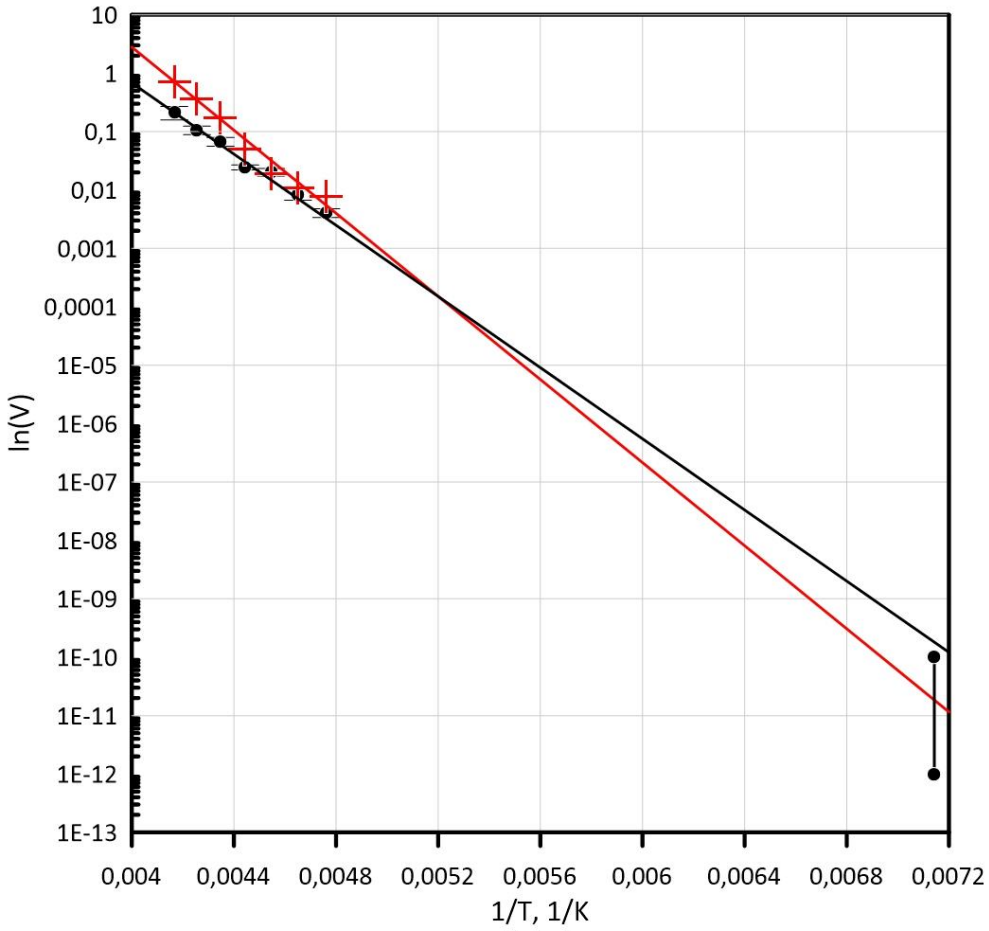
Velocities of melting ice XVII and cubic ice formation





Velocities of melting ice XVII and cubic ice formation





Conclusions

- The model of ice XVII with open surface was used to simulate phase transitions between ice XVII and other polymorphic phases. Within this approach two orientations were analyzed. For z-orientation melting of ice XVII was observed.

- For y-orientation one can notice transition between two ice types: Ice XVII and cubic ice. **First ice XVII melts, then one can observe the formation of cubic ice on the surface of ice XVII.** Thus, the results obtained by this method confirm the possibility of transition of ice XVII into cubic ice.

- For high temperatures, the formation of pure cubic ice is shown, which agrees with experimental data. In some cases hexagonal ice formation with cubic ice is observed.

- The velocity of melting ice XVII and cubic ice formation was calculated. The obtained data are in agreement with experiment.