Scilight

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Monitoring microdroplets to test nucleation simulations

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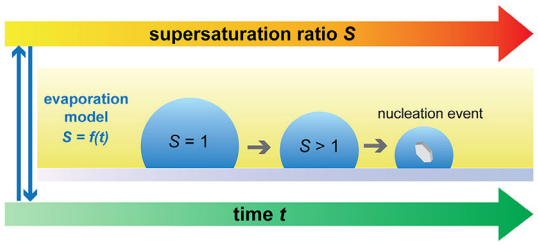
Stochastic approach provides a benchmark to understand nucleation kinetics



Nucleation describes the random formation of a stable cluster. Understanding the phenomenon is essential for applications such as nanosynthesis, energy storage, pharmaceutical production, biomineralization, and climate modeling. However, classical experiments thus far remain deterministic; the nucleation rates of simulations differ from experiments by several orders of magnitude.

Cedeno et. al set to bridge the gap between theory and experiment by generating a large dataset of NaCl nucleation with a stochastic approach.

Using droplet-based microfluidics, the authors created hundreds of NaCl microdroplets with the same composition. Then, with a tailored evaporation model, they extracted NaCl nucleation parameters after measuring the appearance of crystals under a microscope.

“We hoped to illuminate the large discrepancies between measured and simulated nucleation rates. This is essential to confront nucleation theories,” said author Stéphane Veesler. “We also questioned the effect of using smaller and smaller droplets due to the possible interference of confinement with the nucleation process.”

In addition to producing data that can be compared with simulations, the results revealed competition between nucleation-enhancing heterogeneous mechanisms and nucleation-inhibiting confinement effects.

The team aims to inspire a more statistical approach to nucleation and expand the dataset of nucleation parameters — a first step to testing different nucleation theories.

“Future experiments may include studying the impact of the rate of change of supersaturation ratio, investigating a wider range of droplet sizes to investigate quantitatively the impact of thermodynamic confinement, modeling the distributions of the pre-critical clusters, and comparison with salts/molecules of diverse solubilities.” said Veesler.

Source: “CNT effective interfacial energy and pre-exponential kinetic factor from measured NaCl crystal nucleation time distributions in contracting microdroplets,” by Ruel Cedeno, Romain Grossier, Nadine Candoni, Nicolas Levernier, Adrian Flood, and Stéphane Veesler, *Journal of Chemical Physics* (2023). The article can be accessed at https://doi.org/10.1063/5.0143704.

This paper is part of the Nucleation: Current Understanding Approaching 150 Years After Gibbs Collection, learn more here.