



Effect of nanostructures on heat transfer coefficient of an evaporating meniscus



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ABSTRACT

The effect of nanostructures on heat transfer coefficient of an evaporating meniscus in thin film evaporation and nucleate boiling is investigated using combined modeling and molecular dynamics (MD) simulations. The model is developed accounting for the evaporation kinetics, disjoining pressure, conduction resistance, and Kapitza resistance of an evaporating meniscus on a nanostructured surface. The model is then verified using MD simulations for a water–gold system with square nanostructures of varying depth and film thickness. Good agreement is obtained between MD results and model predictions. The results show the existence of a critical film thickness on the order of a few nanometers where the heat transfer coefficient reaches its maximum. For a film thickness below this critical value, the evaporation resistance dominates and the heat transfer coefficient increases with film thickness but decreases with nanostructure depth due to the enhanced disjoining pressure. However, for a film thickness greater than the critical value, the conduction resistance dominates and the heat transfer coefficient decreases with film thickness but increases with nanostructure depth. In addition, both critical film thickness and maximum heat transfer coefficient increase with the roughness ratio of the nanostructure, mainly due to the reduction in Kapitza resistance.

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1. Introduction

Thermal management is becoming a severe bottleneck in ever-increasing demand toward miniaturization of high performance integrated circuits, power electronics, and lasers. Phase change through boiling is one of the most effective heat transfer mechanisms by utilizing the high latent heat of vaporization to dissipate thermal energy, with the maximum theoretical heat flux on the order of $10,000 \text{ W/cm}^2$ [1]. However, there exists a practical limit of boiling heat flux, the critical heat flux (CHF), above which the rapid development of an insulating vapor layer blankets the heat transfer surface. Based on the Helmholtz instability of vapor columns leaving a solid surface, Zuber predicted the CHF of water on a planar surface to be $\sim 110 \text{ W/cm}^2$, which agrees well with pool boiling experiments utilizing planar surfaces [2].

Recent efforts using micro/nanostructured and hierarchical structured surfaces to enhance heat transfer coefficient (HTC) and CHF of boiling experiments have resulted in enhanced CHF on the order of $200\text{--}313 \text{ W/cm}^2$ [1,3–14]. This enhancement in CHF can be attributed to a variety of mechanisms, including

increased nucleation site densities [1,5,15], elongated contact line [7,16], enhanced micro-convection around nucleated bubbles [4,17,18], increased bubble departure frequency [19], and enhanced microlayer evaporation via a strong wicking effect [3,9,13,14,20–22]. Among these possible mechanisms, the enhanced microlayer evaporation through wicking has been widely accepted as the dominant mechanism, where correlations [3,21] and theoretical predictions [22] have been established between the CHF and the wicking rate. For a bubble nucleated on a solid surface during boiling, evaporation occurs both along the apparent liquid–vapor interface and across the thin film (or microlayer) near the bubble contact line as shown in Fig. 1a, where nanostructure-enhanced liquid delivery through wicking stabilizes the evaporating thin film, thereby improving the CHF. In order to better understand nanostructure-enhanced boiling heat transfer, the effect of the nanostructures on the heat transfer coefficient of an evaporating thin film needs to be systematically studied.

The evaporating meniscus near a contact line can be divided into three regions: the non-evaporating film region, evaporating thin film region, and intrinsic meniscus region, as illustrated in Fig. 1b. In the evaporating thin film region, due to the presence of solid–liquid intermolecular forces, an excess pressure known as the disjoining pressure is required for liquid molecules to escape

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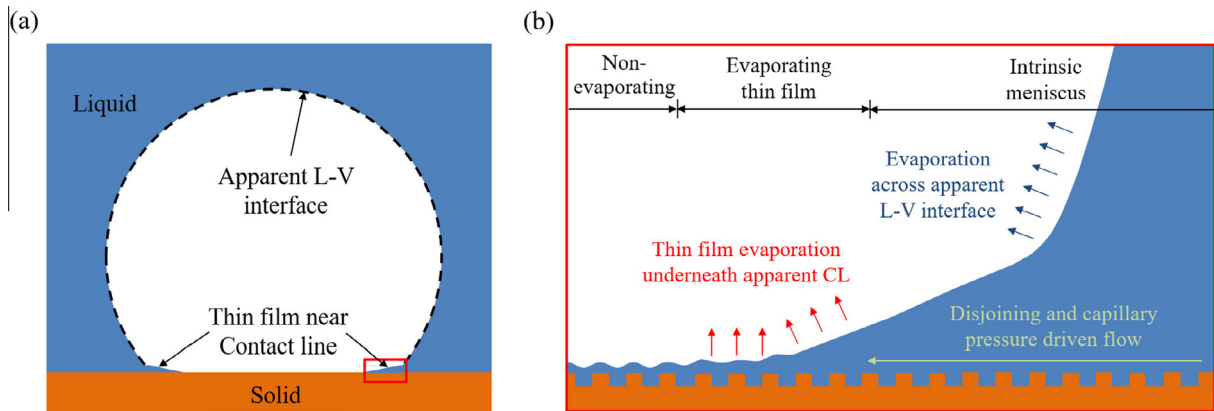


