

Molecular-dynamics simulation of thermoelastic waves in a solid induced by a strong impulse energy

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A molecular-dynamics investigation of thermoelastic waves in a solid at various pressures and temperatures has been studied. The numerical experiments were performed on a two-dimensional $\langle 111 \rangle$ plane consisting of fcc lattice particles having the Lennard-Jones (12-6) interaction potentials. Three types of impulse energy, including thermal, kinetic, and superposition of thermal and kinetic energies, were employed to investigate the origins and characteristics of the generated waves. According to their propagating speeds, three waves, namely, W_1 , W_2 , and W_3 , were observed if a kinetic impulse energy was imposed. But only the W_1 and W_3 waves were detectable if the applied energy was thermal. The W_1 wave, accompanied by a strong compressive stress wave, is the first sound wave and caused by sudden expansion as the impulse energy applied. Due to coupling of thermal and elastic energies, it is a nonequilibrium thermoelastic wave. The W_2 wave was initiated by strong velocity disturbance in the longitudinal direction. If induced by a thermal impulse energy, the W_3 wave is the so-called second sound. The monotonically decreasing of the second sound speed with increasing temperature is also verified.

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I. INTRODUCTION

When energy is transported in a solid medium, it is accomplished through movements of its composed discrete atoms. Thus, the discreteness in atoms has to be taken into account in the discussion of lattice vibrations. However, when the wavelength is long enough the atomic nature can be disregarded and subcollective atoms exist that move in the same direction. Such vibrations are referred to as elastic waves. The interatomic coupling present in a solid allows many different vibrational modes that correspond to elastic waves with different frequency. Just as the energy of an electromagnetic wave is quantized, the energy of the elastic waves can be quantized as phonons and the solid medium can be treated as phonon gas. Thermal energy is transported by those phonons that traveling randomly in all directions. The elastic wave is an ideal mechanism that transfers energy without any dissipation. The heat transfer, however, has been regarded as a diffusionlike process and changes energy into a more disordered state. Of fundamental interest are the occurrence and separation of these two mechanisms, especially at the very beginning of imposed disturbance induced by an energy input.

Classically, the flow of heat in materials has been regarded to be proportional to the temperature gradient. The constant of the proportionality is the thermal conductivity. This is the Fourier's law of heat conduction. As a consequence of this law the speed of heat propagation is infinite. Peshkov¹ first reported his observation of heat propagating in liquid He II in a completely different manner, as a wave. This wavelike thermal behavior was then described as "second sound." Ever since Peshkov's experiment, a considerable effort has been devoted to the possible existence of this phenomenon in solids. Ackerman *et al.*² undertook

temperature-pulse experiments in samples of solid helium, and reported their observations of the propagation of temperature waves, the second sound, at low temperature. In their experiment of heat pulses in NaF, McNelly *et al.*³ found, other than the diffusive propagation of heat, an additional heat pulse existed in a very pure dielectric solid sodium fluoride NaF. Jackson and Walker^{4,5} immediately corroborated this existence and extended the range of observation of second-sound propagation in the same crystal grown independently in their lab. Except for He and pure NaF crystal, Narayanamurti and Dynes⁶ indicated the mechanism of heat pulse propagation in the bismuth has transferred from ballistic phonon through second sound to diffusive propagation. They indicated that the collective second-sound mode is a thermodynamic average of all different modes of the multiple polarization system. Thus, they believed the velocity of the second sound is independent of orientation.

In addition to experimental effort, numerous researchers theoretically studied the phenomena of the thermal waves. From the macroscopic point of view, Chester⁷ indicated that there is a critical frequency for the onset of thermal waves. He also predicted that speed of the second sound wave should be in the third of the square of the phonon velocity. A thermal wave (the second sound) is the propagation of a phonon density disturbance. Guyer and Krumhansl⁸ showed that the condition for the propagation of a temperature wave in a phonon gas is $\tau_N \ll \Omega^{-1} \ll \tau_R$, where τ_N and τ_R are the relaxation times for N -process scattering and momentum-loss scattering, respectively; Ω is the frequency of collision phonon gas. They also indicated the propagation speed of the second sound C can be determined by the way in a N -process approach as $C = v_s / \sqrt{3}$, where v_s is the speed of the first sound wave.⁹ But in the U -process region, Ranninger¹⁰ showed that the speed C should be modified by

$C/\sqrt{1+2\tau_N/\tau_U}$. A Comprehensive review of earlier works regarding the second sound waves was contributed by Ackerman and Guyer.¹¹ The prediction and detection of second sound was one of the great triumphs of the theory lattice vibration. In their articles about the heat waves, Joseph and Preziosi^{12,13} interpreted the concept of transmission of heat by waves. In addition, a nearly complete literature survey of heat waves until the eighties was given in chronological order in these articles. A more recently review on the wave theory in heat conduction was presented by Özisik and Tzou.¹⁴

The use of molecular-dynamics simulation to study the thermal and elastic waves was first seen in Tsai and MacDonald's papers.^{15,16} By applying a strong heat pulse at the boundary of a perfect semi-infinite bcc lattice of α iron, they found the disturbance propagated into the lattice as a combination of the first sound and second sound superimposed on a diffusive background. The first-sound waves, generated by the disturbance when the lattice boundary was rapidly heated or cooled, were stress-induced pulses. These pulses were not in thermal equilibrium and generated their own temperature waves, which contributed to the observed second-sound wave. The propagating speeds of the sound waves were discussed. Another molecular-dynamics study of heat pulse propagation with three-dimensional one-component lattice model was carried out by Schneider and Stoll.¹⁷ The second-sound regime was then located by the spectral density. Recently, Volz *et al.*^{18,19} studied the transient heat conduction and tested the validity of the generalized Fourier's law by both equilibrium and nonequilibrium molecular-dynamics experiments in a Lennard-Jones (12-6) solid argon. The presence of the first- and second-sound waves was confirmed in their simulations.

