

Simulating Hot Nano Beads

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1. Introduction

Single molecule detection and single molecule spectroscopy have been a very important tool in exploring molecular interactions, reaction kinematics, conformational dynamics [1]. The techniques used analyze the time variation of the fluorescent signal emitted by the tagged molecule. An alternative approach to the fluorescent spectroscopy is using metal nano-particles which interact strongly with light. In a recent experiment, Frank Cichos and others [2] introduced a novel method for single molecule detection, known as Photothermal Correlation Spectroscopy. In this method a gold nano particle is heated with a laser which changes the local refractive index. A second laser is used to measure the local change in the refractive index. A correlation analysis similar to Fluorescence Correlation Spectroscopy is then applied to the photothermal signal amplitude. Motivated by this novel experiment we have performed a simulation of a similar system consisting of a gold nano particle surrounded by a Lennard Jones fluid

2. Experiments and Theory

In the simulation of the system we consider a spherical gold nano particle which is surrounded by a Lennard-Jones fluid. The initial configuration for both the fluid and the gold particle is obtained from a FCC lattice. The interaction between the fluid molecules and that of the fluid and the gold particle is of Lennard-Jones type while the interaction between the gold atoms in the nano cluster is of FENE springs [3]. Molecular dynamics simulation has been done to investigate the flow of heat around the gold nano particle. The system is equilibrated at a constant temperature and pressure. After the equilibration process the nano particle is constantly heated at a constant rate. The measured temperature profile shows a discontinuity at the solid-liquid interface which can be associated with the Kapitza resistance, the finite interfacial resistance between the solid and the liquid phases.

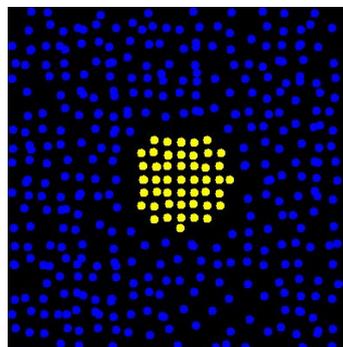


Fig. 1: Simulation snapshot of the gold nano particle in Lennard Jones fluid. The picture is the projection in the x-y plane.

3. Conclusion

Motivated by the recent experiment by F. Cichos and others on the detection of a nano particle heated by a constant laser, we have performed molecular dynamics simulation of

a similar system consisting of a gold nano particle in a Lennard-Jones fluid and have investigated the flow of heat around the gold nano particle. The interfacial resistance across the solid-liquid interface can be attributed to the Kapitza resistance

References

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