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Adsorption kinetics of surfactants at liquid-solid and liquid-vapor interfaces from atomic-scale simulations[1] EUGENIYA K. ISKRENOVA, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA and UES, Inc., Dayton, OH 45432, USA, SOUMYA S. PATNAIK, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA — Nucleate pool boiling of pure liquid is a complex process involving different size- and time-scale phenomena. The appearance of the first nanobubble in the liquid at the bottom of a hot pan, the detachment of the bubble from the solid surface, its subsequent coalescence with other bubbles, all represent complex multiscale phenomena. Surfactants added to water increase the complexity of the process by contributing to the dynamic surface tension at the liquid-vapor and liquid-solid interfaces and thus affecting the heat and mass transfer at those interfaces. We apply molecular dynamics simulations to study the adsorption kinetics of anionic, cationic, and non-ionic surfactants at liquid/solid and liquid/vapor interfaces. The all-atom vs. united-atom approaches for the solid and surfactants are surveyed in view of their applicability at near boiling temperatures and a range of model water potentials is assessed for reproducing the thermal properties of water at boiling conditions.

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