The present work is focused on the propagating energy waves on a two-dimensional $\langle 111 \rangle$ fcc lattice plane composed of the Lennard-Jones solid. At the very beginning of observation, a strong impulse energy was applied to the designated slender heated region which was located either near the lattice boundary or in the center of the computational domain. Evolutions of wave generation, propagating, and dissipation are studied. To examine the disposition of thermoelastic energy, energy transportation, and commencement of thermal waves in an idealized lattice, both ideal thermal and kinetic energy impulses are used. The origins of the thermal waves, wave forms, and wave speeds as well as their dependence on the types of the energy impulse will be studied and discussed systematically. Comparisons with results obtained by previous investigators are discussed. The dependence of wave speeds on temperature and pressure will also be presented.

II. PHYSICAL MODEL AND SIMULATION METHOD

In order to observe energy disposition and transportation in a solid lattice induced by a single energy impulse, we constructed a rectangular plane. This plane was composed of 32 080 solid atoms that were packed by the face-centered-cubic (fcc) arrangement. This designed $\langle 111 \rangle$ plane with dimensions that were 401 atomic layers in the z direction by 80

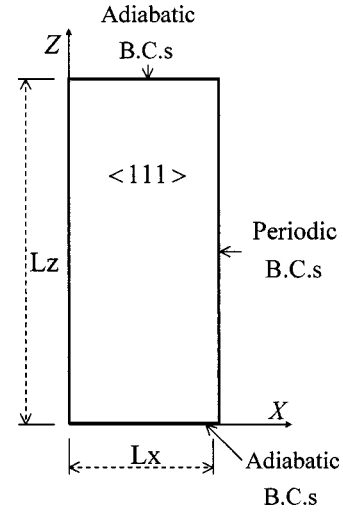


FIG. 1. Schematic diagram showing the dimensions, coordinates, direction and the physical boundary conditions in the computational domain.

atomic layers in the x direction. Two atomic layers, namely, the end layers, on each end side in the z direction were used for boundary conditions. The geometry of the computational model is shown in Fig. 1. The considered atomic system is described by Lennard-Jones interaction potentials of the form

$$u(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right], \quad (1)$$

where the subscript ij represents the connection between pair atoms i and j , r is the distance between the pair atoms to be considered, and the parameters ϵ and σ , providing the scale of energy and distance, represent the bonding energy and effective diameter of the pair atoms, respectively. For computational convenience, we select the energy scale ϵ , length scale σ , and the atomic mass scale m to nondimensionalize all subsequent expressions. The resulting units for time, temperature, velocity, force, and pressure are $t/\sigma\sqrt{m/\epsilon}$, $k_B T/\epsilon$, $v/\sqrt{\epsilon/m}$, $f/(\epsilon/\sigma)$, and $p/(\epsilon/\sigma^3)$, respectively. Here after the quantities we use are all in dimensionless.

The exact dimensions of the computational domain for cases of different pressures and temperatures were determined as the following: a random kinetic energy drawn from a Boltzmann distribution, subjected to the desired system temperature, was first assigned to each atom in the computational plane; the atomic spacing was then determined through adjusting the system's volume to ensure both conditions of the designated system temperature and pressure were reached.²⁰ Once the system was in equilibrium at the designated conditions, the volume was then fixed, and a microcanonical ensemble (NVE ensemble, number of molecules N , system volume V , and total energy E , are fixed) was simulated. The steady value of Boltzmann's H function²¹ and the order parameter²² were used to check if the initial thermal equilibrium was reached. In order to preserve waves propagating in the designated z direction, it was assumed that two end sides in the z direction were insulated and periodic boundary conditions were imposed on the other two sides for

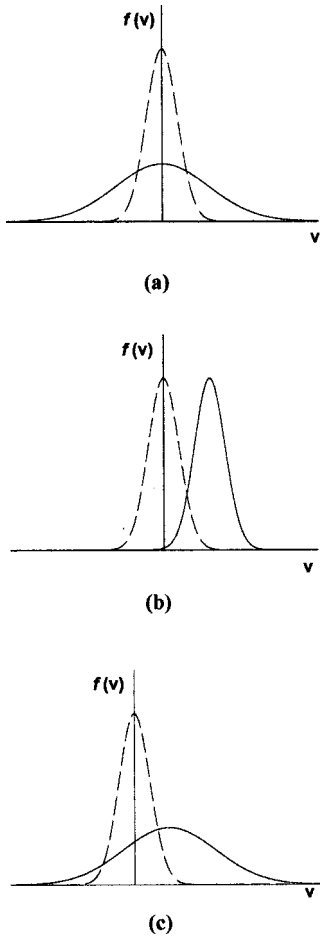


FIG. 2. Schematic diagram showing the velocity distribution functions in the heated region for the three types of impulse energy employed in this study. (a) Type I, (b) type II, and (c) type III. The dashed curves indicate the initial velocity distributions before the impulse energy being imposed and the solid curves represent the new distributions after energy impulse being applied.

getting rid of the boundary effects from the x direction. The thermally insulated boundary conditions were achieved by assuming that the mass of atoms in the end layers was 10^{10} times larger than atoms inside the end layers. This assumption made atoms in the end layers be motionless and resulted in the microscopically insulated.

