Molecular Dynamics Simulation of Power Generation in a Nanofluidic Energy Conversion Device

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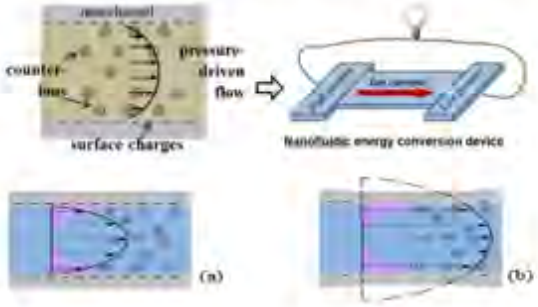
Introduction

Nanofluidic energy conversion devices use a simple structure to convert mechanical energy directly to electrical energy using a pressure differential and a charged fluid to drive an external load.



Electrostatic charges create a mismatch between the ion density profile and fluid density profile in the nanochannel. Theoretical evidence shows ~70% efficiencies can be achieved by slip flow conditions such as that provided by a graphene- lined nanochannel.

Ref: "Lennard-Jones Potential." Chemistry LibreTexts. Ed. Rabia Naeem. Libretexts, 08 Jan. 2017. Web.

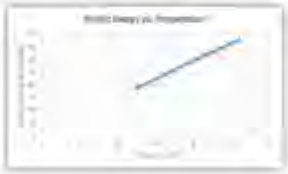
$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

The Lennard-Jones potential equation where ε (epsilon) is the depth of the potential well, σ *(sigma)* is the finite distance at which the inter-particle potential is zero, and r is the distance between the particles.

Box Simulation of Argon

Solid Argon (Ar), FCC lattice, 5x5x5 nm^3 unit cells, LJ potential, 2.5σ cutoff distance, the initial lattice constant set as 5.4 Angstrom, periodic boundary conditions. T = 50 K, P = 10 atm. Equilibrium molecular dynamics (EMD) simulations were ran for 1 ns with a timestep of 0.5 fs.

The plotted graphs above show the relation of K.E/1.5kB and P.E/eps as a function of time at temperature 50 K where kB is the Boltzmann constant and eps is ε.



Simulation of Ar in a box at 50 K and 10 atm. The temperature was gradually increased by an interval of 2 K while the pressure was kept constant. At each temperature the system was equilibrated for 2 ns with a timestep of 0.5 fs.

The KE and PE (after reaching equilibrium) at each temperature was averaged and a phase change was observed at ~87 K where there was a sudden jump in KE and PE. The graphs plotted are KE and PE as a function of temperature.

Simulation of Argon in a Nanochannel With Fixed Boundary Conditions

Ref:
Liang, Zhi, and Keblinski, Pawel. "Slip Length Crossover on a Graphene Surface: The Journal of Chemical Physics: Vol 142, No 13." The Journal of Chemical Physics. American Institute of Physics, n.d. Web.

Made a nanochannel of cross- sectional area 5.3x5.3 nm^2, a FCC lattice of Au as a fixed boundary condition on top and bottom filled with fluid Ar. The system is introduced with 100 atoms at 150 K constant temperature. Atoms are gradually increased at supercritical temperature.

Future Work

Simulations were performed using fixed boundary conditions on top and bottom. In the future, a dynamic boundary condition will be implemented by giving a velocity to one of the fixed boundaries to simulate flow. The slip length velocity will be analyzed along with the ion charge density for the flow between the fluid and the nanochannel.

Acknowledgement

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