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**Numerical and Experimental Study of the Wetting
Characteristics of Water Droplets on Solid Substrates**

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Abstract

In this study, the author first reviewed the background and the mechanism of a highly efficient cooling method – i.e., the thin film evaporative cooling, in which the heat removal performance is highly dependent on the wetting characteristics of the working fluid. Then, the author studied the wetting behavior of water on different solid substrate both numerically and experimentally. By minimizing the free energy, Surface Evolver was used to explore the profile of the static liquid meniscus and the corresponding contact angle of water droplets on plain solid substrate and pillar substrate with sharp edge. Besides, goniometer experiments were performed to study the contact angle of a sessile water droplet on silicon, copper and aluminum substrates with graphene oxide (GO) and reduced graphene oxide (RGO) nanocoatings of different thicknesses. In addition, the author prepared a detailed list of components to be ordered for performing Micro-PIV experiments. An extensive literature study have been done to support the feasibility of the author's work.

Keywords: thin film evaporation, simulation, experiment

Table of Contents

I. Introduction.....	1
1. Background	1
2. Thin-Film Droplet Evaporation Mechanism	3
3. Object.....	4
II. Simulation	4
III. Experiment	7
1. PID Temperature Controller Module	7
2. Contact Angle Measurement Using Goniometer	8
3. Micro-PIV.....	10
IV. Conclusions	10
Reference.....	11

I. Introduction

1. Background

In the past several decades, high performance electronic devices have continued to shrink in size and grow in functions. Although this evolution has brought significant convenience for daily life, there is a long-existing problem that needs to be solved. What comes with a high performance is the challenge of the efficient heat dissipation of the electronic system. As the size of the cooling system should be compatible with the size of the device, different thermal management methods and cooling techniques are used for different electronic applications, with diverse sizes and system powers (as shown in Fig. 1). In addition, the integration of multiple functional units in a single device has led to generation of non-uniform heat flux that varies with space and time. Thus, cooling of hotspot with extremely high heat becomes the bottleneck of the thermal management of the device. How to tackle the hotspots problem spatially and temporally poses a great challenge.

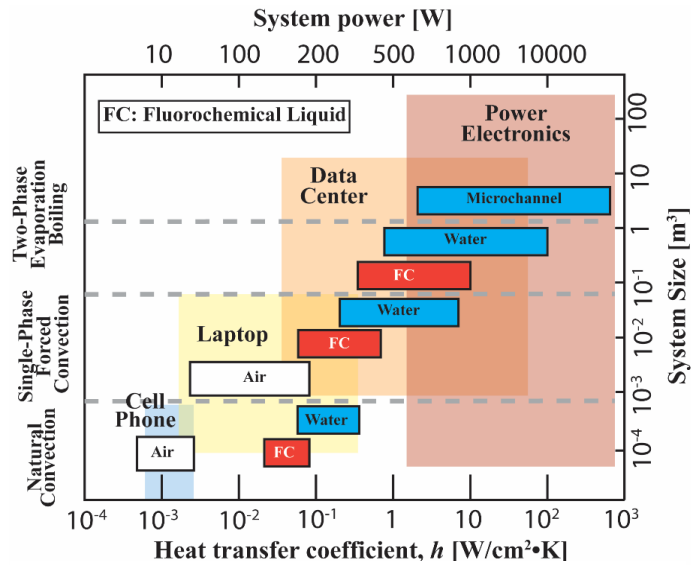


Figure 1. Thermal management map for different electronic applications, power specifications and cooling techniques

Currently, there are three principle methods for cooling: natural convection, single-phase forced convection, and two-phase forced convection. As shown in Figure 1, for small and portable devices such as cell phones, the hotspots presented in the CPU and batteries part have relatively low heating density. Therefore, natural convection with air is enough to remove all the heat produced by these hotspots. For higher heat removal requirements such as personal computers and data centers, both single phase and two-phase (e.g., convective boiling, vapor chamber, heat pipe) liquid cooling methods are feasible approaches for dissipating the moderate excessive heat from high performance computing units ($\sim 100 \text{ W/cm}^2$). In fact, liquid cooling of electronic packaging has been utilized for many years. For example, liquid cooling is used to cool the combustion engine in automotive industries[1]. For working fluid, while water has demonstrated many merits such as high specific heat capacity, low price, low boiling point, and being environmental benign. However, water cannot be used for direct cooling due to their electric conductance. In those scenarios, fluorochemical liquids have been explored as alternative candidates due to their dielectric properties. For two-phase systems, current studies are focusing on jet impingement, convection boiling in microchannels, and evaporation/boiling in porous media [2-5].