Once the NVE system was in equilibrium at the designated temperature and pressure, an impulse energy was then suddenly imposed on the heated region to generate potential propagating energy waves. The heated region was made from the three atomic layers above the bottom end at $z=0$ or centered on $z=1/2L_z$. Three types of impulse energy, representing the thermal, kinetic, and superposition of thermal and kinetic energies, were used in this study. The velocity distributions for atoms in the heated region, after imposing these three types of impulse energy, are qualitatively shown in Fig. 2. For the purpose of discussion and comparison, the amount of energy imposed was adjusted to be about the same for each type of energy impulse. Commencement of our computations was at the moment of energy impulse applied. Newton's law of motion was numerically integrated for each

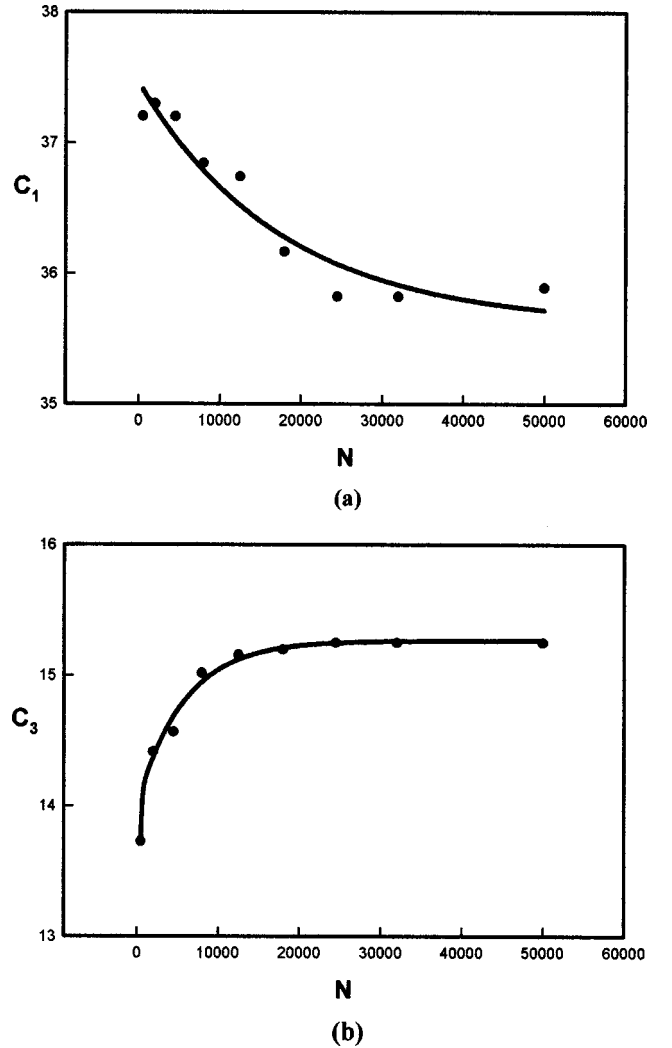


FIG. 3. Dependence of (a) the first sound speed and (b) the second sound speed on the number of atoms in the computational plane. The system pressure is 200 and temperature is 0.4.

atom using a fifth-order Gear's predictor-corrector algorithm, with time steps Δt at 1.9×10^{-3} , 6.0×10^{-4} , and 8.0×10^{-5} for cases of pressure at 10, 200, and 2000, respectively. One unit of time was about 2.09×10^{-12} sec.

The system pressure was set through the virial theorem²¹ as

$$P = \frac{1}{A} \left\langle NT - \sum_{i < j} r_{ij} \frac{du}{dr_{ij}} \right\rangle, \quad (2)$$

where A and N represent area and total number of atoms in the system, respectively. Calculation of local temperature in a two-dimensional space was given by

$$T = \frac{1}{2\mathcal{N}} \sum_i^{\mathcal{N}} (v_i - \bar{v})^2, \quad (3)$$

where $\mathcal{N}$ is the number of neighboring atoms that have been picked up to represent the local temperature, and its value was about 600 in this study. The local mean velocity in Eq. (3) was defined by

