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Optimizing Nanoscale Heat Transfer for Novel Applications

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Independent Study Report

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Nanoscale surface treatments and their effect on liquid film pinning and thin film evaporative heat transfer was studied through published literature and experimental simulation. ANSYS Fluent was utilized to study relevant geometries and to confirm experimental results found in published literature. Vapor chambers were studied to compare their current performance to that of a vapor chamber with a proposed graphene integrated CIO, copper inverse opal, wicking structure. The role of graphene in altering the surface energy and conductive characteristics of a given substrate as well as its performance as a protective coating was studied, yielding results that require further study. Further research will be required to confirm published results on the wettability of graphene as well as building a two-phase fluid flow simulation to study the performance of copper inverse opal wicking structures.

Introduction

The objective for the research conducted this semester was to study nanoscale heat transfer. This along with a goal of developing novel applications for microporous materials meant that vapor chambers became a focus of the research conducted. Vapor chambers are passive cooling devices, used for high heat flux applications such as high powered electronics. They feature a wicking structure, which utilizes capillary action to drive the working fluid from the evaporative section to the condensation section of the heat pipe, that governs the thermal performance of the vapor chamber. Previously published literature showed that copper inverse opal wicking structures were a promising development and thus CIO was studied in detail, utilizing modeling and simulation software such as SolidWorks and ANSYS Fluent. Lastly, a hybrid structure utilizing graphene to increase the specific surface area as well as change the wettability characteristics of CIO was proposed. This led to the need to know more about graphene's intrinsic wettability characteristics and how it could alter the surface energy and properties of an underlying substrate.

Although graphitic materials had been previously studied for many decades, graphene, being relatively new, was still not fully understood. Graphene shows promise for its high thermal and electrical conductivity and high specific surface area to volume ratio. However, the literature available cited contrasting results and thus further research will be required to understand and be able to predict graphene's performance within a CIO wicking structure. Published results were

confirmed for single phase flow through a CIO structure and further developments would include integrating a two-phase flow regime by adding a developed evaporative flux user-defined function, UDF, to our ANSYS Fluent simulation.

Copper Inverse Opal

Optimizing vapor chambers to meet the rising power densities of high powered electronics has become a popular topic of research. The underlying wicking structure is responsible for much of the vapor chamber's performance and it is expected to provide both high liquid permeability as well as high capillary function, two contrasting demands¹. Microporous structures and specifically microporous metals have been studied for their high specific surface area, conductivity, and density of fluid-permeable pores to facilitate heat transfer². Copper inverse opal is a metallic microporous structure that shows the most promise to dissipate high heat fluxes for high powered electronics applications³.

We wanted to develop a sophisticated model of CIO, whose surface energy we could modify according to the effects of graphene. This model could then be used to generate results for our proposed graphene integrated CIO wick. The first step in developing this model was to create a CIO unit cell and subject it to single-phase fluid flow as shown in figures 1 and 2.

