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Molecular simulations of Cavitation Bubbles dynamics

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The observation of a cavitation bubble forming as a nano-scale spherical surface detached from a flat substrate unveiled complexities in capturing the cavitation pattern, hindered by existing methodological constraints. To decode the molecular dynamics and detailed morphology underlying this phenomenon, the study applies molecular dynamics (MD) simulations. This investigation mapped the onset and early development stages of cavitation at the nanoscale, organizing the morphology into four distinct phases and highlighting a pivotal moment where the rates of nucleation and growth find equilibrium. The research further explores the effects of variable pulling speeds and ambient pressures on the dynamics of cavitation through simulations. It was observed that higher pulling speeds amplify the cavitation volume but reduce the bubble's lifetime. On the other hand, ambient pressure variations significantly influence both the maximum volume and the collapse rate of the cavitation. The findings are systematically encapsulated in a phase diagram that displays the effects of varying pulling speeds and ambient pressures. Significantly, the study corroborates a Family-Vicsek scaling law, predicting the maximum volume and lifetime.

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