The author's research focuses on the use of two-phase flow and aim to achieve high heat transfer by forming a stable, ultrathin evaporation liquid film at the walls of heat exchanger even at extreme high heat fluxes.

2. Thin-Film Droplet Evaporation Mechanism

Recent studies have revealed the potential of transitioning from nuclear boiling to thin-film evaporation, resulting in increasing thermal performance of heat exchanger[6, 7].

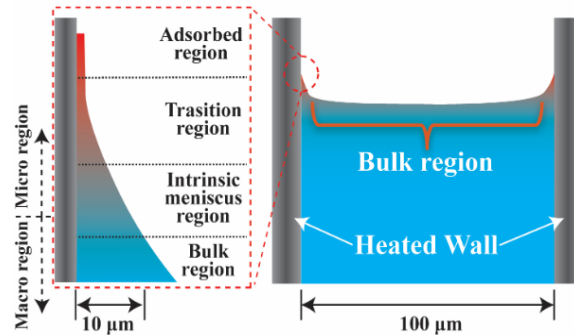


Figure 2. Schematic of different evaporating regions in traditional thin-film evaporation

As is seen from Figure 2, the meniscus near the boundary of the bulk water region can be divided into several regions: (1) the adsorbed region (< 10 nm), (2) the transition region (10-1000 nm), and (3) the intrinsic meniscus region (1-10 μ m). The area and the properties of each region are influenced by several interfacial forces, including the disjoining pressure at the adsorbed region, capillary force in the transition region, and thermocapillary effects in the intrinsic meniscus/bulk[8, 9]. Due to the small conduction resistance in the micro region (i.e. transition region and intrinsic meniscus region), extremely high local heat transfer coefficients can be achieved.

However, traditional thin film evaporation from wicking materials usually involves a concave evaporating meniscus that yield negative Laplace pressure and potential risk of early boiling. Droplet evaporation, on the other side, resolves such issue. When a sessile droplet is placed on a heated surface, the convex shape will yield a positive Laplace pressure ($\Delta p = 2\sigma/R$), which not only suppresses the boiling in the liquid but also enables higher evaporation rate. When the size is within millimeter scale, the conduction resistance through the liquid will dominant the evaporation from the bulk, but when the size goes down to ~ 10 μ m, this resistance will be in the same magnitude with the evaporation resistance. This leads to an average heat

transfer coefficient approaching $10^6 \text{W m}^{-2} \text{K}^{-1}$. Compared with the traditional droplet evaporation with concave meniscus, the whole evaporation region can be defined as the thin-film droplet evaporation region.

While most previous studies of liquid droplet evaporation were focused on spherical configurations. Sáenz et al.[10] showed recently that for two droplets with same contact line perimeter and liquid-vapor interfacial area, the droplet resting on triangular substrate evaporates 17% faster than the droplet resting on circular substrate. Therefore, understanding the shape effect on the evaporation rate is also important for realizing a higher total heat flux.

3. Object

The primary object of this independent study is to do a preliminary research on the thin-film evaporation phenomena – i.e., to explore the wetting characteristics of water droplets on solid substrates with different configurations numerically and experimentally. Such a study will help understand the evaporative heat transfer performance from a thin film droplet and the influence of working fluid-substrate configuration. For the simulation tasks, Surface Evolver is employed to study the profile of the liquid meniscus by minimizing the total free energy with a given surface tension. Molecular dynamics (MD) simulation is employed to study the relationship between water molecules, graphene coatings, and silicon substrate. For the experimental tasks, a goniometer and micro-PIV system are employed to observe the change of contact angles, and the internal flow of droplets, respectively. Multiple simulations and experiments were performed to ensure repeatability and mitigate artificial errors.

II. Simulation

For small enough droplet, the surface tension force dominates over gravity in the droplet. Thus, the shape of the drop interface is only affected by the surface tension, where the minimization of the total free energy will lead to a capped spherical geometry of droplets resting on infinite plane substrate. However, for droplets resting on a confined substrate (i.e., a pillar with sharp edge and axisymmetric shape), the droplet may exhibit different equilibrium geometry, and the apparent contact angle at the sharp edge may extend beyond its intrinsic contact angle on plane surface before the liquid burst out from the edge. Surface Evolver[11] was used to

demonstrate the phenomenon of pinning and bursting for droplets on pillar edges with various shapes. In addition, the axisymmetric geometry will result in non-uniform curvature when the droplet gets pinned on the pillar edge under steady conditions. This may result in different evaporation rate.

