

Physics Colloquium, University of South Florida

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A Tale of Fire and Ice: Beyond Classical Nucleation Theory in the Solidification of Water at High Pressure

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The metastability and kinetics of non-equilibrium phase transformations in water present one of the greatest mysteries of condensed matter physics and chemistry. Owing to its unique inter- and intra-molecular interactions, water is likely the most polymorphic material in existence -- having over 17 ice phases, most of which are accessible only at high pressure. Indeed, it's believed that the vast majority of water in the universe remains in an ultracold, amorphous state. Developing an understanding of the nucleation of ice at high pressure has direct implications for the origins of life on extrasolar "super-earths", ocean worlds that have been detected by NASA's Kepler telescope. Recently, experiments that solidify water into the high-pressure ice VII phase, by using shock-waves, have presented seemingly contradictory results regarding the nucleation of ice far from equilibrium. Here we show that, under these extreme conditions, classical nucleation theory can remain successful but only if amended to include new aspects that are unique to the non-equilibrium state, and that by doing so we are able to reconcile the apparent discrepancies between various nucleation experiments. Finally, we highlight the potential for application of this formalism to other self-organization processes, such as the self-assembly of viral capsids and metal-organic materials.

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Dr. Jon Belof is a physicist, Group Leader for Theoretical Physics within the Weapons and Complex Integration Directorate, and Program Leader for Physics and Engineering Models (PEM) under the Advanced Simulation and Computing Program at Lawrence Livermore National Laboratory (LLNL). In addition to his work leading the theory and computational model development for dynamic material properties, Jon is also the PI for a Laboratory R&D program to experimentally investigate phase transformations under shock-wave loading using high-powered lasers. Jon's areas of scientific interest include non-equilibrium statistical mechanics, pattern formation and self-assembly, multiscale physics and high energy density physics. He is a subject matter expert in nuclear weapon physics, applications of science and technology to non-proliferation and nuclear counter-terrorism, and is a member of the Capabilities for Nuclear Intelligence. With a focus on supramolecular chemistry, he earned his B.A. (2005) and Ph.D. (2009) in Chemistry from the University of South Florida and then joined LLNL as a Postdoctoral Fellow in High Energy Density Physics (2010). More recently, Dr. Belof received the Presidential Early Career award (conferred by President Obama) for his work in non-equilibrium phase transitions, a Global Security Gold Award for his work in nuclear forensics and attribution, and LLNL Director's Award for contributions to shock-wave compression of condensed matter.