

Office of Naval Research (ONR)

Final Performance Report

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Phase Change in High-Density Confined Liquids for Thermal Management

Prime Offeror

Syracuse University, Syracuse NY 13244

Principal Investigator/Technical Contact

Shalabh C. Maroo

Associate Professor

Dept. of Mechanical & Aerospace Engineering

Syracuse University

Link Hall 251, Syracuse NY 13244

Tel: 315-443-2107, Email: scmaroo@syr.edu

Technical Representative at ONR

Mark S. Spector, Ph.D.

Office of Naval Research

Advanced Naval Platforms Division, Code 331

875 N. Randolph Street, Arlington VA 22203-1995

Phone: 703-696-4449

E-mail: mark.spector.civ@us.navy.mil

Administrative Contact at Syracuse University

Amy S. Deppa

Research Administrator, Office of Sponsored Programs

Syracuse University

Lyman Hall 211, NY 13244

Tel: 315-443-9355, Email: asdeppa@syr.edu

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N00014-18-1-2357: Phase Change in High-Density Confined Liquids for Thermal Management

Final Performance Report

Submitter: Shalabh C. Maroo, Principal Investigator, Syracuse University

Major Goals

The proposed research comprises of three main tasks which involve water, dielectric coolants and glycols/alcohols as the working fluids: 1. Estimation of heat transfer related properties of water confined in nanochannels 2. Visualization, thermal characterization and modeling of bubble formation in water confined in nanochannels 3. Visualization and experimental heat transfer analysis of bubble formation in confined dielectric coolants as well as glycols/alcohols. In addition to nucleation experiments and simulations, we are also utilizing wicking in such nanochannels to estimate the disjoining pressure in experiments with validation from theory and CFD, followed by implementing those pressure values in CFD simulations and modeling the bubble nucleation process. Further, we have utilized a novel design of buried channels with micropores to estimate the heat flux capability and vapor velocity from the menisci in such channels.

Accomplishments Under Goals

Key Outcomes

(1) Disjoining pressure and bubble nucleation in nanochannels

Disjoining pressure of water was estimated from wicking experiments in 1D silicon-dioxide nanochannels of heights 59 nm, 87 nm, 124 nm and 1015 nm. The disjoining pressure was found to be as high as ~1.5 MPa while exponentially decreasing with increasing channel height. Such a relation resulting from curve fitting of experimentally-derived data was implemented and validated in computational fluid dynamics. The implementation was then used to simulate bubble nucleation in water-filled 59 nm height nanochannel to determine the nucleation temperature. Simultaneously, experiments were conducted by nucleating a bubble in a similar 58 nm height nanochannel by laser heating. The measured nucleation temperature was found to be in excellent agreement with the simulation, thus independently validating the disjoining pressure relation developed in this work. The methodology implemented here integrates experimental nanoscale physics into continuum simulations thus enabling numerical study of various phenomena where disjoining pressure plays an important role.

Summarizing the scientific achievements realized in this work:

- a) The first experimentally-derived disjoining pressure values for sub-100 nm water thin films.
- b) The first observation that disjoining pressure of water can be as high as ~1.5 MPa under confinement, i.e. 15 times the atmospheric pressure.
- c) The first implementation of experimentally-derived disjoining pressure values in CFD and its validation against experimental data.

- d) The first experimental work of bubble nucleation in water-filled-nanochannel of height <100 nm and measurement of nucleation temperature.
- e) The first continuum simulation work of bubble nucleation in water-filled-nanochannel of height <100 nm and estimation of nucleation temperature.
- f) The first study to show that nucleation temperature in confined nanochannel is higher than bulk water due to the dominance of disjoining pressure in such confinement, and independent validation of the nucleation temperature values obtained in experiments and continuum simulations.

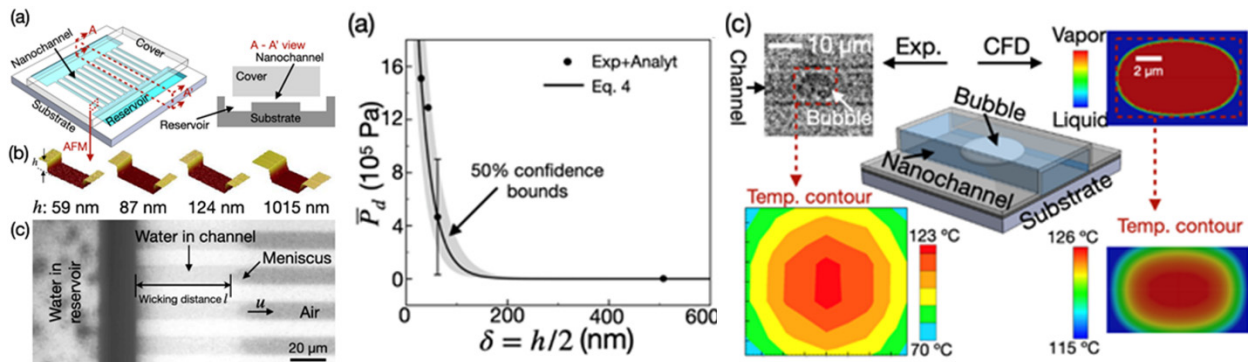


Figure 1: Disjoining pressure and bubble nucleation in nanochannels

Reference: An Zou, Sajag Poudel, Manish Gupta & Shalabh C. Maroo, Disjoining Pressure of Water in Nanochannels, [Nano Letters](#), 18, 7769-7774, 2021

