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Supplementary Materials: Machine Learning Based Prediction of Nanoscale Ice Adhesion on Rough Surfaces

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Citation: Ringdahl, S.; Xiao, S.; He, J, and Zhang, Z. Machine Learning Based Prediction of Nanoscale Ice Adhesion on Rough Surfaces. *Coatings* **2021**, *11*, 33. https://doi.org/10.3390/coatings11010033

Received: 11 December 2020
Accepted: 27 December 2020
Published: 31 December 2020

1. Roughness Effect on the Amorphous Liquid Layer

There is an interfacial amorphous layer of water in all the simulation systems. The amorphous water layers had an initial thickness of 8 Å, which is an arbitrary initial height and can change in equilibration simulations. Nevertheless, all the systems with this set-up should have a composite structure of ice, amorphous layer and substrate from top to down in equilibrium before nanoscale ice adhesion testing. In order to verify this, the rough substrate shown in Figure 1 in the main text with amorphous water layer of varied thickness and ice was devised for comparing the dynamic change of the amorphous layer. In longer equilibration simulations of 50 ns, the systems stabilized with the aimed structure for ice adhesion testing, despite different amorphous water layer thickness and interaction strength between the substrate and the water molecules, as results shown in Figure S1.

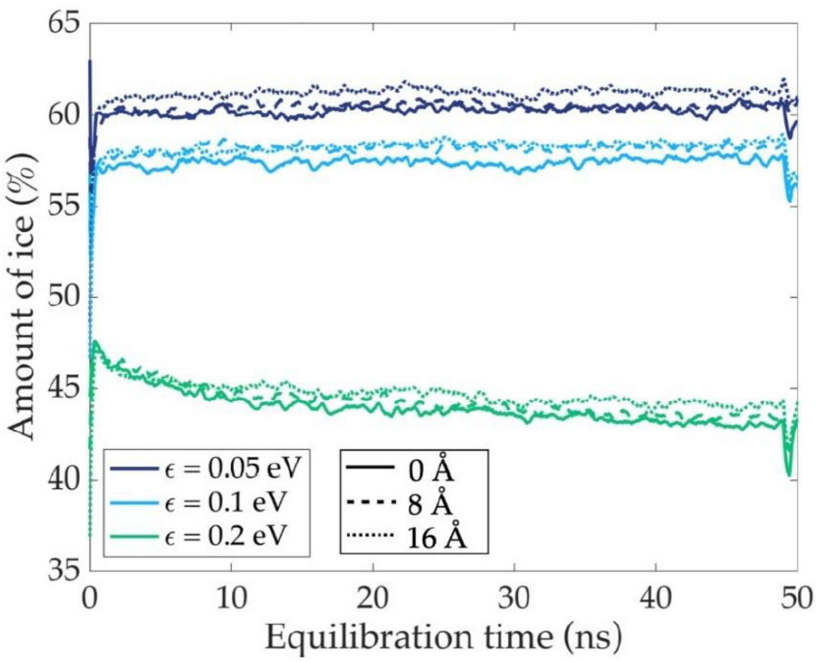

Figure S1. Percentage of water molecules in ice structure on a representative rough surface with different interaction strength in equilibration simulation. The rough surface with three LJ potential depth (ε) and three initial amorphous layer thickness were equilibration for 50 ns. The amount of ice molecules in the simulations were identified by the CHILL + algorithm.

2. Loading Rate Dependency of Nanoscale Ice Adhesion Strength on Rough Surfaces

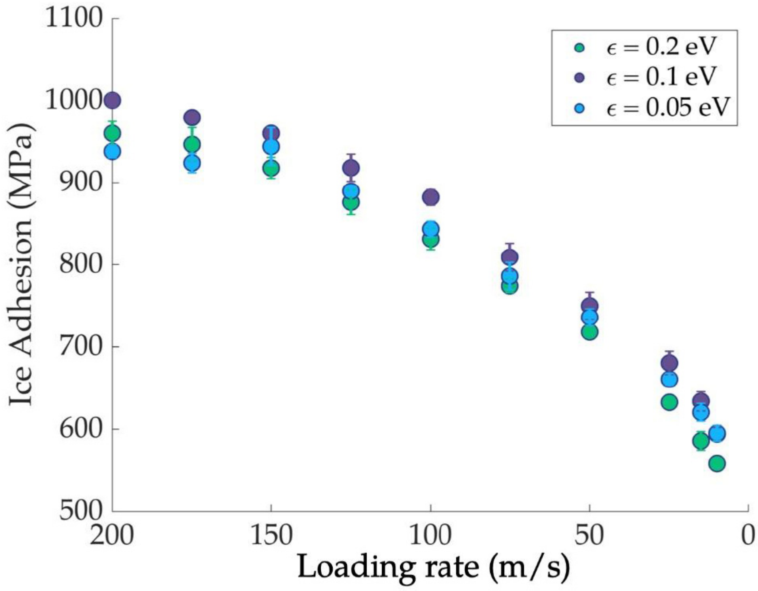

Figure S2. Ice adhesion strength monitored on a representative rough surface with different moving speed of the surface (Loading rate). With all the three LJ potential energy depth (ε) between water and the substrate, the ice adhesion strength changes with the loading rate (tensile pulling speed). The lowest speed of the loading rate (2 nm/ns) was used in all the simulations for data collection in this study.