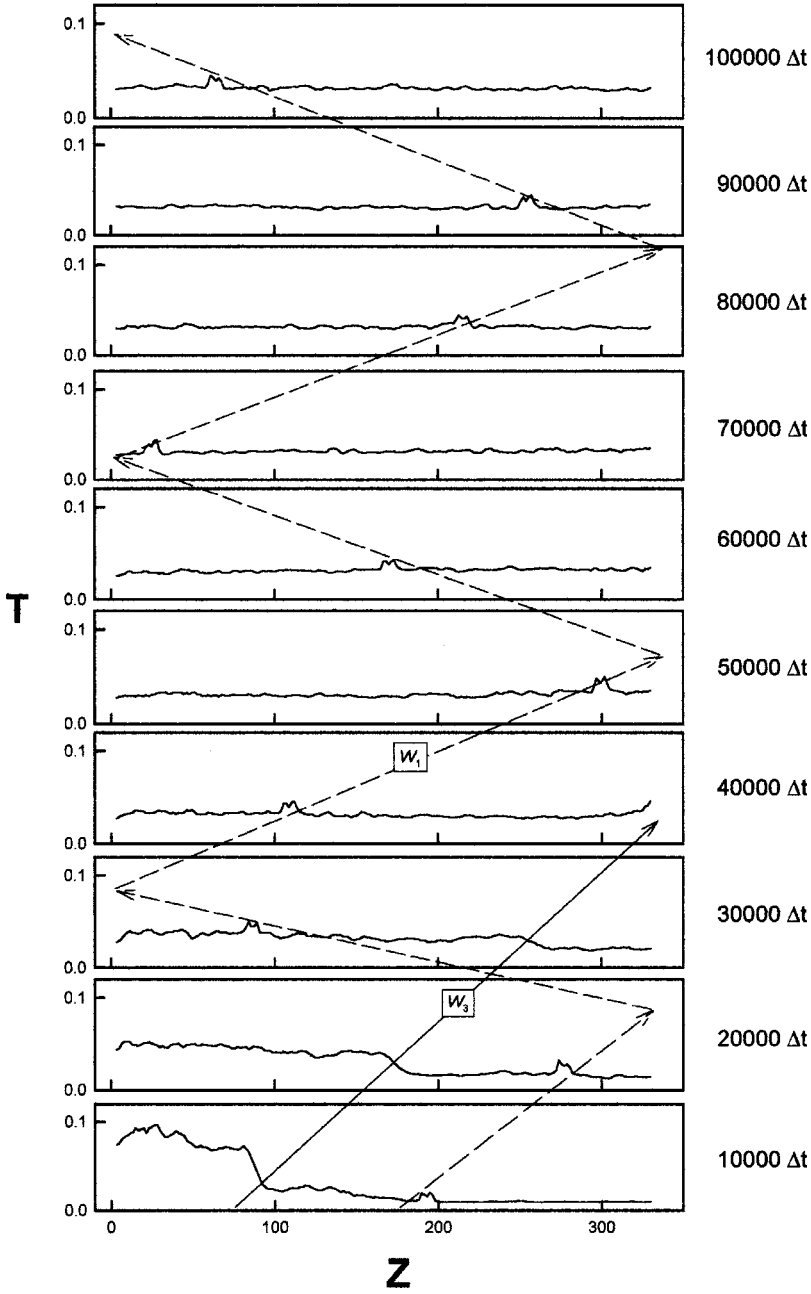


FIG. 4. Time history of the two thermal waves W_1 and W_3 , propagating in the computational plane after a thermal impulse energy was imposed on the heated region. The system pressure and temperature are 200 and 0.01, respectively.

$$\bar{v} = 1/N \sum_i^N v_i. \quad (4)$$

The local longitudinal stress was calculated according to²³

$$S = \frac{1}{A} \left\langle \mathcal{N}T + \sum_{i < j}^N r_{ij} \frac{du}{dr_{ij}} \right\rangle. \quad (5)$$

The simulated plane, once the impulse energy applied, was treated as an isolated system. Conservation of system's total energy was monitored every time step during the computation. The potentials of atom interactions were cut off at 2.5. In what succeeding discussion section, the local thermal equilibrium has been judged when the following two conditions are reached: the stress distribution is uniform and the

two components of the H function H_x and H_z based on velocities of v_x and v_z , defined by

$$H_x = \int_{-\infty}^{+\infty} f(v_x) \ln f(v_x) dv_x$$

$$H_z = \int_{-\infty}^{+\infty} f(v_z) \ln f(v_z) dv_z \quad (6)$$

are coincidental. The first condition means that no stress induced by any nonisotropic thermal effects while the second condition indicates the medium is close to thermally isotropic.