(2) Disjoining pressure driven water transport from macro-reservoir to nanochannel

The work lays a foundation advanced heat transfer devices where appropriate macro-to-micro-to-nano channel-system network can be designed to passively flow water from a reservoir to an evaporating nanoscale liquid meniscus. This work uses 3D CFD simulations to mimic the stomata-xylem-soil pathway in a 100 m tall tree. In nanoscale conduits of height <100 nm, disjoining pressure has been found to play a significant role in determining liquid water pressure. Thus, to capture the proper physics of water transport in a nanopore, a disjoining pressure model is developed and implemented into the simulations, following which the transpiration mechanism is simulated. Disjoining pressure is found to be capable of inducing absolute negative pressures as high as -23.5 atm at the nanopore meniscus during evaporation, thus presenting a sufficient stand-alone explanation of the transpiration mechanism. It is also observed that, for very high evaporation rates (5000 kg/m²s in our study), the disjoining pressure driven supply of water cannot balance the evaporation at the meniscus, resulting in complete dewetting of meniscus from the nanopore and the consequent failure of the transpiration mechanism.

Summarizing the scientific achievements realized in this work:

- a) The first study of transpiration in a tree using continuum-based computational fluid dynamics (CFD) simulations
- b) The first study to develop an expression of disjoining pressure in a water film as a function of distance from the surface from experimental findings

- c) The first integration of near-surface nanoscale effects of disjoining pressure in continuum CFD simulations
- d) The first study to show absolute negative pressures as high as -23.5 atm at liquid-vapor meniscus in a nanopore during evaporation, thus presenting disjoining pressure to be a sufficient and stand-alone explanation of the transpiration mechanism

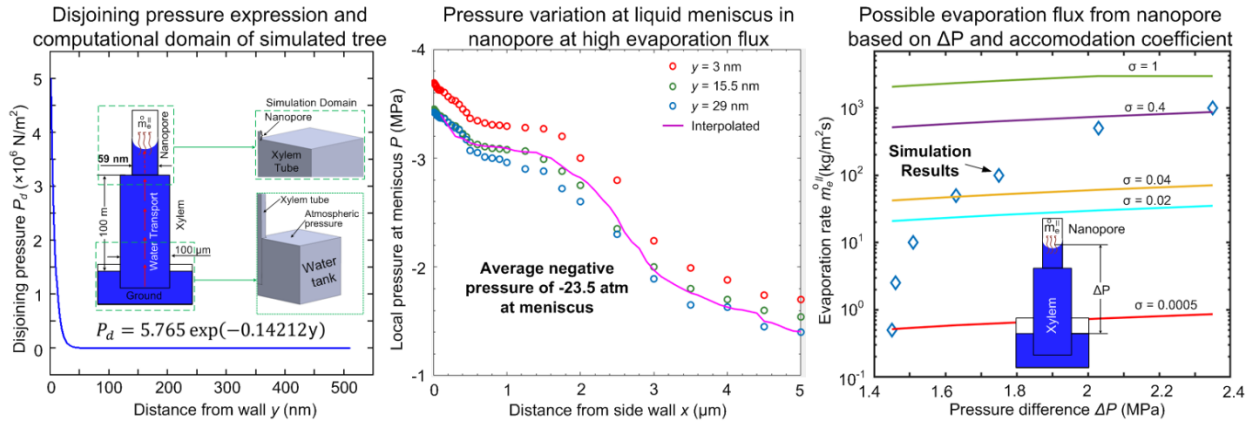


Figure 2: Disjoining pressure driven water transport from macro-reservoir to nanochannel

Reference: Sajag Poudel, An Zou & Shalabh C. Maroo, Disjoining Pressure Driven Transpiration of Water in a Simulated Tree, [Journal of Colloid and Interface Science](#), 616, Pages 895-902, 2022

(3) Bubble nucleation in a water-filled 59-nm nanochannel

Vapor bubble nucleation in nanochannel filled with polar liquid water is numerically simulated using computational fluid dynamics. The findings of the prior work on disjoining pressure of water in nanochannels is utilized to invoke the effect of nanoscale confinement on the liquid-vapor phase-change phenomenon. By means of CFD simulation, the pressure within the nanoscale liquid film can be set at different levels as dictated by the expression of disjoining pressure and the phase-change process is studied by specifying a constant heat-flux boundary condition at the channel wall. The bubble nucleation phenomenon is studied at varying heat-flux and the nucleation temperature is found to be $\sim 125^\circ\text{C}$ for a nanochannel of height 59 nm which matches well with the prior experimental finding. Nucleation temperature is found to be independent of supplied heat-flux; however at very high heat-flux ($> 50 \text{ W/cm}^2$), the rewetting of the channel wall ceases, and the three-phase contact line is formed. The present work sheds light on the lesser-known parameters of homogeneous nucleation like the liquid-film thickness underneath the bubble, the heat-flux supplied, as well as the maximum disjoining pressure the liquid-film in water-SiO₂ pair can sustain.