The author first simulate the processes of droplet spreading through surfaces with different shape (i.e., triangle, square, hexagon, and circle). The Surface Evolver is an open-source software without a user interface, thus all simulations are written in codes and are executed in the command lines. The simulations can be divided into the following steps: (1) Define parameters for future use (e.g. Gravity should be set to zero due to the scale of the droplet). (2) Draw the initial geometry, determine coordinates for all vertices and number all edges, facets, and bodies. (3) Set the boundary conditions for the droplet (i.e., the droplet should be pinned on the outer edge of the surface and should not go down the surface). (4) Create Macros to execute the codes in the command lines.

After refining 4 times and iterating 3000 times, droplets with varies geometries can be obtained as shown in figure 3.

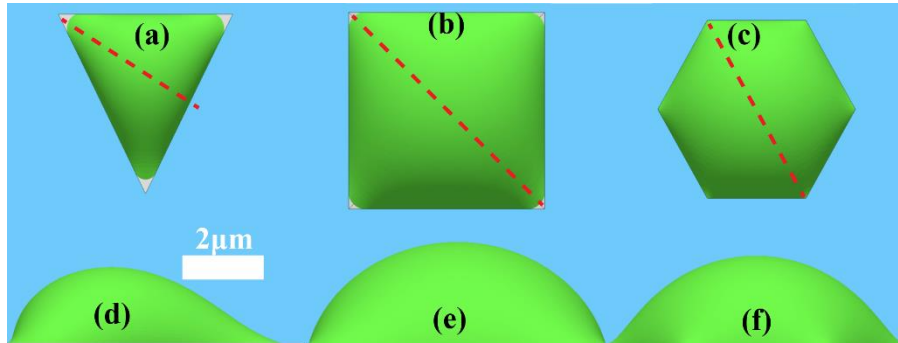


Figure 3. Demonstration of top view and side view for droplet on triangle (a,d), square (b,e), and hexagon (c.f) using Surface Evolver

Next, the author output the images and x, y, z coordinates of droplets, and employed MATLAB to calculate surface curvatures.

Table 1. Curvature for different shapes

Droplet shape	Mean curvature (1/m)	
	Water	FC-40
Triangle	571.3	536.0

Square	607.9	591.1
Hexagon	634.9	632.7
Circle	503.4	492.3

As is seen from this table, with the same perimeter and interfacial area, triangle has a higher mean curvature than circle, thus resulting in higher evaporation rate.

Then author modified the constraint conditions with increasing volume of the droplets. When the volume is increased, the droplet grows larger and eventually bursts from the outer edge of the pillar structure. If the initial volume is more than critical burst condition, and once the liquid front reaches the outer edge of the pillar, it should spontaneously spread downwards along the outer wall of the pillar. This is numerically realized in Surface Evolver by applying a new geometric constraint on the side wall of pillar. The dynamic process is shown in Figure 4.

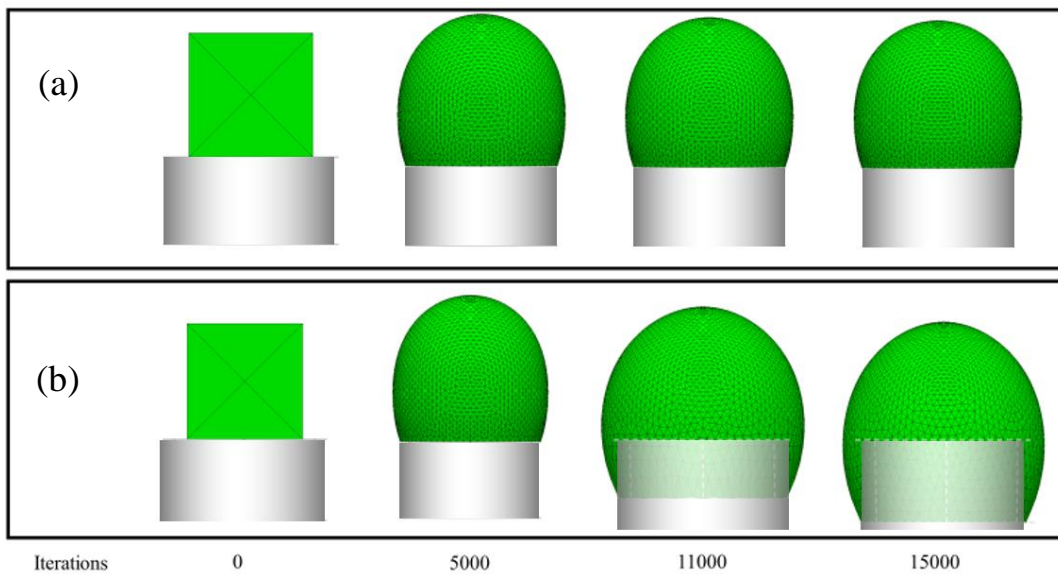


Figure 4. Demonstration of pinning and bursting phenomena on symmetric pillar with different liquid volume (a) $V = 7.20 \times 10^{-6} \mu\text{L}$; (b) $V = 7.25 \times 10^{-6} \mu\text{L}$