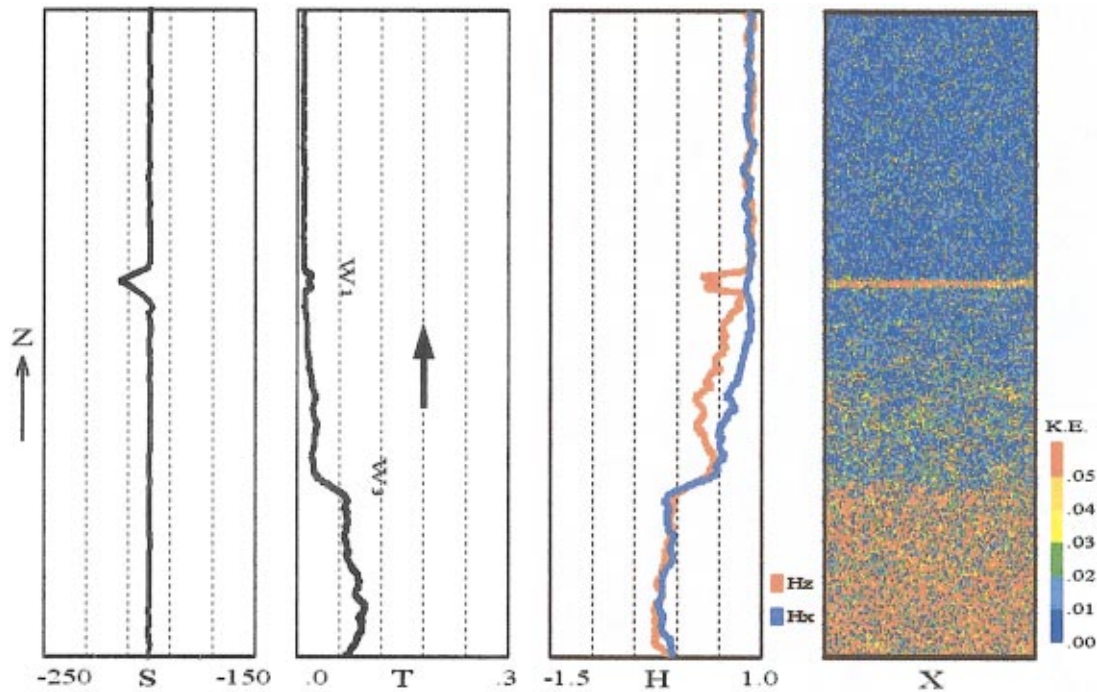


FIG. 5. (Color) Panels showing the distributions of stress, temperature, Boltzmann's H function, and the kinetic energy of each atom in the computational plane at $t=6.0$. The impulse energy is the type I, an ideal thermal impulse energy, and the system pressure and temperature are 200 and 0.01, respectively. In the panel for Boltzmann's H function, the blue and red curves represent H_x and H_z , respectively. Numerical values along the color index denote magnitudes of the kinetic energy.

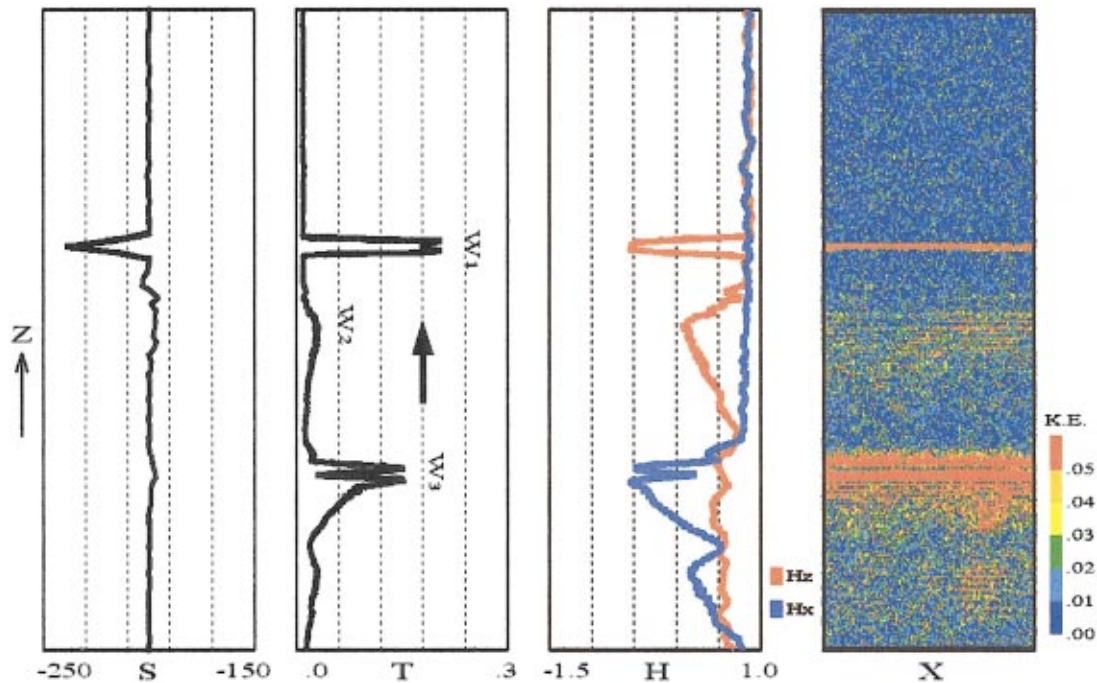


FIG. 6. (Color) Panels showing the distributions of stress, temperature, Boltzmann's H function, and the kinetic energy of each atom in the computational plane at $t=6.0$. The impulse energy is the type II, an ideal kinetic impulse energy, and the system pressure and temperature are 200 and 0.01, respectively. In the panel for Boltzmann's H function, the blue and red curves represent H_x and H_z , respectively. Numerical values along the color index denote magnitudes of the kinetic energy.

