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Adsorbed Layer Transport Dominates Thin Film Evaporation in Nano Scale Confinements

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Evaporation studies focus on the identification and characterization of heat transfer and flow dynamics in the vicinity of the solid-liquid-vapor contact line. The meniscus is often characterized by the following three regions: non-evaporating adsorbed layer, thin-film, and capillary regions. The adsorbed layer, which has a thickness on the order of nanometers, is traditionally believed to be non-evaporating due to the strong intermolecular forces producing a strong disjoining pressure that suppresses evaporation. Despite this classical view, recent molecular dynamics (MD) simulations have shown that adsorbed layer plays a significant role during thin film evaporation [1]. Utilizing a new energy-based interface detection method [2], we present nonequilibrium MD simulation results of thin film evaporation of liquid argon sandwiched between two parallel platinum plates. One end of the platinum channel is heated by energy addition, while the other end is cooled at the same rate to ensure constant energy of the simulation system. Liquid argon evaporates in the heater and travels to the condenser region. As a result, the utilized MD simulation system exhibits statistically steady transport. Here we present the shapes of the evaporating menisci for 4 different channel heights varying from 2 nm, 4 nm, 8 nm, and 16 nm, at three different wall-fluid interaction parameters and under several different heating/cooling rates. Depending on the surface wettability and applied heat flux the meniscus can be in the pinned or receding regimes. The latter case creates adsorbed layers suitable for investigating its dynamics. The higher wettability cases exhibit thicker and more stable adsorbed layers, with reduced radius of curvature (ROC) and reduced evaporation rate. They are more stable and can handle higher heat fluxes. The lower wettability cases exhibit more evaporation but can easily lead to dry out. For channel sizes less than 10 nm, the adsorbed layer and evaporating thin film regions are intertwined, and evaporation from the adsorbed layer can contribute up to 80% of the total evaporating mass flowrate. Even for the largest channel case (16 nm), the adsorbed layer contributed about 10% of the total evaporating mass flowrate [3]. The talk will focus on these findings and gear towards consolidation of our findings towards a universal behavior of adsorbed layer transport in nanoscale confinements.

Participation

In-Person

References

[1] Akkus, Y., Koklu, A., Beskok, A., "Atomic Scale Interfacial Transport at an Extended Evaporating Meniscus,"Langmuir, 35 (13), pp 4491–4497, 2019.

[2] Ozsipahi, M., Akkus, Y., Nguyen, C.T., and Beskok, A., "Energy-Based Interface Detection for Phase Change Processes of Monatomic Fluids in Nanoconfinements,"Journal of Physical Chemistry Letters 12(34), 8397-8403, 2021.

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