Summarizing the scientific achievements realized in this work:

- a) The first study to simulate bubble nucleation in a water-filled sub-100 nm nanochannel using CFD
- b) The first continuum work to show that bubble nucleation is homogeneous (rather than heterogeneous) in 59-nm nanochannel where disjoining pressure is dominant
- c) The first work to map and create a phase diagram between phase transition coefficient and supplied heat-flux

d) The first study to show that liquid-dewetting occurring at the surface underneath a bubble is directly related to the liquid film thickness and disjoining pressure in the liquid film

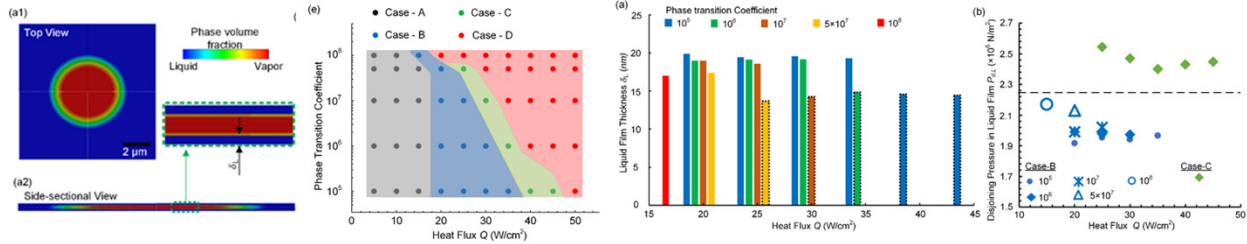


Figure 3: Bubble nucleation in a water-filled 59-nm nanochannel

Status: Sajag Poudel, An Zou & Shalabh C. Maroo, Bubble nucleation in a water-filled 59-nm nanochannel, *draft completed and in process of being submitted to journal*

(4) Heat Dissipation via Nanochannels using Dielectric Coolants

Parallel nanochannels have been fabricated to create a thermal management device (Figure 4a) towards the use of dielectric coolant as the working fluid. Microfluidic reservoirs have been fabricated at channel ends, and then enclosed with an opening at the top, to provide a pathway for the coolant to be filled in. The sample will be heated from underneath in <1 cm width to initiate bubble nucleation within the channels creating a single bubble in each nanochannel which then behaves as a heat pipe dissipating heat to the surrounding liquid. Such a device is based on patent published (Figure 4b) where ONR funding has been instrumental in expanding our fundamental understanding of the technology, beneficial in further de-risking the technology, providing critical data to support the patent prosecution and improve commercialization viability. The patent describes a cooling device for a heat source, such as an electronic component, has a single or set of nano-and/or micro-sized channel(s) connected to a single or multiple reservoir(s). The heat source causes nucleation within a channel, and a vapor bubble forms removing heat from the heat source via evaporation of liquid to vapor in the bubble and condensation of the generated vapor at the cooler ends of the bubble. Thus, the channel operates as a passive heat pipe and removes heat from the source by passively circulating the cooling fluid between the vapor bubble and the reservoir(s).

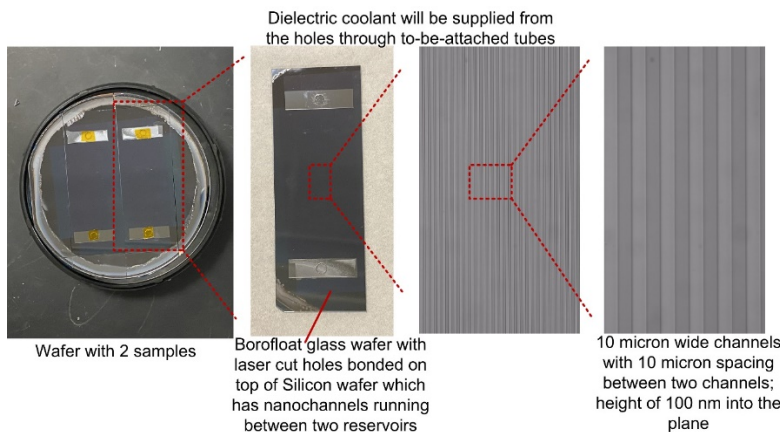


Figure 4a: Heat Dissipation via Nanochannels using Dielectric Coolants

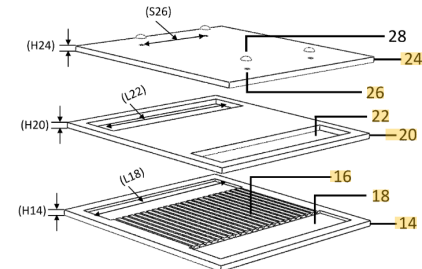


Figure 4b: Passive nano-heat pipes

Status: Durgesh Ranjan, An Zou & Shalabh C. Maroo, *fabrication complete and experiments being conducted*

Reference: Shalabh C. Maroo, An Zou, Manish Gupta, Passive nano-heat pipes for cooling and thermal management of electronics and power conversion devices, *US Patent 10,881,034*, 2020