Fig. 1. (a) Schematic of a bubble in nucleate boiling. (b) Zoomed-in schematic of the contact line region of the bubble on a nanostructured surface.

from the thin film. This disjoining pressure increases rapidly with decreasing liquid film thickness and its gradient, induced by the change in liquid film thickness of the evaporating meniscus, drives the liquid to flow from the intrinsic meniscus to the evaporating thin film region such that a high heat flux in the thin film region is maintained. Modeling of heat transfer in an evaporating thin film was pioneered by Wayner et al. [23], where the role of disjoining pressure in both liquid delivery and evaporation suppression was identified. A thin film evaporation model was further developed to include the effects of slip boundary [24], thermocapillary [24,25], electrostatic on disjoining pressure [25], heat conduction through thin film [25–27], and capillary suppression [27,28]. Wang et al. [27] analyzed the evaporation of a meniscus in nanochannels and found that the evaporating thin film region (from the non-evaporating film to the location of film thickness $\sim 1 \mu\text{m}$) accounts for more than 50% of the total heat transfer. Narayanan et al. [25] showed that the electrostatic disjoining pressure elongates the thin film region and increases the total evaporation rate. Despite their proven success, to the best of authors' knowledge, existing thin film evaporation models have been developed based on planar surfaces where the effects of nanostructures on disjoining pressure, capillary pressure, heat conduction, and thus the overall heat transfer performance are not accounted for.

Recently, Hu et al. developed a closed-form model to account for the effect of nanostructures on disjoining pressure [29,30]. However, how the nanostructure-enhanced disjoining pressure affects the heat transfer rate of an evaporating thin film has not been systematically investigated. Furthermore, existing thin film evaporation models neglected the Kapitza resistance, i.e., the interfacial thermal resistance caused by the mismatch in thermal properties between two contact materials. It is important to note that the Kapitza resistance at a water–gold interface is $\sim 10^{-8} \text{ m}^2\text{K/W}$ [31,32], equivalent to the conduction resistance of a 10 nm water film. As the non-evaporating water film becomes as thin as a few nanometers [25], the Kapitza resistance, which is significantly affected by nanostructures, becomes nontrivial [32,33]. Molecular dynamic (MD) simulations have become a powerful tool to investigate nanoscale heat transfer, including disjoining pressure [34] and Kapitza resistance [32]. However, atomistic simulations are limited by the specific material systems and geometries studied, making the generalization to other systems difficult.

In the present study, a closed-form model is developed to determine the heat transfer coefficient of an evaporating meniscus on a nanostructured surface by integrating evaporation kinetics with disjoining pressure and Kapitza resistance so as to better quantify the impact of nanostructures on heat transfer performance of thin film evaporation and nucleate boiling.

Molecular dynamics simulations are performed for thin water films evaporating on square nanostructured gold surfaces of varying film thickness and nanostructure depth to verify the model predictions. The effects of film thickness and nanostructure depth on heat transfer coefficient are examined. The results presented here will be used to guide design of nanostructured surfaces with a variety of materials and geometries for enhanced thin film evaporation and boiling heat transfer.

2. The model

In this section, a model is developed to predict the heat transfer coefficient of a thin liquid film evaporating on a nanostructured surface by integrating evaporation kinetics, disjoining pressure, and Kapitza resistance. The schematic of a thin liquid film of thickness δ_0 evaporating on a two-dimensional periodic nanostructure of wavelength L and depth D is shown in Fig. 2a using a square nanostructure as an example. The basic assumptions of the model are:

- (i) The van der Waals interactions are the dominating intermolecular interactions between the liquid film and the nanostructured surface.
- (ii) The vapor near the thin film is assumed to behave as an ideal gas.
- (iii) The meniscus shape, ζ_1 , is periodic with the same wavelength L as that of the substrate surface ζ_s .
- (iv) The thin liquid film wets the nanostructured surface in Wenzel state, where liquid is in full contact with the nanostructured surface.
- (v) The evaporation and condensation at the liquid–vapor interface can be determined based on evaporation kinetics.
- (vi) The vapor phase is not far from equilibrium. Specifically, the difference between the liquid temperature at the liquid–vapor interface, T_{lv} , and the vapor temperature, T_v , is small, i.e., $|T_{lv} - T_v| \ll T_v$ and $|P_{\text{equ}}(T_{lv}) - P_v(T_v)| \ll P_v(T_v)$, where $P_{\text{equ}}(T_{lv})$ is the equilibrium pressure at the liquid–vapor interface and is different from the saturation pressure due to the presence of the disjoining and capillary pressures.
- (vii) The temperature of the solid surface is uniform at T_s .
- (viii) The conduction in the liquid phase is one dimensional (along z direction).

Fig. 2b shows the resistance network model of thin film evaporation, which includes the Kapitza resistance at the solid–liquid interface, R_K , the conduction resistance in the liquid film, R_{cond} , and the evaporation resistance at the liquid–vapor interface, R_{evap} . Based on the kinetic theory, the evaporative heat flux at the liquid–vapor interface is given following Schrage's derivation [35,36]

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