ABSTRACT
Molecular dynamics simulations are carried out to study the thermal and mechanical phenomena of ultra-high heat flux conduction induced by ultrafast laser heating in thin Si films. Nanoscale Si films with various depths in heat flux direction are treated as a semi-infinite model for the study of ultrafast heat conduction. A distribution of internal heat source is applied to simulate the absorption of the laser energy in films and the induced temperature distribution. Stress distribution and the evolution of the displacement are calculated. Thermal waves are observed from the development of temperature distribution in the heat flux direction, though the average temperature of the simulated Si films increases monotonically. The average stress shows periodic oscillations. The time development of strain has the same trend as the average stress, and the net heat flux shows the same trend as the stress at different depths of the Si films in the direction of heat flux. This reveals a close relationship between stress and net heat flux in the Si films in the process of ultrafast laser heating.

Keywords: Molecular dynamics simulation; Heat conduction; Si thin films; Ultrafast laser heating

INTRODUCTION
Ultrafast lasers have been widely used in industries such as medical science and engineering, super fine micro-processing, high-density information storage, and laser controlled fusion. Ultrafast laser pump-probe technology [1-4] has also become an important means for basic experimental research. Understanding thermodynamic phenomenon of interaction between ultrafast lasers and materials is important for ultrafast laser processing and non-destructive testing.

The mechanism of energy conversion and transport process is one of important problems of basic research in the fields like energy, information technology, material science, micro-processing, etc. It manifests the interaction of energetic-particles at the nano/pico level, whereas the time and space scales of these interactions are in the range of femtosecond-picosecond and nanometer, respectively. Ultrafast laser pump-probe technology can distinguish and observe the interaction of these energetic-particles to provide experimental means for the observation of conversion and transport of nanoscale energy and the research on rule, which is now the only way to observe nano interaction of energetic-particles.
In 1980s, ultrafast laser pump-probe technology was first applied to the research on micro heat transport in an experimental study by Eesley [1-3] of American GM laboratory on ultrafast laser pulse exciting heat transport in metal films. The ensuing series of meticulous and in-depth work last until today, mainly focusing on metal materials [5-14]. The theoretical research on micro/nano non-equilibrium heat transport has been staying ahead of experimental research, and the successively developed theoretical models include heat wave model proposed by Vernotte and Cattaneo [15]; Anisimov's [16] dual temperature semi-classical theoretical model (TTM model) when ultrafast laser illuminates metal; and Tzou's [17] dual-phase-lagging model. Specially, TTM model can effectively describe heat transport in metal films under ultrafast laser irradiation. With the mutual verification and promotion of experiments and theories, research on micro/nano non-equilibrium heat transport in metals has become very mature today. However, few people have conducted research on nano heat transport in semiconductors and super-lattices, a large class of materials. Though some models have been proposed for the micro/nano heat transport in semiconductors, they have never been fully accepted for lack of experimental verification. Research on micro/nano heat transport in semiconductor materials has not been carried out in a systematic way.

In the field of micro/nano electronics or photo-electronics, semiconductors are used more widely than metals, which make the research on the mechanism of micro/nano heat transport in semiconductor materials bear practical significance. With the improvement of integration of micro/nano electronic and photo-electronic devices, heat problem of chips like temperature fluctuation begins to influence the performance of chips. The heat dissipation of chips becomes a key obstacle in further improving the integration. On the other hand, as a complete theoretical system, micro/nano heat transport cannot hold without research on semiconductor materials. Conducting experimental and theoretical research on semiconductors is scientifically significant for establishing a complete theoretical system for heat transport system at micro/nano scale.

In this treatise, molecular dynamics (MD) simulation is utilized to study the thermal and mechanical phenomena in silicon semiconductor films heated by an ultrafast laser. Calculations include temperature distribution, stress distribution, strain distribution and the generation and transmission of the stress waves. It is discovered that the temperature fluctuation is the result of coupling between the heat transfer quantity and strain rate.

MODEL DESCRIPTION

Due to extremely short heating time, the triggered pressure waves develop rapidly, which brings many obstacles for the research on the thermo-mechanical waves in materials. Under such extreme conditions, continuum body hypothesis is questionable for dealing with heat transfer and thermal-mechanical coupling. Use of MD direct simulation of atomic or molecular motion plays an important role in revealing the heat effect during ultrafast laser-material interaction and the mechanism of internal deformation. The Si film is considered as a semi-infinite medium for ultrafast heat transfer modeling. For the present MD simulations, Si crystal atoms in the heat direction are inside an analog box with various lengths of 32.3 nm, 40.4 nm, 48.4 nm, 60.5 nm and 75.6 nm, respectively. To reduce fluctuation errors of statistical mechanics caused by short heat-conducting direction of semiconductor compromising with balanced computation power, all the present simulations use the same number of molecules, namely 288,000 Si atoms.