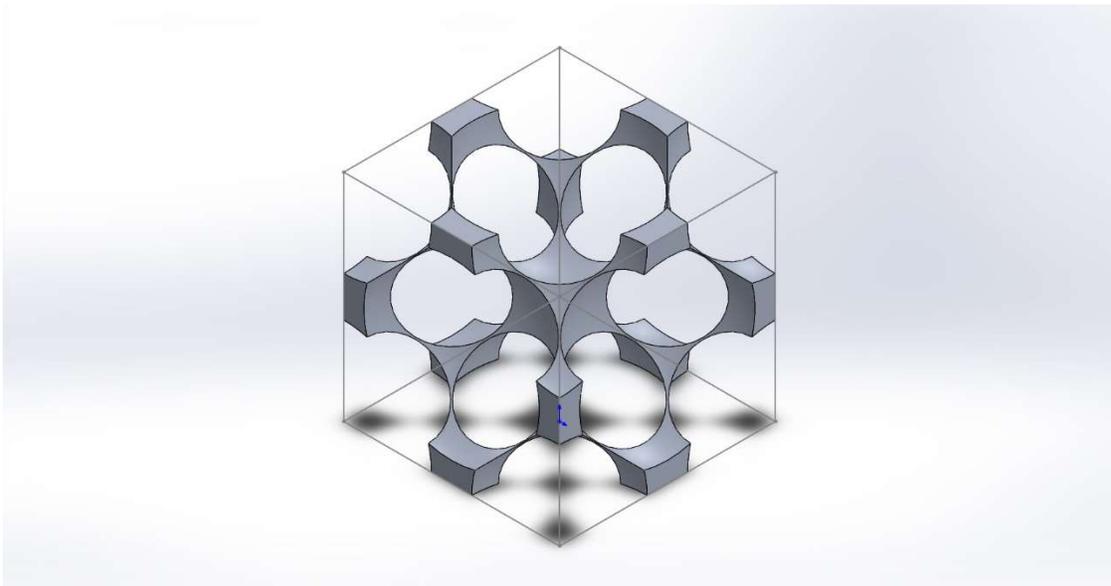


Figure 1: A SolidWorks model of a CIO unit cell (FCC)

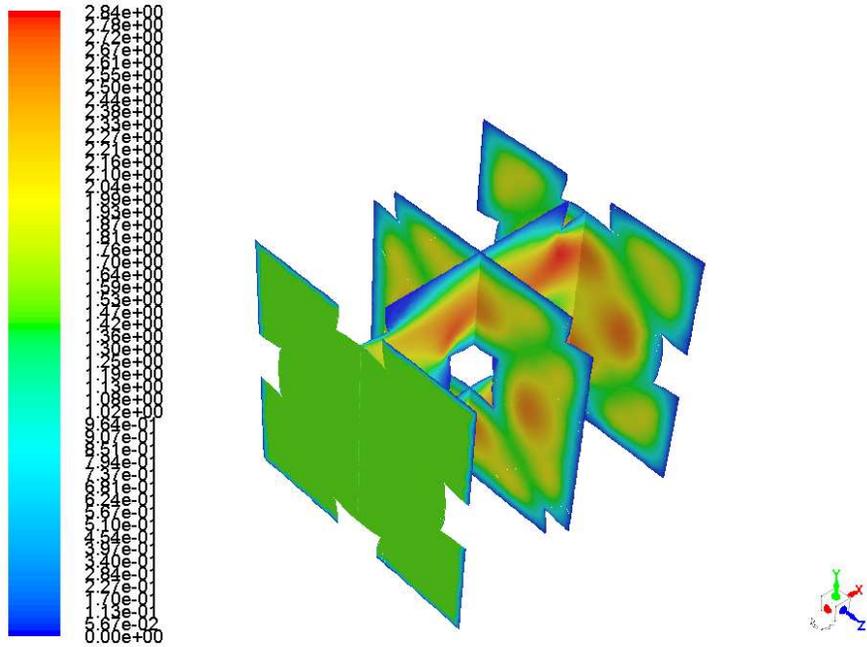


Figure 2: The resulting velocity contour plot for single phase flow

The resulting velocity contour plot resembled and thus confirmed the general findings of Thomas Dusseault et al as shown below in figure 3⁴.

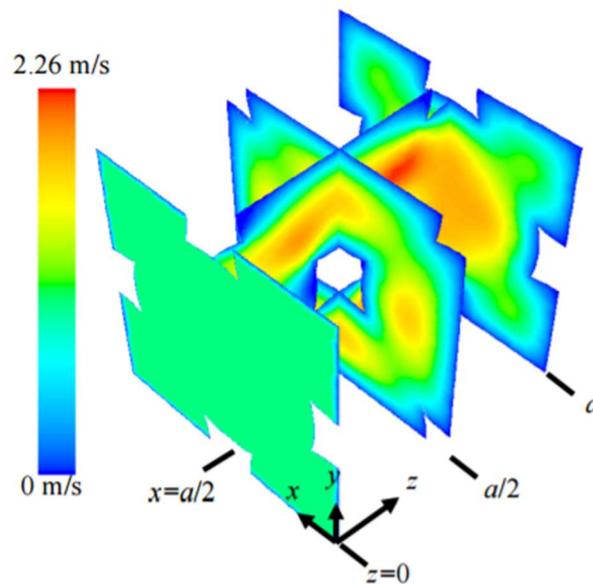


Figure 3: Velocity contour plot for CIO in the FCC geometry⁴

By comparing and confirming our results with previously published results, we know that we are on the right track for eventually creating the sophisticated model mentioned above.