(5) Droplet Evaporation on Porous Nanochannels for High Heat Flux Dissipation

Droplet wicking and evaporation in porous nanochannels is experimentally studied on a heated surface at temperatures ranging from 35°C to 90°C. The fabricated geometry consists of cross-connected nanochannels of height 728 nm with micropores of diameter 2 μm present at every channel intersection; the pores allow water from a droplet placed on the top surface to wick into the channels. Droplet volume is also varied and a total of 16 experimental cases are conducted. Wicking characteristics such as wicked distance, capillary pressure, viscous resistance and propagation coefficient are obtained at the high surface temperatures. Evaporation flux from the nanochannels/micropores is estimated from the droplet experiments, but is also independently confirmed via a new set of experiments where water is continuously fed to the sample through a microtube such that it matches the evaporation rate. Heat flux as high as ~294 W/cm² is achieved from channels and pores. The experimental findings are applied to evaluate the use of porous nanochannels geometry in spray cooling application, and is found to be capable of passively dissipating high heat fluxes upto ~77 W/cm² at temperatures below nucleation, thus highlighting the thermal management potential of the fabricated geometry.

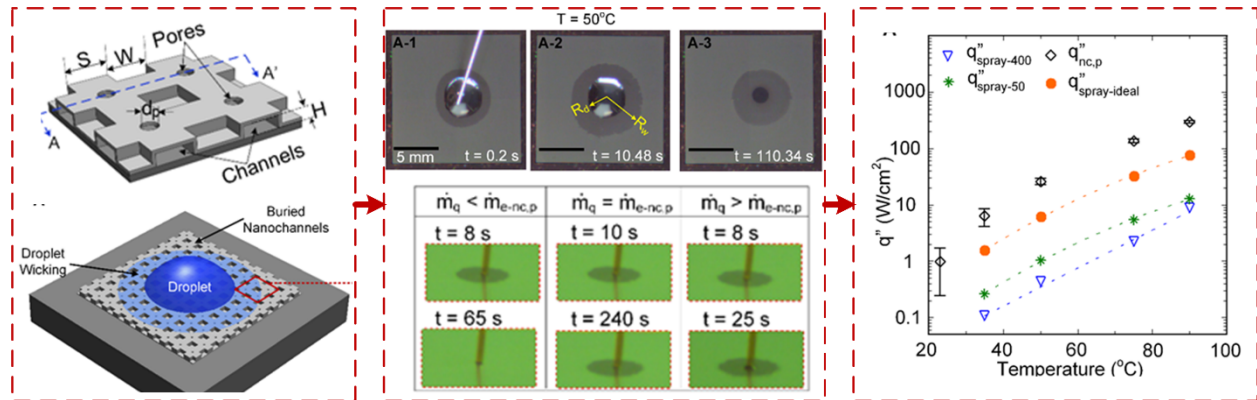


Figure 5: Droplet Evaporation on Porous Nanochannels for High Heat Flux Dissipation

Summarizing the scientific achievements realized in this work:

- The first experimental study of droplet coupled thin-film evaporation in porous nanochannels by surface heating.
- The first observation that initial wicking in such nanochannels is independent of surface temperature and droplet volume.
- The first observation that, at high surface temperatures, maximum wicking distance in porous nanochannels is independent of droplet volume.
- The first experimental estimation of steady thin-film evaporation heat flux in porous nanochannels can be as high as 294 W/cm².
- The fundamental experimental findings and obtained data is directly utilized to study the potential use of porous nanochannels in spray cooling thermal management applications;

heat flux dissipation as high as 77 W/cm^2 (based on projected sample area) at surface temperatures below nucleation can be achieved.

Reference: Sajag Poudel, An Zou & Shalabh C. Maroo, Droplet Evaporation on Porous Nanochannels for High Heat Flux Dissipation, *ACS Applied Materials & Interfaces*, 13, 1, 1853-1860, 2021

(6) Evaporation Dynamics in Buried Nanochannels with Micropores

We conducted computational fluid dynamics (CFD) simulations and experiments of wicking-coupled-evaporation in cross-connected buried nanochannels of height $\sim 728 \text{ nm}$ with $\sim 2 \mu\text{m}$ diameter micropores at each intersection. Two different samples of nanochannel widths $\sim 5 \mu\text{m}$ and $\sim 10 \mu\text{m}$ were studied. The experimental study of water droplet spreading in the porous structure provided results on the evolution of wicking radius and droplet base radius with time. Concentrating on the evaporation dominant regime of wicking phenomenon, evaporation flux in channels/pores is estimated from both experiment and CFD, and found to be in good agreement. CFD simulations demonstrated that evaporation of water wicked in channels/pores is independent of evaporation of the bulk water droplet sitting above the channels. When the meniscus recedes, new contact line regions form underneath the pores causing the observed increase of evaporation flux. Wicking flux velocity, pressure distribution inside nanochannels and curvature motion associated with wicking were also independently computed, from which the variation of viscous resistance with time is estimated. Viscous resistance is found to initially increase with time before achieving a steady value, thus implying that it is directly related to the driving force. Hence, this work articulates a wider perspective of wicking by estimating local spatial and temporal parameters which govern the phenomenon. Through CFD simulations supplemented by experiments, we are able to comprehend the lesser understood parameters, such as evaporation flux, wicking flux velocity, and pressure distribution, in wicking of water in sub-micron porous nano/micro structures, with potential design applications in heat pipes and spray cooling technologies.