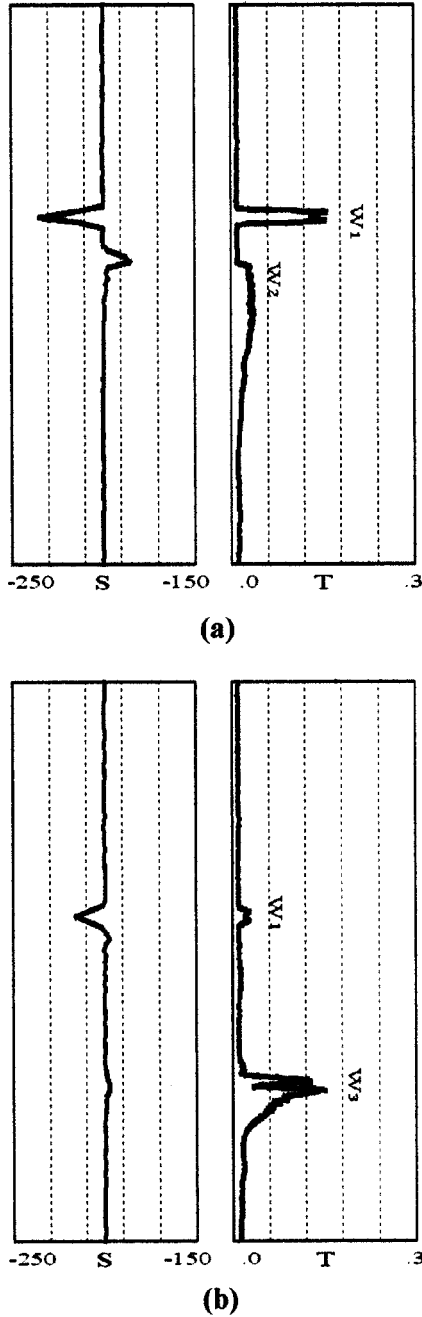


FIG. 7. Panels showing the distributions of the stress and temperature in the computational plane when a kinetic impulse energy is solely imposed in the heated region to change the velocity distribution of v_z for (a) and v_x for (b). The system pressure and temperature are 200 and 0.01, respectively.

III. RESULTS AND DISCUSSION

To understand the size effect on the computational results, cases with different sizes, atom numbers ranging from 2000 to 50 000, were employed in size-independence tests. Figure 3 presents the dependence of wave speeds of W_1 and W_3 upon the atom numbers when a thermal impulse energy was applied in the heated region. Results indicate that saturated wave speeds were reached if the number of atoms was larger than 25 000. Thus results presented in this study are based on

the size of 32 080 atoms. It is also noted that several three-dimensional calculations, with dimension of $8a \times 8a \times 100a$ (where a was the lattice constant) and total 25 600 atoms, were also performed for comparison. It was found that, except the wave speed, other fundamental phenomena of waves, such as patterns, types, as well as sequences of generation and propagation, were qualitatively similar to the two-dimensional results. Our three-dimensional simulations showed that the speed ratio of the first sound to the second sound C_1/C_3 was about $\sqrt{3}$, which is consistent with the theoretical predication.⁷ Without loss of fundamental characteristics, we adopt two-dimensional model in this study because it is more easily for observation and presentation of the wave phenomena as well as much more economic in computation time.

Initially atoms in the computational domain were thermally fluctuating and the system was equilibrium at the designated temperature and pressure. At the moment of an impulse energy applied, atoms in the heated region were instantaneously promoted to a new velocity distribution. Through the atomic interaction potential, this disturbance first affected mainly atoms near the heated region and then propagated in the z , longitudinal, direction, due to the periodic boundary conditions in the x , the transverse, direction. Figure 4 shows time history of the temperature distribution in the computational plane after imposing an impulse thermal energy. The system temperature and pressure were at 0.01 and 200, respectively. Two apparently separated temperature waves, namely respectively the W_1 and W_3 waves, were observed. The W_1 wave propagating with a higher speed hit the top end side around $22\,000\Delta t$ and reflected back due to the adiabatic boundary condition. The W_3 wave, which encountered the reflecting W_1 wave around $26\,000\Delta t$, has different wave form from the W_1 wave and moved with lower speed. After passing through each other, both waves proceeded without changing velocities. The W_3 wave was attenuated gradually and became undetectable after $40\,000\Delta t$. The W_1 wave, however, could sustain much longer until 1 800 000 computational time steps, about 2.3 ns. It is noted, as compared with the W_1 wave, that a perceptible background temperature increase was seen after the W_3 wave passed.

For telling the fundamental difference of these two waves, distributions of stress, temperature, the Boltzmann's H function and kinetic energy of atoms in the computational plane at a particular time of $10\,000\Delta t$ are shown in Fig. 5. The impulse energy and system's initial conditions were the same as those in Fig. 4. In order to separate contribution of energy carried by the elastic wave from the thermal energy, the local temperature, defined by Eq. (3), was used in this study. From the panel of stress distribution, it is found there is a stress wave moving the same speed with the W_1 wave, but no any apparent stress wave accompanying with the W_3 . From the distribution of the H function, it is shown that the value of H_z was deviated abruptly from its initial equilibrium value and separated from H_x when the W_1 wave had passed. H_z and H_x coincided with each other again and reached a new equilibrium value until the W_3 wave arrived. Since the impulse energy of type I was pure thermal, the occurrences of