Graphene

Graphene, a two-dimensional monolayer of carbon atoms condensed in a honeycomb lattice⁵, has become a material of significant interest due to its mechanical, thermal, and electrical properties¹. It is the building block for graphitic materials such as nanotubes and graphite⁶. It was first mechanically exfoliated by Kostya Novoselov and Andre Geim, physicists from the University of Manchester, through an experiment involving scotch tape and a block of graphite⁷. Epitaxial graphene can be produced through the chemical vapor deposition of hydrocarbons on metal substrates and thermal decomposition in which epitaxially grown SiC is exposed to high enough temperatures so that the Si atoms evaporate, leaving only carbon and thus forming graphene⁶. Because of its recent discovery, the characteristics of graphene aren't well agreed upon as will be shown by the contradictory findings from experiments. Thorough literature searches were conducted to explore the wettability and surface energy effects of graphene so we can eventually run simulations of our proposed wicking structure. General findings are presented below.

Applications

As a coating: Since graphene is atomically thin and flexible it is thought to be promising as a coating to prevent or slow down the oxidation of metals¹. Graphene's impermeability as well as its thermal and chemical stability, graphene was found to be stable in extremely high temperatures exceeding 1500°C, are what makes graphene such an outstanding candidate as a protection layer⁸. Chen et al showed that graphene successfully protected metal substrates from O₂ and H₂O₂ oxidation while keeping the added benefit of not drastically changing the thickness of the substrate or its physical properties⁸.

Schrifer et al recently showed that graphene offered Cu substrates effective short-term protection from oxidation, over the scale of minutes to hours, but proved to greatly promote galvanic corrosion over longer time scales, months to years, and thus may be an even worse corrosion barrier than leaving the substrate bare⁹. Zhou et al concluded that the long-term oxidation of a Cu substrate was accelerated by the presence of graphene over a time period of 6 months and attributed this accelerated corrosion effect to graphene's ability to promote electrochemical corrosion in Cu¹⁰.

These contradictory findings suggest that more work is needed to fully evaluate graphene's performance as an anti-corrosion coating.

Wettability: Many recent studies concluded that graphene is hydrophobic, exhibiting similar wetting properties to graphite: Epitaxial graphene was shown to have a WCA of 92° while CVD graphene exhibited WCAs of 90.4° and 93.8° when grown on Ni and Cu respectively¹¹.

However, Li et al concluded that graphene might be a lot more hydrophilic than previously thought, showing a WCA of 44° when freshly produced, and its wettability characteristics are dominated by the effects of surface contamination through ambient hydrocarbons, which was seen by an increase in its WCA to 80° when exposed to air for a day as shown in figure 4¹¹.

Amadei et al confirmed these findings and attributed the transition between hydrophilicity to hydrophobicity for highly ordered pyrolytic graphite, HOPG, to the adsorption of contaminating molecules from the ambient air¹². (Both groups used atomic force microscopy, AFM, and Fourier transform infrared spectroscopy to confirm the presence of hydrocarbons as the cause of graphitic material's change in wettability)

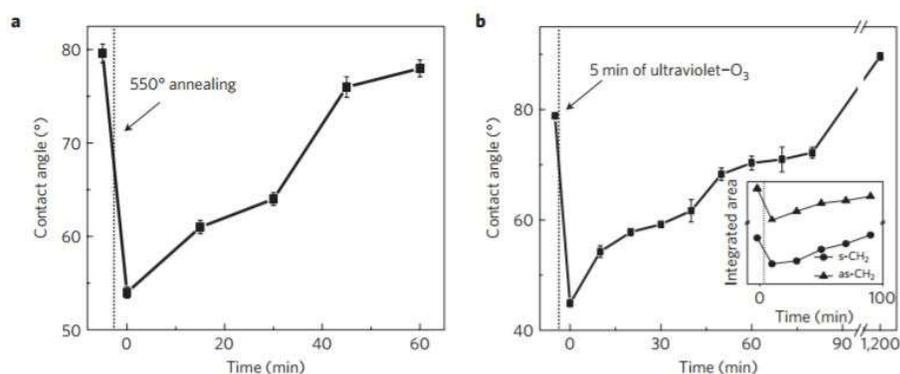


Figure 3 | Removal of hydrocarbon contaminants from a graphene/copper sample reduces its WCA. a,b Effect of thermal annealing in Ar at 550°C (a) and ultraviolet- O_3 treatment (b) on the wettability of a graphene/copper sample. The inset in b shows the integrated peak area versus time for the ATR-FTIR peaks at $2,930\text{ cm}^{-1}$ (asymmetric CH_2 stretching, triangles) and $2,850\text{ cm}^{-1}$ (symmetric CH_2 stretching, circles). The thermal annealing and ultraviolet- O_3 treatment ended at time 0. Error bars correspond to ± 1 standard deviation of three measurements.