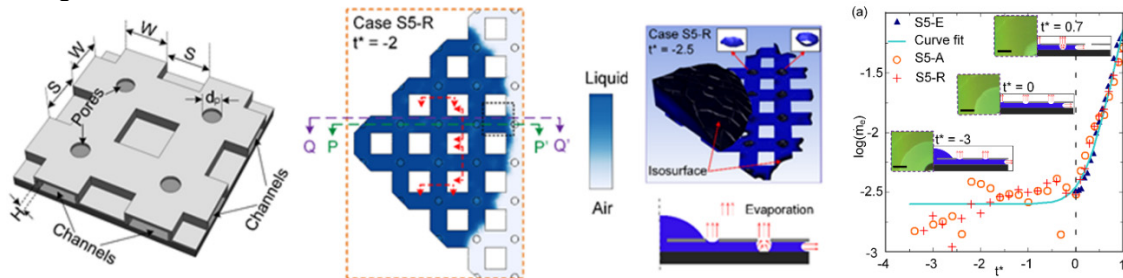


Figure 6: Evaporation Dynamics in Buried Nanochannels with Micropores

Summarizing the scientific achievements realized in this work:

- The first CFD study presenting *one-to-one* comparison with experiments on evaporation flux in sub-micron porous structures.
- The uniformly structured cross-connected buried nanochannels with micropores have a well-defined porosity allowing for CFD simulations and experiments to be performed on the exact same geometry.
- The first observation of local contact line regions forming underneath the micropores as meniscus recedes in the nanochannels, thus rapidly enhancing evaporation flux as a power-law function of time.

- d) The first independent estimation of wicking flux velocity and pressure-gradient in such nanochannels from which viscous resistance can be computed.

Reference: Sajag Poudel, An Zou & Shalabh C. Maroo, Evaporation Dynamics in Buried Nanochannels with Micropores, Langmuir, 36, 27, 7801-7807, 2020

(7) Thermal Management of Photovoltaics using Porous Nanochannels

The photoelectric conversion efficiency of a solar cell is dependent on its temperature. When the solar radiation is incident on the photovoltaics (PV) panel, a large portion of it is absorbed by the underlying material which increases its internal energy leading to the generation of heat. An overheated PV panel results in a decline in its performance which calls for an efficient cooling mechanism that can offer an optimum output of the electrical power. In the present numerical work, thermal management with a porous nanochannels device capable to dissipate high heat flux is employed to regulate the temperature of a commercial PV panel by integrating the device on the back face of the panel. The spatial and temporal variation of the PV surface temperature is obtained by solving the energy balance equation numerically. By evaluating the steady-state PV surface temperature with and without thermal management, the extent of cooling and the resulting enhancement in the electrical power output is studied in detail. The nanochannels device is found to reduce the PV surface temperature significantly with an average cooling of 31.5°C. Additionally, the enhancement in the electrical power output by ~33% and the reduction in the response time to 1/8th highlight the potential of using porous nanochannels as a thermal management device. Furthermore, the numerical method is used to develop a universal curve which can predict the extent of PV cooling for any generic thermal management device.

Summarizing the scientific achievements realized in this work:

- The first numerical study integrating porous nanochannels for thermal management of photovoltaics.
- Porous nanochannels can provide an average cooling ~31.5°C of the photovoltaics surface and can enhance its electrical power output by ~33%.
- A universal curve is also developed to predict the extent of photovoltaics cooling for any generic thermal management device.

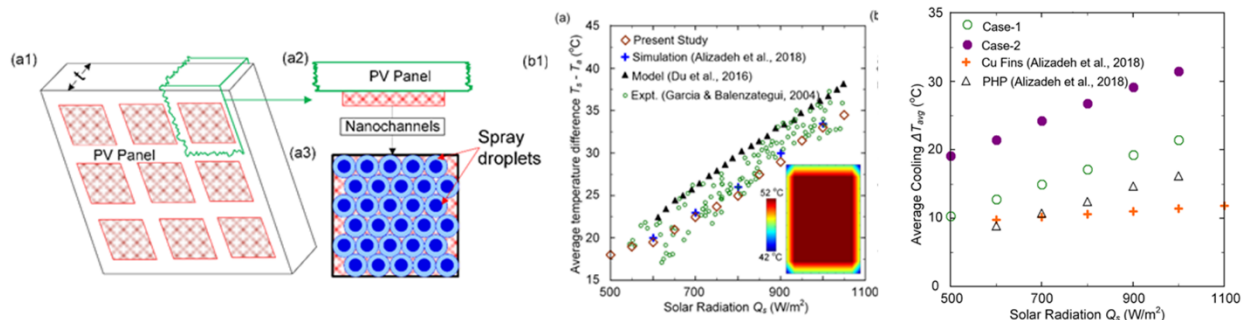


Figure 7: Thermal Management of Photovoltaics using Porous Nanochannels

Reference: Sajag Poudel, An Zou & Shalabh C. Maroo, Thermal Management of Photovoltaics using Porous Nanochannels, ACS Energy & Fuels 36, 8, 4549–4556, 2022

(8) Transpiration Mechanism in Confined Nanopores

We report a fundamental atomistic study of liquid pressure in confined nanopore. The liquid pressure in such pores can be high (positive) but thermodynamically stable due to strong surface-liquid interaction causing structured liquid layers to form. Due to evaporation, small reduction in these high pressure values can cause liquid to flow from the low pressure bulk region to the high pressure pore region. Pressure in the structured liquid layers can also transition from high to negative values when its density decreases from its equilibrium state. These insights can assist in further understanding of liquid transport in biological systems, thin film evaporation in phase change processes, as well as design and creation of passive flow devices.

