

Nucleation Under Shear Flow

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Abstract:

We present a general formalism for calculating the nucleation rates of simply sheared systems [5-6]. We have derived an extension to the conventional Classical Nucleation Theory, explicitly embodying the shear rate. The framework can be used for moderate supercooling, at which temperatures brute-force methods are practically infeasible. We show how the theory can be used to identify shear regimes of ice nucleation behavior for the mW water model, unifying disparate trends reported in the literature [7].

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- [6] Goswami, A, Dalal IS, Singh JK, J. Chem. Phys, 153, 09502 (2021)
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Bio: Prof. Jayant Singh holds the Poonam and Prabhu Goel Chair, and is the Head of the Department of Chemical Engineering at IIT Kanpur. He received his B. Tech. in Chemical Engineering from the Indian Institute of Technology, Kanpur in 1997. He subsequently completed his M.S. in Computer Science and Engineering, in 2002, and Ph.D. in Chemical Engineering, in 2004, from SUNY Buffalo.

Dr. Singh's current research interests are in drug discovery, material modelling, machine learning, energy storage, selective adsorption and separation, and development of novel molecular simulations tools. Dr. Singh has authored over 160 peer reviewed articles in international journals. He is a recipient of prestigious awards including Herdillia Award of IChE, SERB STAR Award, JSPS Invitation Fellowship, Alexander von Humboldt Research Fellowship, Young Engineers of Indian National Academy of Engineering, Amar Dye Chem Award of IChE, BRNS Young Scientist Award and DST-BOYSCAST Fellowship. He is an elected fellow of National Academy of Science, India. Dr. Singh has guided 14 PhDs and 34 Masters and 30 post-doctoral students. Dr. Singh is currently an Associate Editor of the Journal of Chemical Engineering Communications and serves on the advisory board of ACS Chemical Engineering Data, ACS Omega, Fluid Phase Equilibria. He is the founder of Prescience Insilico Pvt. Ltd, a deep tech company in scientific research.