MOLECULAR FORCE FIELD AND ABSORPTION OF LASER ENERGY

The common force fields suitable for Si crystals include EAM (embedded—atom method) potential, MEAM (modified embedded—atom method) potential, Tersoff potential and SW potential. SW potential is selected in the present simulation as the interaction potential between Si atoms, since it can better embody multi-body potential interaction, ensuring calculation precision and avoiding complex calculation of Tersoff potential to enable more atoms to be engaged in the simulation. Generally, laser heating can be treated as heat flux boundary condition of the second kind. The heat flux boundary condition acts as an alternative heat source [19]. The internal heat source S converted from laser energy can be obtained as:

\[ S(x, t) = 0.94 \frac{(1 - R)}{A t_p} \exp \left[ -\frac{x}{\delta} - 4 \ln 2 \left( \frac{t}{t_p} \right)^2 \right] \tag{1} \]

where \( R \) is the reflectivity of semiconductor film surface, \( J \) is the single pulse power, \( A \) is the sectional area of laser beam, and \( \delta \) is the depth of absorption.

In the present MD simulations, the internal heat source joins the simulation system in the form of kinetic energy. The Si film model consists of two zones, as shown in Fig. 1. Zone 1 is of the research interest. Zone 2 is Langevin heat bath to transfer the heat generated by the inner heat source in Zone 1 out of the system through Langevin damping force. Zone 1 is divided into 10 parts. Each part acts as a node of inner heat source. The atom corresponding to this node adds the heat derived from Eq. (1) to the node through speed acceleration. With the inner heat source of Zone 1 and Langevin heat bath of Zone 2, the net heat in the system is maintained to be in the range that film has no phase change.

In the present simulations, \( t_p = 10 \) ps, \( \delta \) is the length of Zone 1 [20].
OTHER PARAMETERS AND STEPS OF SIMULATION

In the heat transfer modeling, the silicon crystals of different thicknesses are assumed to be a semi-infinite heat conduction model. The laser heating end in Zone 1 of the model adopts fcc surface model. Langevin heat bath model is applied in Zone 2.

The simulation steps are divided into equilibrium stage and non-equilibrium stage. In the stage of equilibrium simulation, the silicon crystal films are assumed a same initial equilibrium temperature at 300 K. The silicon volume is determined according to the lattice constant of silicon crystal. Equilibrium simulation is NVT ensemble simulation.

In the stage of non-equilibrium simulation, speed calibration is carried out for atoms in zones of different thicknesses in the heat flow direction of silicon crystal in each step to simulate the inner heat source term.

In the course of simulation, the boundaries deviating from the heat flow direction are in periodic boundary condition while that in the heat flow direction is surface boundary condition. The boundary far away from the heat flow direction is phantom boundary condition of constant temperature heat flow. The time step used in simulation is 0.1 fs. Newton motion equation is in the format of leap-frog.

RESULTS AND DISCUSSION

The Si crystal films of different thicknesses are equally divided into same number of grids along the heat flow density direction. Because the total number of molecules of films of different thicknesses is the same, the number of molecules in each corresponding grid is the same for films of different thicknesses.

TEMPERATURE

Figure 2 shows the change of temperature with time along the heat-flux direction for the thickness of 32.3 nm. It demonstrates the existence of heat waves, though the calculated temperature curve concavity may lessen the heat wave appearance. In the stage of laser heating, the overall mean temperature of the film increases monotonically. From the change of temperature with time at different normal depths, it is seen that in the process of constant heat-flux laser heating, the change rate of temperature with time is different at different normal depths. The change is greater as the distance is closer to the laser heating surface.

The whole Si crystal film is divided into 20 grids and each grid makes temperature statistics for different times. The development of temperature with time at 65nm thicknesses of the Si crystal film is shown in Fig. 3.
STRAIN AND STRESS

The strain corresponds to the displacement absolute value of each grid of Si film of various thicknesses along the heat flux relative to the initial centroid and the interactive force on the boundary of each grid.