Summarizing the scientific achievements realized in this work:

- The first study detailing a new mechanism of high-pressure driven passive liquid flow in a nanopore.
- The first atomistic observation of (counterintuitive) liquid flow from low pressure bulk region to high pressure nanopore region.
- The first study of transition from high pressures to negative pressures in thin liquid films.

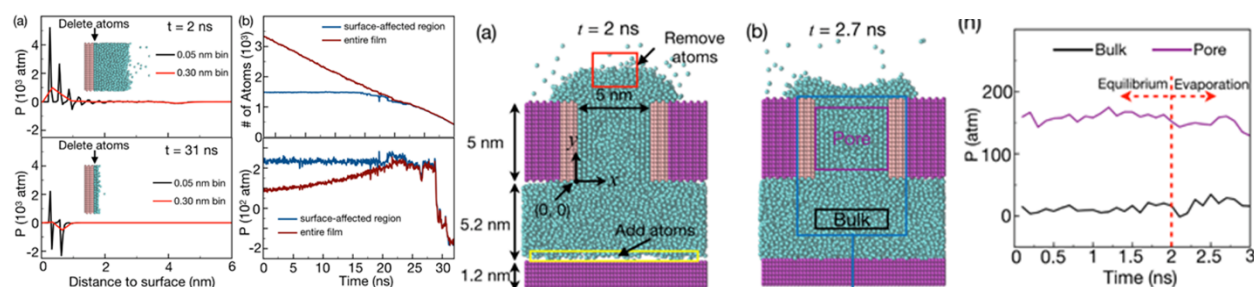


Figure 8: Transpiration Mechanism in Confined Nanopores

Reference: An Zou, Manisha Gupta & Shalabh C. Maroo, Transpiration Mechanism in Confined Nanopores, [Journal of Physical Chemistry Letters](#), 11, 9, 3637-3641, 2020

(9) Onset and critical radius of heterogeneous bubble nucleation

We studied the onset of bubble nucleation process using molecular dynamics (MD) simulations and experiments. In MD simulations, we first implemented our surface heating model into open source software LAMMPS and validated it against the classical heat conduction theory for heat transfer in argon liquid between two platinum surfaces. We utilize this surface heating model to initiate heterogeneous bubble nucleation on a partially heated platinum surface submerged in a pool of liquid argon. Over 40 simulations are run for varying width and temperature of heated part of the surface. We observed that if the heated width is less than a critical width for nucleation, the bubble collapses. The bubble remains stable near the critical heated width, while the bubble grows with time if the heated width is larger than critical width. Local thermodynamic data of density, internal energy, pressure, temperature and entropy are estimated to calculate the change in Gibbs free energy. The 'energy barrier' corresponds to the stable bubble case with the growing bubble achieving free energy change above this value while the collapsing bubble unable to reach and pass this barrier, thus showing very good agreement between MD simulations and classical nucleation theory. A high pressure and temperature fluid region is

found to exist in the liquid monolayer next to the surface which initiates nucleation. A heat transfer based analytical model is developed to predict the critical radius of nucleation using the MD simulation data. Experiments of bubble nucleation in water on a silicon-dioxide surface are conducted by laser heating. High speed camera images of onset of bubble nucleation are obtained along with surface burn mark from which the initial bubble radius is estimated and found to match well with a theoretical prediction. Thus, the surface-to-fluid heat transfer model implemented in LAMMPS in this work can allow for large molecular-level study of near-surface transient and thermodynamically-sound heat transfer problems which have not yet been possible.

Summarizing the scientific achievements realized in this work:

- a) The first atomistic MD study on heterogeneous bubble nucleation from a heated surface showing collapsing, steady and growing bubbles, as described in theory, while estimating their Gibbs free energy.
- b) The first experimental study to capture the bubble radius at onset of nucleation and demonstrate good agreement with theoretical critical radius of nucleation.
- c) The first implementation of a surface-to-liquid heat transfer algorithm in LAMMPS (MD software) allowing for differential fluid heating/cooling at surface and study of near-surface transient heat transfer problems which have not yet been possible

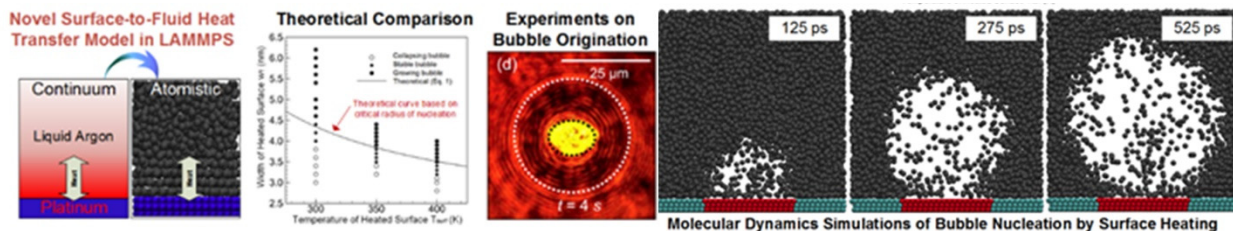


Figure 9: Onset and critical radius of heterogeneous bubble nucleation

Reference: Manisha Gupta, An Zou & Shalabh C. Maroo, Onset and critical radius of heterogeneous bubble nucleation, [Applied Physics Letters](#), 116, 103704, 2020

