Molecular Dynamics Simulation on Thermodynamic Properties and Transport Coefficients

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Molecular dynamics simulation (MDS) is used to study the thermodynamic properties and transport coefficients of an argon system with Lennard–Jones potential. The results on the velocity distribution, mean free path, mean collision time, specific heat and self-diffusion coefficient agree well with the existing theoretical/experimental data. It shows that molecular dynamics method is another bridge to connect microworld and macroworld.

Keywords: molecular dynamics simulation, thermodynamic property, transport coefficient.

INTRODUCTION

With the rapid development of microelectronics and microelectronics mechanic system microscale heat/mass transfer becomes an important subject of research such as cooling of electronics circuit (up to 0.1 μm level), convection in the micro channels, heat conduction in thin films and so on. It was discovered from experiments that microscale heat transfer may be quite different from macroscale heat transfer. For example, convective heat transfer in microchannels can exhibit one order of magnitude higher than in the ordinary sized channels, the heat conductivity of thin films may reduced two orders of magnitude compared to that for the bulk materials. These phenomena can't be explained reasonably by the classic macroscopic theory. Furthermore, in some fields such as phase change and interface interaction, some problems remain unsolved, which can be clarified from the point of view of molecular level.

It is well-known that statistics mechanics is used to describe the macroscopic properties in term of microscopic information, but it can only explain some phenomena based on thermodynamic equilibrium hypothesis. On the contrary, molecular dynamics as a powerful tool starts from the basic physical model and simulates molecular motion completely, so that it can describe and reveal complex phenomena being far away from the thermodynamic equilibrium.

Molecular dynamics method has been widely used in Japan and the United States. Kotake advanced the following five future aspects in molecular heat and mass transfer study: 1) Control and enhancement of heat and mass transfer on the basis of atomic and molecular kinetics using thin-film and fine-particle technology. 2) Application of interfacial kinetics between phases to controlling energy transfer, adhesion and lubrication. 3) Improving and modifying to macroscopic physical and chemical properties with dynamic feature of molecular motion. 4) Controlling the phase change of condensation and evaporation with clustering process. 5) Application of light interaction with matter to spectroscopic energy transfer and control, and so on.

MOLECULAR DYNAMICS SIMULATION

Molecular dynamics simulation method is divided into molecular dynamics method and Monte Carlo method. Depending on the fact whether the quantum effect is considered or not, it can be further subdivided into four types: quantum molecular dynamics method, classic molecular dynamics method (i.e., molecular dynamics simulation), quantum Monte Carlo method and classic Monte Carlo method. At thermal energy level, the quantum effect is usually negligible. This leads to the concept of molecular dynamics in which molecular motions obey the classic Newton's equation.
of motion. Molecular dynamics thus may provide a direct route from the microscopic details of a system to macroscopic properties of both theoretical and experimental interest (the equation of state, transport coefficient and process, and structural order parameters, and so on).

The main steps of molecular dynamics simulation are as follows:

Selection of System Size, Boundary Condition and Potential Among Molecules

Macroscopic properties of a system are determined by the motion states of all the molecules in it, which are statistical average of corresponding microscopic quantities. In principle, the more the number of molecules the examined system consists of, the more accurate the macro properties obtained from micro average are. However, due to the limitation of computer speed and storage, the considered molecules can not be too many. The molecule number of system is from several hundred to several thousand. In the present study, two thousand five hundred argon molecules are included.

Implementing periodic boundary conditions can dramatically reduce the molecule number needed for computation on the one hand, and overcome the problem of surface effect on the other hand. The cubic box is replicated throughout space to form an infinite lattice, as shown in Fig.1(a). The central box simply forms a convenient axis system for measuring the coordinates of the \( N \) molecules. When the system is isolated, the mirror boundary condition should be used, as shown in Fig.1(b).

The potential among molecules determines the macroscopic properties of a system. The widely used potential model is Lennard–Jones dual potential:

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

(1)