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Coarse-grained modeling of polycrystalline ice in supercooled water. HENRY CHAN, MATHEW CHERUKARA, BADRI NARAYANAN,, CHRIS BENMORE, STEPHEN GRAY, SANKARANARAYANAN SUBRAMANIAN, Argonne National Laboratory — Formation and growth of grains of ice is ubiquitous, influencing naturally occurring phenomena such as glacier formation and processes happening at the nanoscale, like intracellular freezing. Despite the exponential growth in computing resources, it remains a grand challenge to simulate phase transitions and dynamical processes in deeply supercooled systems due to limitations imposed by system sizes and timescales which is further compounded by their sluggish kinetics. We will present our work on probing the formation and grain growth in polycrystalline ice using coarse-grained molecular dynamics on multi-million molecule systems for up to microsecond time scales. Our findings highlight the distinct differences between grain growth mechanisms of ice compared to those in metals and ceramics.

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