Abstract Submitted
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Pool boiling investigations via non-equilibrium molecular dynamics: the role of surface topography in heterogenous nanobubble nucleation[1] ALESSIO LAVINO, Imperial College London, EDWARD SMITH, Brunel University London, MIRCO MAGNINI, University of Nottingham, OMAR MATAR, Imperial College London — Molecular dynamics (MD) is emerging as a robust and powerful tool in the modelling of pool boiling processes. The main advantage of discrete molecular models over a continuum based approach is the ability to capture the atomistic nature of phase transition together with solid-liquid and liquid-vapor interfacial phenomena. Here, we study the onset of nanobubble nucleation and transition to film-like boiling regimes at the molecular scale by means of non-equilibrium molecular dynamics (NEMD). We investigate the surface topography effects on pool boiling using a cavity on the solid surface. The interplay of the cavity aspect ratio, surface wettability and wall superheat is investigated to explore the main mechanisms that control nanobubble nucleation. NEMD results are summarized in a phase diagram which captures the main phenomena observed at the different operating conditions. Classical nucleation theory (CNT) and continuum-scale heat transfer models are applied to reach a solid understanding of the MD results, showing a promising way to link the latter to larger-scale models in a more general multi-scale framework.

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