Hybrid Collisional-Radiative/Molecular-Dynamics Studies of Anisotropic Melting of Ice Induced by Ultrafast Non-thermal Heating

I. Dawod[1,2], K. Patra[1], S. Cardoch[1], O. H. Jönsson[3], J. A. Sellberg[3], A. V. Martin[4], J. Binns[4], O. Gråsäs[1], A. P. Mancuso[2,5,6], C. Caleman[1,7]*, and N. Timneanu[1,2]

[1]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden
[2]European XFEL, Holzkoppel 4, DE-22869 Schenefeld, Germany
[3]Department of Applied Physics, KTH Royal Institute of Technology, SE-106 91 Stockholm, Sweden
[4]School of Science, RMIT University, Melbourne, Victoria 3000, Australia
[5]Diamond Light Source, Harwell Science and Innovation Campus, Didcot OX11 0DE, U.K.
[6]Department of Chemistry and Physics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria 3086, Australia
[7]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron, Notkestraße 85 D-22607 Hamburg, Germany

Water and ice are routinely studied with X-rays to reveal their diverse structures and anomalous properties. We developed a hybrid collisional-radiative/molecular-dynamics code, MolDstruct [1], to explore how femtosecond X-ray pulses interact with hexagonal ice. We find that ice makes a phase transition into a crystalline plasma where its initial structure is maintained up to tens of femtoseconds. The ultrafast melting process occurs anisotropically, where different geometric configurations of the structure melt on different time scales. The transient state and anisotropic melting of crystals can be captured by X-ray diffraction, which impacts any study of crystalline structures probed by femtosecond X-ray lasers [2].

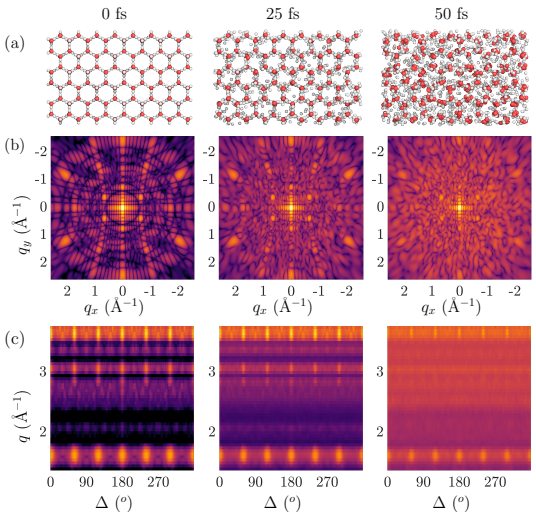

Figure 1. Dynamics of hexagonal ice investigated with an intense 50 fs long X-ray pulse, with 8 keV photons and intensity of 10^{18} Wcm^{-2}. (a) Snapshots of the structures from the hybrid CR/MD simulation of ice at 3 different time points. (b) Diffraction patterns of ice at corresponding time points, with sample to detector distance of 70 mm. (c) Angular correlation of the intensity in the diffraction patterns as a function of angle and momentum transfer.

References

[1] I. Dawod et al. J. Chem. Phys. **160**, 184112 (2024).

[2] I. Dawod et al. , ACS Phys. Chem. Au **6**, 385?392 (2024).

*E-mail: carl.caleman@desy.de