Figure 4 shows the change of the static pressure with time in the Si film 48.4 nm thick. The variation of the static pressure of films of other thicknesses is similar to Fig. 4. It is seen that the film static pressure changes periodically with time when laser energy is deposited in the semiconductor film. The period is calculated as 650 fs.

\[
y = y_0 + A \sin \left( \frac{\pi (x - x_c)}{\omega} \right)
\]

where \(y\) means vertical axis static pressure, \(x\) means horizontal axis time.
Figure 5 shows the detailed change of the static pressure of the Si film 75.9 nm thick at different locations along the heat flow direction with time.

![Pressure-time graphs for different depths](image)

**Figure 5 Development of Pressure at Diverse Depths in the Direction of Heat Flux in 75.9 nm-Thick Si Thin Film (The Red Curve is the Fitting Curve)**

Figure 6 shows the development of centroid displacement fitted according to Eq. (2) at different locations.

![Displacement-time graphs for different depths](image)

**Figure 6 Development of Centroid Displacement at Diverse Depths in the Direction of Heat Flux in 75.9 nm-Thick Si Thin Film (The Red Curve is the Fitting Curve)**

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Figure 7 examines the relationship of static pressure, centroid displacement and grid net heat flow, where statistics for grid net heat flow at each thickness of the Si semiconductor film is considered. The statistical method Green-Kubo [24] is the same method of making statistics for heat flow when calculating heat conductivity.

FIG. 6 DEVELOPMENT OF CENTROID DISPLACEMENT IN THE DIRECTION OF HEAT FLUX IN THE 75.9nm-THICK Si THIN FILM (THE RED CURVE IS THE REGRESSION CURVE)
Sine wave equation regression is applied in Fig. 5, Fig. 6 and Fig. 7 to analyze the relationship between the pressure change and each factor at different thicknesses. In Fig. 5, $A^*$ represents the amplitude of pressure term varying with time and marks the fluctuation of pressure statistics; $\omega$ means the frequency of the pressure term varying with time. $\omega$ takes on periodic change with depth, suggesting that the transfer of heat wave in the film makes pressure fluctuation frequency fluctuates along the depth. In Fig. 6, due to the statistical method, the vertical coordinates are coordinate in the calculation model without any practical meaning. However, values of $A^*$ and $\omega$ derived from regression function suggest the transmission of vibration wave in the direction of depth. The displacement vibration wave also displays periodicity with depth, which is related to the heat wave generated by the laser irradiation. It is known from Fig. 4 and Fig. 6 that the static pressure of the whole semiconductor film is closely related to the displacement at each thickness of the film.

It is known from Fig. 6 and Fig. 7 that among the physical quantities developing with time at different grids in the direction of heat flux, displacement of centroid in the direction of heat flux presents periodic changes when the laser heat flux is deposited in the semiconductor film. The overall mean temperature of the film in the present simulation system increases monotonically, while the mean pressure oscillates periodically and increases slowly. In the heating stage, the normal strain of crystals at different normal depths has same trend with the mean pressure of the whole film, namely periodic oscillation and slow increase. The oscillation period of all the centroid changes is 650 fs. The strain change at different normal depths and the net heat flux change in the course of heating show the same trend, suggesting that the strain change has a close relationship to the net heat flux under heating and that the strain increases when the net heat flux increases, and vice versa.

**CONCLUSIONS**

MD simulation is carried out to study the thermal phenomenon and mechanical phenomenon caused by picosecond laser heating of silicon semiconductor films. The temperature distribution, stress distribution, strain distribution, generation and transmission of stress wave are calculated. The results of the MD simulation show temperature fluctuation is caused by the coupling between the temperature and the strain rate, which shows the propagation velocity of temperature wave is the same as the stress wave. The following conclusion can be obtained:

1. In the stage of laser heating, the overall mean temperature of the films increases monotonically, but the mean pressure oscillates periodically and increases slowly.
Development of thermal waves for local temperatures is observed.

(2) In the heating stage, the normal strains of crystals at different normal depths have the same trend with the mean pressure of the whole film, namely periodic oscillation and slow increase. The oscillation period of all the centroid changes is found to be 650 fs. The strain change at different normal depths and the net heat flux change in the course of heating show the same trend, suggesting that the strain change has a close relationship with the net heat flux under heating and that the strain rises when the net heat flux increases, and vice versa.

NOMENCLATURE

\[ A \] area
\[ A^* \] amplitude of pressure term varying with time
\[ J \] single pulse power
\[ R \] reflectivity of semiconductor film surface
\[ S \] heat source
\[ t \] time
\[ x \] depth of thin films
\[ x_r \] regression parameters
\[ y \] vertical axis static pressure
\[ \delta \] the length of Zone
\[ \omega \] frequency of the pressure term varying with time.

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REFERENCES

