Popular science summary of the PhD thesis

PhD student	Wenfu Situ
Title of the PhD thesis	Nanoscale Heat Transport in Multiphase Systems: A Molecular Dynamics Study
PhD school/Department	Department of Civil and Mechanical Engineering

Science summary

* Please give a short popular summary in Danish or English (approximately half a page) suited for the publication of the title, main content, results and innovations of the PhD thesis also including prospective utilizations hereof. The summary should be written for the general public interested in science and technology. Before the thesis defence, the summary is sent to DTU's Office for Communication and Media and to the media *Ingeniøren*:

This PhD thesis advances the design of next-generation micro-/nanoscale thermal management systems by demonstrating the critical role of air removal in liquid cooling architectures and establishing pressure/electric field modulation as viable optimization strategies. Employing molecular dynamics frameworks, this work elucidates atomic-scale heat transfer mechanisms in multiphase systems, resolving persistent knowledge gaps.

Non-equilibrium molecular dynamics (NEMD) simulations were used to investigate thermal transport in copper-water-air systems. Physical accuracy was ensured through force field calibration, air solubility quantification, and modification of the PPPM solver. Contrary to air's detrimental impact on interfacial heat transfer, high pressure enhances phonon transport across interfaces by inducing ordered water layers near copper substrates, thereby reducing Kapitza resistance. In nanoscale boiling, literature has long contested the boiling state and air's influence. This work clarifies that boiling occurs exclusively as the Leidenfrost phenomenon—not bubble nucleation—and quantifies the adverse effects of air dissolution in water nanofilms. To optimize nanoscale thermal transport, we examined how bulk ion concentration and electric field intensity jointly modulate Kapitza resistance at copper-electrolyte interfaces. Below 4 Vnm^{-1}, ion hydration dominates interfacial heat transfer with strongly temperature-dependent Kapitza resistance. Electric fields exceeding 4 Vnm^{-1} suppress this effect.

By understanding nanoscale heat transfer dynamics, this research establishes a fundamental framework for thermal management in micro-/nanoelectronics, batteries, and energy harvesters. These findings bridge molecular interactions with macroscopic thermal performance, providing a roadmap for energy-efficient solutions in next-generation electronics and renewable energy systems.

Please email the summary to the PhD secretary at the department