However, there are also limitations for using Surface Evolver to model the bursting behavior. Since the volume of liquid is given by the user, and it cannot be changed during the simulation. Thus, a theoretical calculation should be done before the simulations. In addition, due to the possible system errors, the real value may be different with the calculated value, and the only approach is to change the input parameters (e.g., surface tension) manually in the program each time to continuously

approach the theoretical value. Furthermore, Surface Evolver cannot capture the dynamic behaviors from pinning to bursting. Nevertheless, it is still helpful in studying the static liquid meniscus.

III. Experiment

During the independent study, the author performed the cleaning procedure for graphene oxide (GO)/reduced graphene oxide (RGO)-coated substrates, measured the contact angles of droplets on substrates, and prepared the order list of components for micro-PIV system.

The substrate materials are silicon, copper and aluminum. The airborne particles are the primary contaminants on these substrates. After researching in several literatures, the following method is developed to clean the substrates. Contaminants on GO-coated substrates can be tackled with low-density plasma or UV-O₃ cleaning, while contaminants on RGO-coated substrates can be solved by two steps: (1) Under an argon atmosphere, GO will be thermally reduced at 200 °C for 2 h at a heating rate of 1°C/min; (2) Using acetone and water to wash GO and dry it in the vacuum oven at 40 °C for 24 h.

To start with, the author modified the oven in NEIT lab by adding a PID temperature controller module for maintaining a predefined temperature more accurately.

1. PID Temperature Controller Module

A PID temperature controller module is primarily composed of a PID Temperature Controller, a Solid State Relay (SSR) and temperature sensor. The first step is to calibrate the temperature sensor, which is a Type K thermocouple.

The author calibrated the temperature sensor by comparing numbers displaying on its screen with the calibrated and standard thermometer. Since the experimental temperature range is from 0°C to 200°C, the author thus chosen ice bath, boiling water, and 200 °C engine oil as the reference liquid. Next, the author plotted the two numbers and found the fitting curve for the relationship between these two numbers, as is seen from Figure 5. Thus, the calibration process was completed.

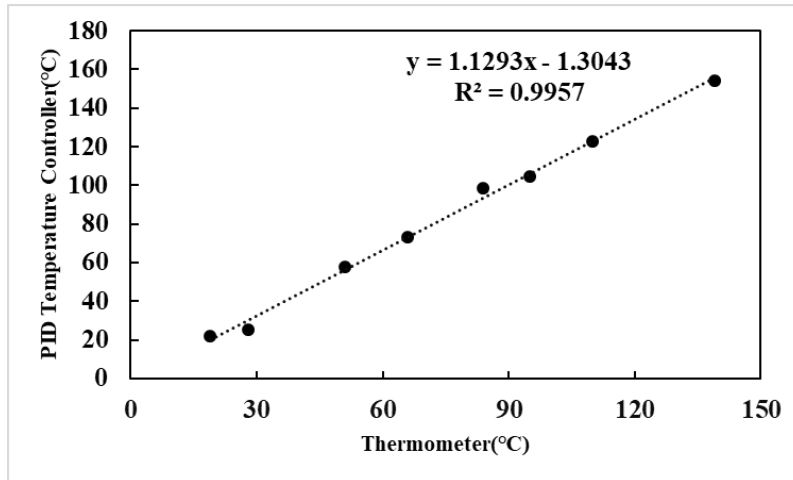


Figure 5. Fitting curve of reading value for PID temperature controller as a function of thermometer values

For other components, SSR is a switch with no moving parts. By using a small trigger voltage (from the PID), it is able to switch a much larger voltage (240VAC from the wall), while the PID is for setting various parameters and required temperature values.

The PID module actually replaces the role of knobs on the oven, therefore, the author unplugged the knobs from the oven and plugged the PID into the oven, and Figure 6 is the oven with the PID module.