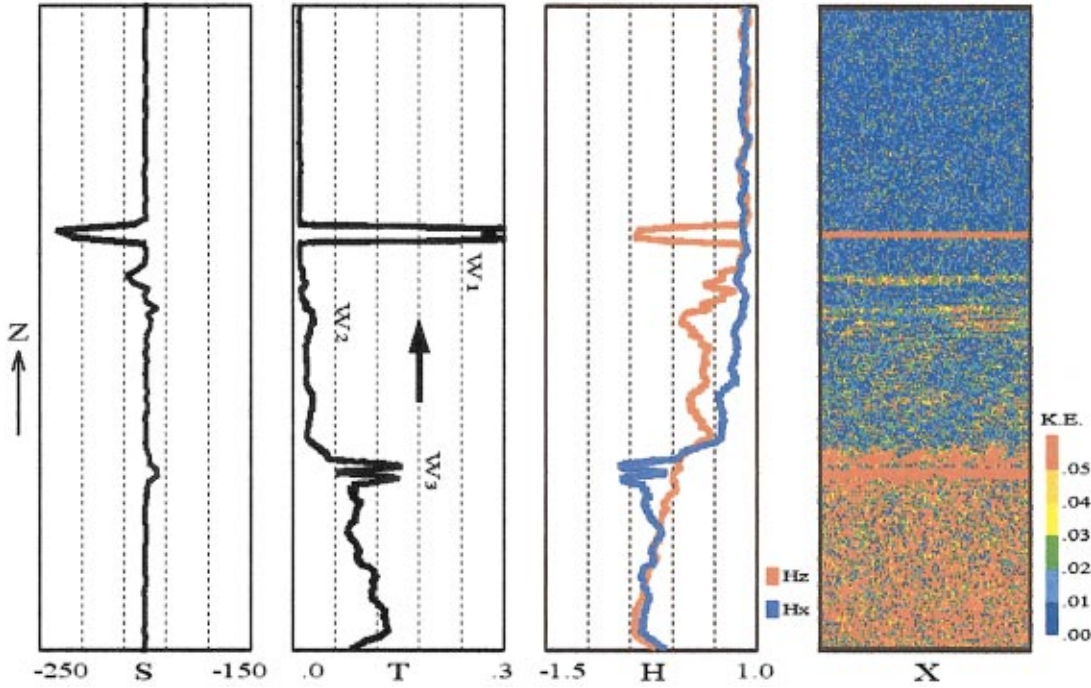


FIG. 8. (Color) Panels showing the distributions of stress, temperature, Boltzmann's H function, and the kinetic energy of each atom in the computational plane at $t=6.0$. The impulse energy is type III, and the system pressure and temperature are 200 and 0.01, respectively. In the panel for the Boltzmann's H function, the blue and red curves represent H_x and H_z , respectively. Numbers along the color index denote magnitudes of the kinetic energy.

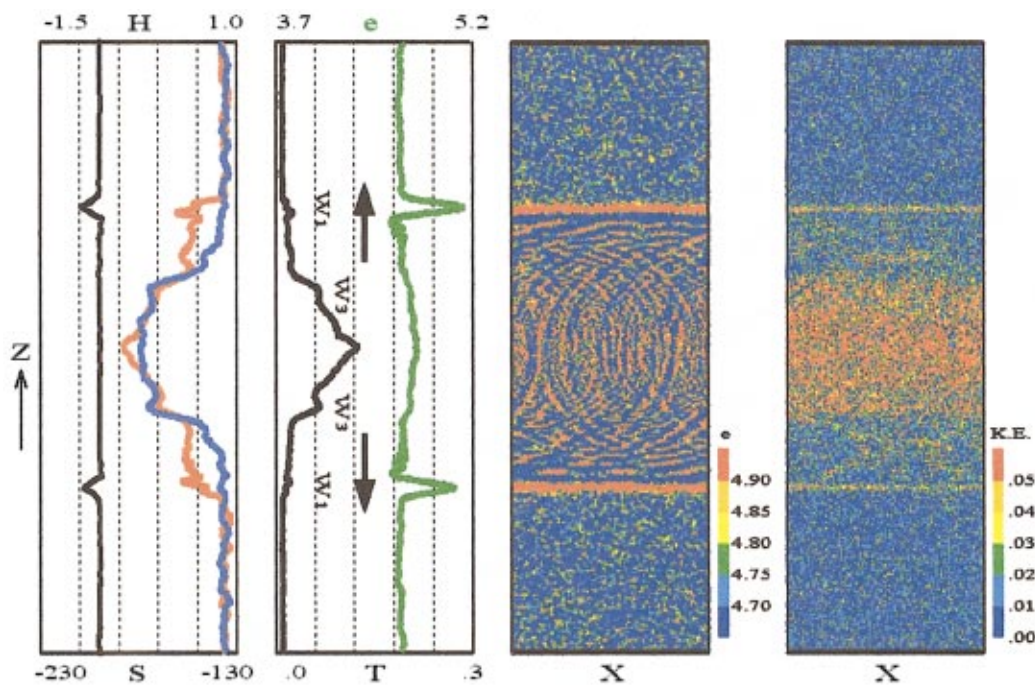
the W_1 wave and its accompanied compressive stress wave are believed from the disturbances in the longitudinal direction that was caused by the sudden expansion in the heated region at the moment of the impulse energy applied.

