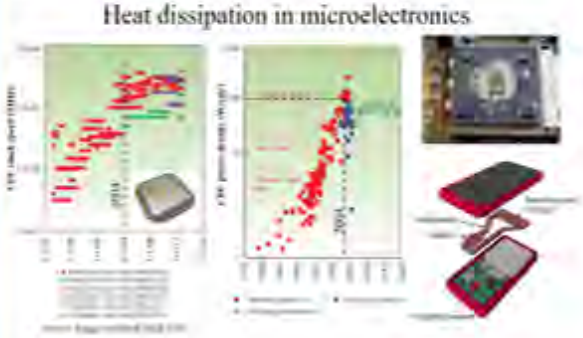
Molecular Dynamic Simulation of Thin Film Evaporation/Condensation in Nanoscale Heat Pipes

Mechanical Engineering
Students: Tyler Hinton & Aaron Singh
Advisor: Dr. Zhi Liang

FRESNO STATE
Lyles College of Engineering

Introduction

As technology has advanced, CPUs have exceeded power densities of 100 W/cm^2 (close to that of a nuclear reactor). This leads to overheating and CPU failure. One solution can be found by examining microscale heat pipes in smartphones and using phase change cooling to decrease internal temperatures. Our research revolves around the use of a Molecular Dynamics simulation program called "LAMMPS" in order to evaluate a simpler argon system. The argon system will undergo evaporation which we study and discuss.



MD Simulation Setup

The system we studied was based upon the following criteria:

- Controlled, set volume
- Leonard-Jones potential
- Temperature of 85 K
- Pressure of 10 atm
- Time step of 5 fs

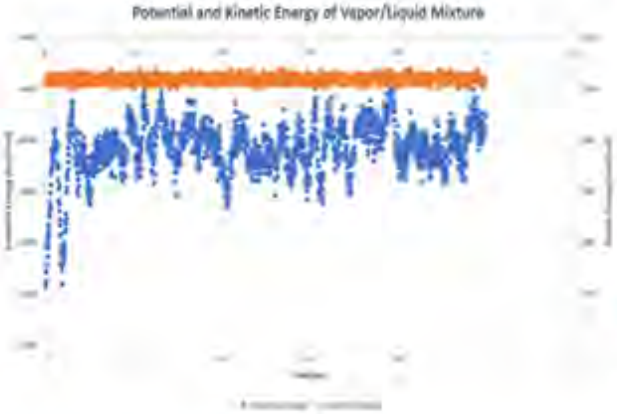
Once these conditions were met, the simulation box was then populated with liquid Argon atoms.

MD Simulation

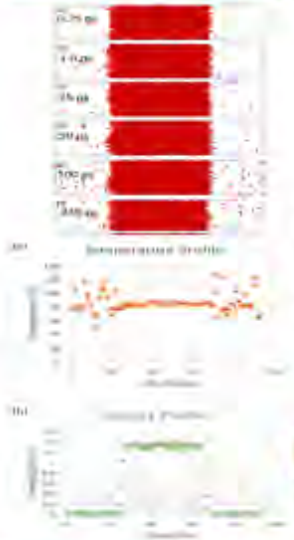
1. Ran simulation with set volume of liquid Argon until it reached equilibrium.
2. Created vacuums on both sides and ran until equilibrium with both liquid and gaseous atoms.
3. Once equalized, split up simulation box into different bins to record the temperature and density

Results

The results show that after about 250 picoseconds, the argon reaches a equilibrium vapor/liquid state. The potential and kinetic energy of the vapor/liquid mixture can be seen in the figure below and shows that the system has reached equilibrium since it is fluctuating about a constant.



Results



The evaporation rate of argon also shows the density profile of argon in the system which is another key factor in determining power densities in electronics. In order to validate our findings, we compared our data to a paper written by Dr. Liang and his results are displayed below.[1]

Conclusion and Future Work

The research project conducted with Dr. Liang gave us extensive knowledge on the fundamentals of phase change cooling. The results of this research not only served to show the significance of phase change cooling but also the tremendous potential in cooling of CPUs. This could lead to revolutionary advancements in technology and allow for more powerful processing. If this project was extended, we would study the same set of properties but with a mixed system that included different types elements in addition to Argon.

Acknowledgments

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(1) Zhi Liang and Pawel Keblinski, "Coalescence-induced jumping of nanoscale droplets on superhydrophobic surfaces", Appl. Phys. Lett. 107, 143105 (2015)