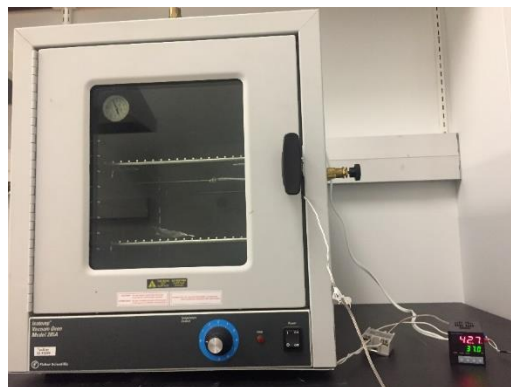


Figure 6. Oven with PID temperature controller module

2. Contact Angle Measurement Using Goniometer

The contact angle is the result of three interfacial surface tensions interaction: liquid-solid, solid-air, air-liquid, and by measuring the contact angles of droplets sitting on

different substrates, the properties of substrates can be studied. A basic actual picture of goniometer system is like Figure 7, and it consists of a camera, a light source, an automated syringe pump, and a sample platform. By programming the syringe pump, a steady flow rate is maintained, thus the volume for different case is the same.



Figure 7. Goniometer System

The experiments were performed during a 24-hour period on GO-coated/ RGO-coated substrates.

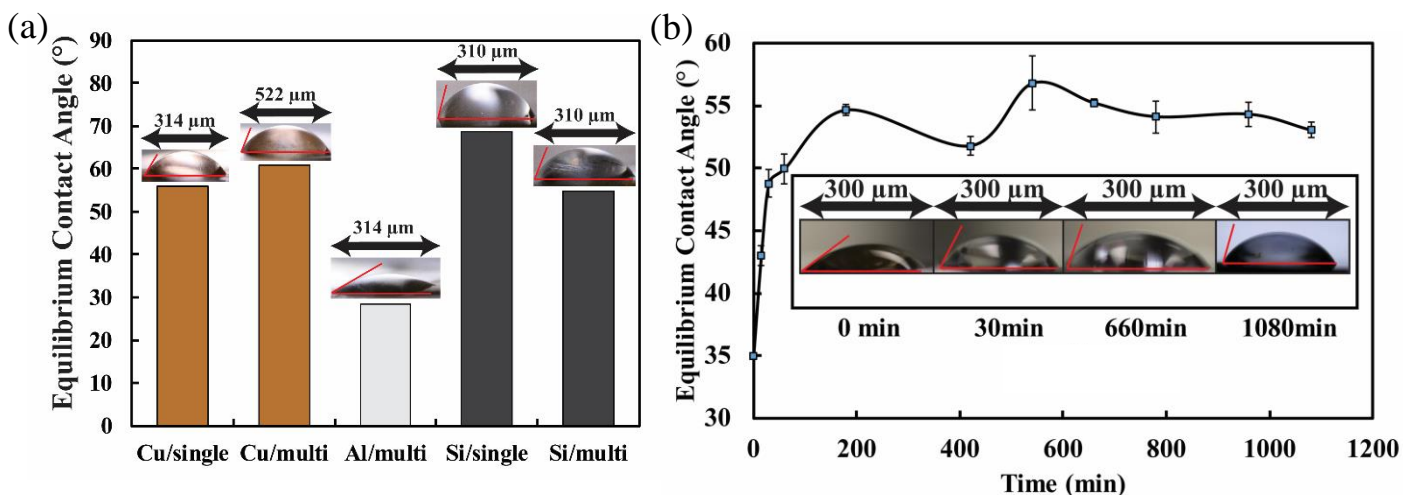


Figure 8. Results for contact angle measurement

Figure 8(a) demonstrates the effect of substrate and RGO thickness on the apparent contact angle of water droplet; Figure 8(b) shows the evolution of contact angle with time of water droplet on RGO coated (single layer) silicon substrate. The trend indicates the degradation of the nanocoating on the substrate by the contaminant in ambient air.

3. Micro-PIV

Micro-particle image velocimetry (μ PIV) is used to measure flow field for different experimental conditions. The μ PIV system consists of a ND-YAG laser (The wavelength and pulse width of the laser beam are 532 nm approximately 3-5 ns, respectively), a high-speed camera with a high objective and a band filter. Some fluorescent particles are added into the observed liquid, and when laser beam is shoot on the liquid, only the particles will be captured by the camera, thus the internal flow of liquid can be observed.

However, during this semester, the components were still in lack for doing the μ PIV experiment, the author ordered a band filter, laser goggles, black screens for absorbing the laser beam, and fluorescent particles for future use.

IV. Conclusions

During the one semester independent study, several achievements were made, while there were still some problems left. For myself, I have learned valuable lessons in computational simulations, experiments, and team-building. For the team, the equipment that I researched and helped purchase will be used in high-quality, vital work in the field of heat transfer. Every member in this lab offered me a lot of experience and guidance, and I offer my highest gratitude to them. I hope that the experiments and simulations I have done can continue to help NEIT lab to do future research on improvement of electronics and heat transfer applications.

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