(10) Molecular Simulation of Bubble Nucleation in Hydrophilic Nanochannels by Surface Heating

Single bubble nucleation in liquid confined in nanochannel is studied using molecular dynamics simulations and compared against nucleation in the bulk liquid (i.e. without confinement). Nucleation is achieved by heating part of a surface to high temperatures using a surface-to-liquid heating algorithm implemented in LAMMPS. The surface hydrophilicity of nanochannels is increased to understand its effect on nucleation behavior. Liquid structuring is found to play a significant role in altering thermodynamic properties of density and pressure in the nanochannels, which in turn changes the enthalpy of vaporization. Increased surface hydrophilicity in nanochannels results in the delay of bubble formation as more energy is required for nucleation. Thus, bubble nucleation in hydrophilic nanochannels can dissipate higher heat fluxes and can potentially be used towards the thermal management of hot spots in power electronics.

Summarizing the scientific achievements realized in this work:

- The first molecular study which simulates bubble nucleation in nanochannel by partially heating the surface.
- The first study to capture the changes in thermodynamic properties of bubble nucleation due to increasing surface hydrophilicity in nanochannel.
- The first study to show that enthalpy of vaporization can increase by 30% due to combination of nanochannel confinement and surface hydrophilicity.

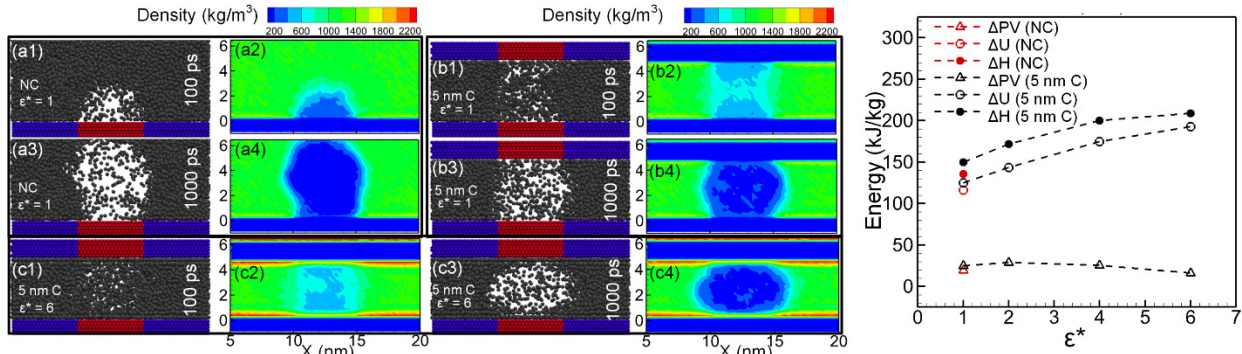


Figure 10: Molecular Simulation of Bubble Nucleation in Hydrophilic Nanochannels by Surface Heating

Reference: Manish Gupta and Shalabh C. Maroo, Molecular Dynamics Simulation of Bubble Nucleation in Hydrophilic Nanochannels by Surface Heating, *Molecular Simulation*, under revision

Results Dissemination

Journal Publications

- Sajag Poudel, An Zou & Shalabh C. Maroo, Thermal Management of Photovoltaics using Porous Nanochannels, *ACS Energy & Fuels* 36, 8, 4549–4556, 2022
- Sajag Poudel, An Zou & Shalabh C. Maroo, Disjoining Pressure Driven Transpiration of Water in a Simulated Tree, *Journal of Colloid and Interface Science*, 616, Pages 895-902, 2022
- An Zou, Sajag Poudel, Manish Gupta & Shalabh C. Maroo, Disjoining Pressure of Water in Nanochannels, *Nano Letters*, 18, 7769-7774, 2021
- Sajag Poudel, An Zou & Shalabh C. Maroo, Droplet Evaporation on Porous Nanochannels for High Heat Flux Dissipation, *ACS Applied Materials & Interfaces*, 13, 1, 1853-1860, 2021
- An Zou & Shalabh C. Maroo, Nano-confinement effects on liquid pressure, *Physics of Fluids*, 33, 042007, 2021
- Sajag Poudel, An Zou & Shalabh C. Maroo, Evaporation Dynamics in Buried Nanochannels with Micropores, *Langmuir*, 36, 27, 7801-7807, 2020
- An Zou, Manisha Gupta & Shalabh C. Maroo, Transpiration Mechanism in Confined Nanopores, *Journal of Physical Chemistry Letters*, 11, 9, 3637-3641, 2020
- Manisha Gupta, An Zou & Shalabh C. Maroo, Onset and critical radius of heterogeneous bubble nucleation, *Applied Physics Letters*, 116, 103704, 2020
- Manish Gupta and Shalabh C. Maroo, Molecular Dynamics Simulation of Bubble Nucleation in Hydrophilic Nanochannels by Surface Heating, *Molecular Simulation*, under revision

