

Supporting materials

**Statistically Understanding Roles of Nanostructure Features in
Interfacial Ice Nucleation for Enhancing the Icing Delay
Performance**

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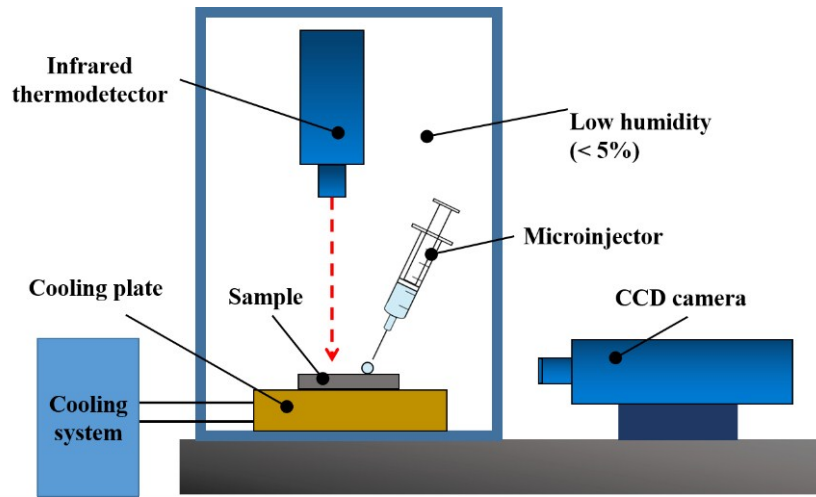


Figure S1. A self-made measurement device for the icing delay performance.

Calculated process for the ice nucleation rate

The ice nucleation behaviors of the water droplets on these sample surfaces were investigated *via* employing the classical nucleation theory. In this work, we describe the nucleation rate (unit: nuclei s⁻¹ in a certain volume) of water droplet on cooled surface, building upon the framework developed by A. Alizadeh and B. Zobrist.^{1,2}

$$J_{total}(T) = J_{bulk}(T) V + J_{lg}(T)S_{lg} + J_{sl}(T)S_{sl} \quad (1)$$

Where $J_{total}(T)$, $J_{bulk}(T)$, $J_{lg}(T)$, and $J_{sl}(T)$ are the corresponding temperature-dependent total, bulk, liquid-gas, solid-liquid interface nucleation rates, respectively. V , S_{lg} , S_{sl} represent the volume of the liquid, the liquid-gas contact area, the solid-liquid contact area, respectively. Also, the $J_{bulk}(T)$ can be expressed by:

$$J_{bulk}(T) = \frac{kT}{h} \exp\left[-\frac{\Delta Q_{diff}(T)}{kT}\right] \times n \exp\left[-\frac{\Delta G^*(T)}{kT}\right] \quad (2)$$

Where k and h are the Boltzmann (1.38×10^{-23} J/K) and Planck constant (6.626×10^{-34} J s). T is the absolute temperature, and n is the volume number density (3.1×10^{28} m⁻³) of water molecules. The Gibbs free energy $\Delta G^*(T)$ and diffusion activation energy $\Delta Q_{diff}(T)$ are provided by:

$$\Delta G^*(T) = \frac{16\pi \gamma^3 T_m^2}{3 \Delta H_{m,v}^2 (T_m - T)} \quad (3)$$

$$\Delta Q_{diff}(T) = \frac{kT^2 E}{(T - T_0)^2} \quad (4)$$

Where the E and T_0 are the fit parameters, and the values of $T_0=118$ K and $E= 892$ K have been determined via the experimental results by Smith and Kay.³

We assumed that the ice nucleation occurring at the interface of liquid-solid is only dominated by the heterogeneous nucleation. The $J_{sl}(T)$ can be given by:

$$J_{sl}(T) = \frac{kT}{h} \exp\left[-\frac{\Delta Q_{diff}(T)}{kT}\right] \times n \exp\left[-\frac{\Delta G^*(T)f(\theta)}{kT}\right] \quad (5)$$

In this case, n (10^{19} m^{-2}) is the number density of water molecules at the interface, and $f(\theta)$ is the wetting parameter, determined by the chemical component, ranging from 0 (complete heterogeneous nucleation) to 1 (homogeneous nucleation). $f(\theta)$ can be given by:

$$f(\theta) = \frac{1}{4}(2 + \cos \theta)(1 - \cos \theta)^2 \quad (6)$$

For the nucleation occurring at the interface of liquid-gas, we assumed that it was the homogeneous nucleation. As a consequence, the $J_{ig}(T)$ approximately equals to $J_{bulk}(T)$ except the value (10^{19} m^{-2}) of n . Furthermore, to calculate the actual water-solid contact area, the apparent contact area S^* between the water droplet and solid surface with a radius (r) can be calculated by:⁴

$$S^* = \pi r^2 \quad (7)$$

$$r = \left[\frac{3V}{\pi(2 - 3\cos \theta^* + \cos^3 \theta^*)} \right]^{1/3} \sin \theta^* \quad (8)$$

Where V is the volume of the reference water droplet ($V=4 \text{ }\mu\text{L}$ in this work), θ^* is the WCA of the water droplet on the sample surface. The reference droplet on the superhydrophobic nanostructure surfaces well conforms to the Cassie-Baxter wetting model:

$$\cos \theta^* = r^* f \cos \theta + f - 1 \quad (9)$$

Where f is the fraction of the projected area of the solid surface that is wet by the liquid and r^* is the roughness factor of the wetting area.⁵ In this wetting case, the contact

interface mainly consists of the solid-liquid and solid-air interfaces. Also, the fraction (f) of the projected area of the solid surface that is wet by the liquid is very small (approximately 10%), therefore the wetting interface can be considered to follow the Young's equation and the r^* is considered to be approximately equal to one. Lastly, the actual water-solid contact area can be easily calculated to be 6.934 mm² for the flat substrate surface, 0.953 mm² for the layered nanoporous structures, and 0.035 mm² for the nanocone structures. Consequently, combining our experimental results about the 4 μ L water droplet on the sample surfaces, we gave the ice nucleation as a function of temperature.

Reference

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