Figure 4: Graphs showing the how airborne contaminants alter the CA of graphene¹¹

As previously stated, the characteristics of graphene aren't well known and thus further research requires us to grow our own graphene and conduct experiments using the goniometer setup that was built over the course of the semester.

Conclusion

Throughout the course of the semester, nanoscale heat transfer and specifically its applications in addressing the demand to cool high power density electronics was studied. Research was conducted on the performance of vapor chambers and a new wicking structure, whose performance determines the performance of the vapor chamber as a whole, was proposed. The new wicking structure features graphene integrated with a CIO substrate in the hopes of maximizing both capillary function as well as permeability. Models were created and progressively improved upon, stopping to compare them with published literature to ensure that we were on the right track. Graphene, being relatively new, required extensive research to understand its characteristics, ultimately so that we can create a model to generate predictions for our proposed wicking structure's performance before experimentally testing a prototype. Further research will be comprised of directly testing graphene's wettability within the NEIT lab and generating a two-phase flow regime that accounts for the effects of applying graphene to CIO.

Current Progress

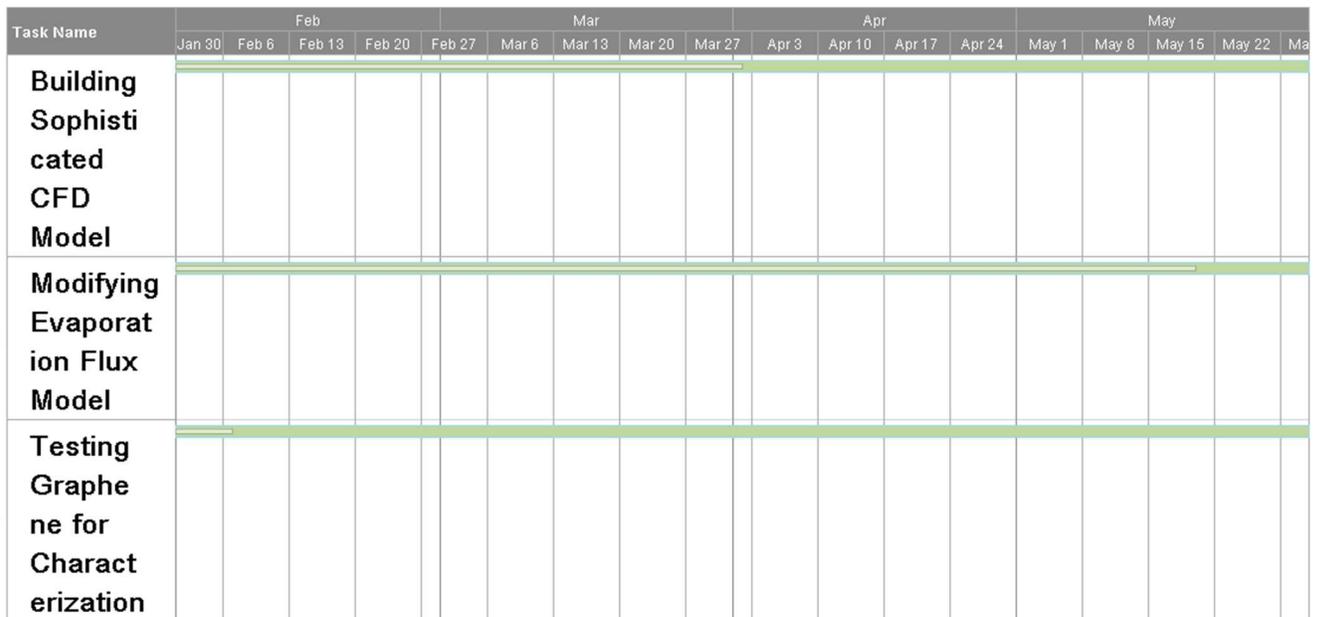


Figure 5: A gantt chart showing our progress throughout the various projects

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