Bridging the Atomistic Deformation Mechanisms to the Microscopic Adhesive-to-Cohesive Fracture at the Ice-Metal Interfaces

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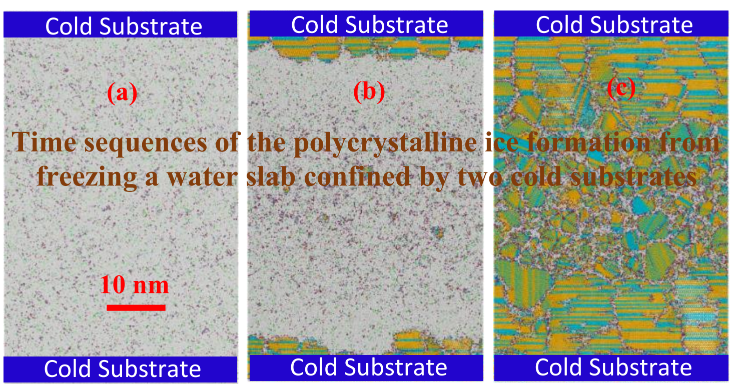
Project Objectives: Ice accretion over the surfaces of materials exposed to the cold environment is a topic of great concern for airplanes, wind turbines, and marine vessels sailing near the arctic area. However, a strategy of de-icing (detaching ice from cold surfaces) with minimal power cost is not well-established yet due to the lack of answers to a fundamental question on how the ice forms and sheds from a material surface. **The goal** of this project is to answer this question by identifying the atomistic mechanisms responsible for the fracture of the ice-metal interface. **Two specific aims** are: (i) to correlate the ice adhesion strength with the ice-metal interface structure; and (ii) to support the search of de-icing strategies that consume far less power than existing approaches. A series of high-fidelity computer simulations will be performed under a correspondence with the relevant experimental measurements in an Icing Research Tunnel at the PIs' institute. *This project will facilitate a rational design of materials that inhibit ice adhesion, with implications for safety-critical infrastructures operating in arctic areas, including telecommunication equipment, power lines, automotive vehicles, marine vessels, offshore oil platforms, and among many others*.

Keywords: icing and de-icing, ice-metal adhesion, crack propagation in ice, multiscale simulation



Progress to Date/Future Plans: through atomistic simulations, the PIs recently found a microstructure transition from "the columnar grain structure" to "the equiaxed grain structure" nearby the ice-substrate interface. Such a microstructure transition in turn, may dictate the commonly observed "adhesive-to-cohesive" fracture involved in a de-icing process. This is to be confirmed by experiments and higher length scale computer models in the next, which may be then utilized to guide the design of novel de-icing strategies.

Highlights of the Expected Outcomes: one main expected outcome of this research will be an integrated experimental and computational platform that can be used to understand how the ice is formed and how it should be removed from the surfaces of engineering infrastructures exposed to the cold environment in arctic areas.

NNA Community Collaboration and Research Coordination: the PIs do not conduct field experiments in any geographic areas nearby the arctic region yet, the gained knowledge thus far may not be directly applicable to understand the ice accretion on the infrastructures in arctic areas due to the lack of the information about the humidity, temperature, wind speed, water droplet size and chemistry in the field. If the support from the NNA community on this aspect is provided, an experimentally-validated computer software can be expected and will be delivered for predicting how the ice is formed from water freezing and how it fractures in arctic areas. This may also enable researchers to explore how the glacier fractures under current global warming conditions from the bottom up.

Advice for Overcoming NNA Project Challenges: if the support from the NNA community is not leveraged, it remains impossible for the PIs to directly use their platform on the infrastructures in arctic areas, although they have practiced in engineering, especially in computational mechanics of materials and experimental icing physics, for tens of years. The PIs believe that all the ongoing and overcoming NNA projects are multidisciplinary in nature, which remains as a challenge to each NNA project team, and should be clearly addressed whenever possible.