10. Sajag Poudel, An Zou & Shalabh C. Maroo, Bubble nucleation in a water-filled 59-nm nanochannel, *draft completed and in process of being submitted to journal*
11. Manish Gupta & Shalabh C. Maroo, Accommodation coefficients of evaporation and condensation in nanochannels using molecular simulations, *draft completed and in process of being submitted to journal*
12. Durgesh Ranjan, An Zou & Shalabh C. Maroo, *fabrication complete and experiments being conducted*

Conference Publications

1. An Zou & Shalabh C. Maroo, Confinement Effects on Molecular Mechanics and Structure of the Liquid Layers at Solid-Liquid Interface, ASME IMECE 2021, Virtual
2. Sajag Poudel, Durgesh Ranjan, An Zou & Shalabh C. Maroo, Numerical Investigation of Photovoltaics Cooling Using Wicking Channels, ASME SHTC 2021, Virtual
3. An Zou, Shalabh C. Maroo, Manish Gupta, Equilibrium Pressure of Liquid Confined in Nanopores Using Molecular Dynamics Simulations, HT2020-9089, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual

Conference Presentations Only

1. Manish Gupta & Shalabh C. Maroo, Prediction of Heat Transfer in Nano-Channels Using Neural Networks, ASME SHTC 2021, Virtual
2. An Zou, Sajag Poudel & Shalabh C. Maroo, Experimentally Characterizing Average Disjoining Pressure of Water in SiO₂ Nanochannels, ASME SHTC 2021, Virtual
3. Sajag Poudel, An Zou & Shalabh C. Maroo, CFD Simulation of Wicking in Nanochannels, ASME SHTC 2021, Virtual
4. Sajag Poudel, An Zou, Manish Gupta & Shalabh C. Maroo, Numerical Simulation of Bubble Nucleation in Nanochannel, ASME SHTC 2021, Virtual
5. An Zou, Manish Gupta & Shalabh C. Maroo, Counterintuitive flow from low-pressure bulk to high-pressure nanopore, 73rd Annual Meeting of the APS Division of Fluid Dynamics, November 22-24, 2020; Virtual
6. Sajag Poudel, An Zou & Shalabh C. Maroo, Droplet-Coupled Wicking in Nanochannels with Micropores, 73rd Annual Meeting of the APS Division of Fluid Dynamics, November 22-24, 2020; Virtual
7. An Zou, Manish Gupta & Shalabh C. Maroo, Will Liquid Flow From Low Pressure Region to High Pressure Region?, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual
8. An Zou, Sajag Poudel, Durgesh Ranjan & Shalabh C. Maroo, Buried Nanochannels: A Tool for Exploring Solutions for High Heat Flux Removal, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual
9. Manish Gupta, An Zou & Shalabh C. Maroo, A Molecular Dynamics Study of Onset Heterogeneous Bubble on Super-Heated Surface, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual
10. Manish Gupta & Shalabh C. Maroo, Analysis of Accommodation Coefficients Using Molecular Dynamics, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual
11. Sajag Poudel, An Zou & Shalabh C. Maroo, Experimental and Numerical Investigation of Evaporation Dynamics in Nanochannels With Micropores, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual
12. Sajag Poudel, An Zou & Shalabh C. Maroo, Stability of Evaporating Liquid Meniscus in Cross Connected Buried Nanochannel Wicks, ASME 2020 Heat Transfer Summer Conference, July 13-15, 2020, Virtual

Other Products

1. Manish Gupta and Shalabh C. Maroo, Modified LAMMPS software with integrated surface heating algorithm (developed in PI's lab) will be publicly available for download post-publication

Honors and Awards

Nothing to Report

Training Opportunities and Outcomes

A senior personnel Dr. An Zou (Research Assistant Professor) and 3 PhD students, Sajag Poudel, Durgesh Ranjan and Manish Gupta, worked on the project under the guidance of PI which includes continuous discussions, one-on-one meetings and group discussions. The skills learnt include cleanroom nano-fabrication and characterization methods, conducting experiments, ANSYS CFD simulations, running LAMMPS MD simulations, data processing, preparing manuscripts, and disseminating results at conferences.

1. Sajag Poudel graduated with his PhD in January 2022 and joined Argonne National Lab as a post-doc. Sajag also completed a 5-month internship at Oak Ridge National Lab through NSF INTERN grant.
2. Manish Gupta graduated with his PhD in August 2021, and joined Future Inc as a Machine Learning Engineer
3. An Zou joined MiTeGen as R&D scientist in August 2021
4. Durgesh Ranjan is on track to graduate with his PhD by May 2023

Technology Transfer

Shalabh C. Maroo, An Zou, Manish Gupta, Passive nano-heat pipes for cooling and thermal management of electronics and power conversion devices, *US Patent 10,881,034*, 2020, Publication date: Dec 19, 2020. The patent filing pre-dates the ONR funding but the research work performed in this project is directly instrumental in expanding our fundamental understanding of the technology, beneficial in further de-risking the technology, and providing critical data to support the patent prosecution and improve commercialization viability.

Participants

Name	Role
Maroo, Shalabh	PD/PI
Zou, An	Research Assistant Professor
Poudel, Sajag	Graduate Student
Gupta, Manish	Graduate Student
Ranjan, Durgesh	Graduate Student

REPORT DOCUMENTATION PAGE

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