The panel for kinetic energy in Fig. 5 shows that there were two regions where atoms with higher energy were located. One was long and thin and centered on the W_1 wave. The other was broad and coincided with the region where the W_3 wave had passed. This difference can also be told from the temperature distribution panel. Temperature was promoted after the W_3 had passed and could not return back to the state that the wave had not arrived. This reveals that the energy associated with the W_3 wave was thermal. Due to the nature of a thermal energy, more isotropic and dissipated, the W_3 wave attenuates faster and becomes imperceptible from the background thermal noises earlier than the W_1 wave. Because of the perfect adiabatic boundary conditions imposed on both ends in the z direction, an ideal elastic wave once generated should persist forever in the current simulation system. The finite lifetime of the first wave indicated that the W_1 wave, even intrinsically more similar to an elastic wave, was still coupled with thermal energy.

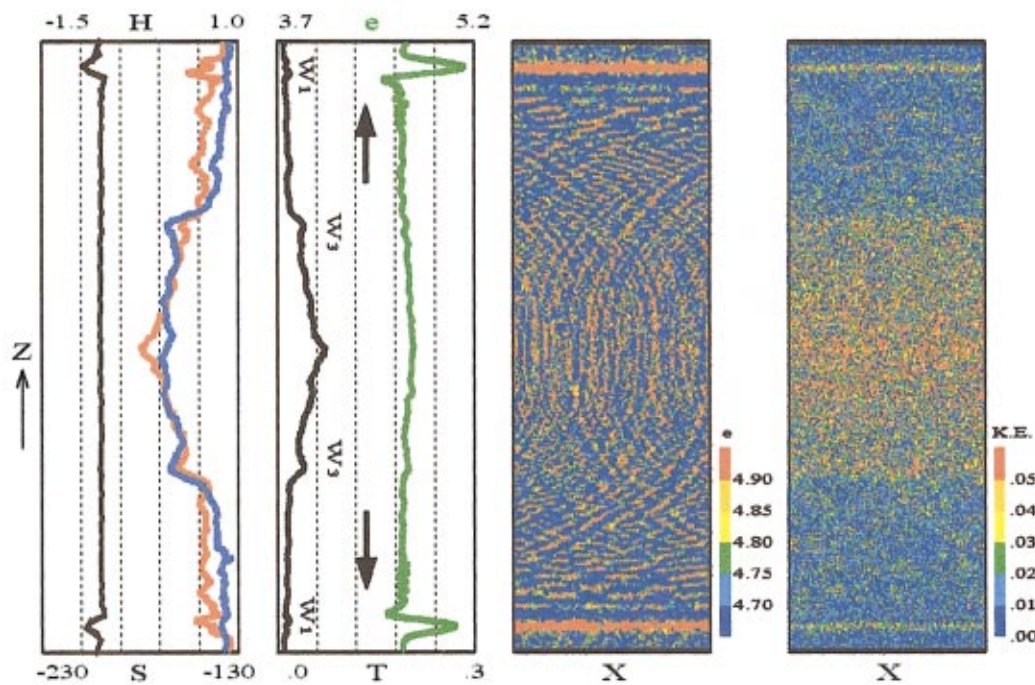
In Fig. 6 we present the distributions of the same variables as in Fig. 5, but the heated region was subjected to the type-II impulse energy. Three waves were detected from the panel of temperature distribution. The W_1 wave in Fig. 6 is similar to the W_1 wave in Fig. 5 because both were generated by the sudden expansion in the longitudinal direction at the moment of energy imposed. The propagating speed of the W_3 wave in Fig. 6 was the same as the W_3 wave in Fig. 5. In between the W_1 and W_3 waves, there was a new wave named

W_2 . To trace the origins of this wave, two cases, which changed the initial velocity distribution of v_x and v_z independently for atoms in the heated region, were studied. Figures 7(a) and 7(b) show distributions of stress and temperature in the computational plane when the type-II energy solely changed the initial velocity distributions of v_z and v_x , respectively. It was found there were two temperature waves in both Figs. 7(a) and 7(b). The first wave in both Figs. 7(a) and 7(b) is the W_1 wave. The second thermal wave in Fig. 7(a) W_2 propagated faster than the second thermal wave W_3 in Fig. 7(b). The occurrence of the W_2 wave was thus due to the longitudinal velocity disturbance. In other words, it was the energy separating from the thermoelastic energy propagating with the W_1 wave.

From the panel of the stress distribution in Fig. 7(a), it is interesting to note, except the compressive stress wave corresponding to the W_1 wave, there was a bumping wave, with relatively positive stress to the system stress, propagating with the W_2 wave. The analogous stress wave to the W_3 wave was not that apparent but still detectable in Fig. 7(b). Due to the relative positive value, the stress waves with the W_2 and W_3 are expansive waves. The strengths of the accompanying stress waves with the W_2 and W_3 waves were smaller than the strength of the accompanying stress wave with the W_1 wave. This indicates energy transported with the W_2 and W_3 is more close to thermal than the energy that transported with the W_1 . This can be further manifested by distribution of the H function in Fig. 6. Separations of H_z from H_x are shown around the three waves. The first two portions of departure were mainly caused by the strong dis-



(a)



(b)

FIG. 9. (Color) Panels showing the distributions of stress, temperature, Boltzmann's H function, and, total and kinetic energies of each atom in the computational plane at $t=2.4$ for (a) and $t=4.8$ for (b), respectively. The impulse energy is type III, and the system pressure and temperature are 200 and 0.01, respectively. Numbers along the color index denote magnitudes of energy.

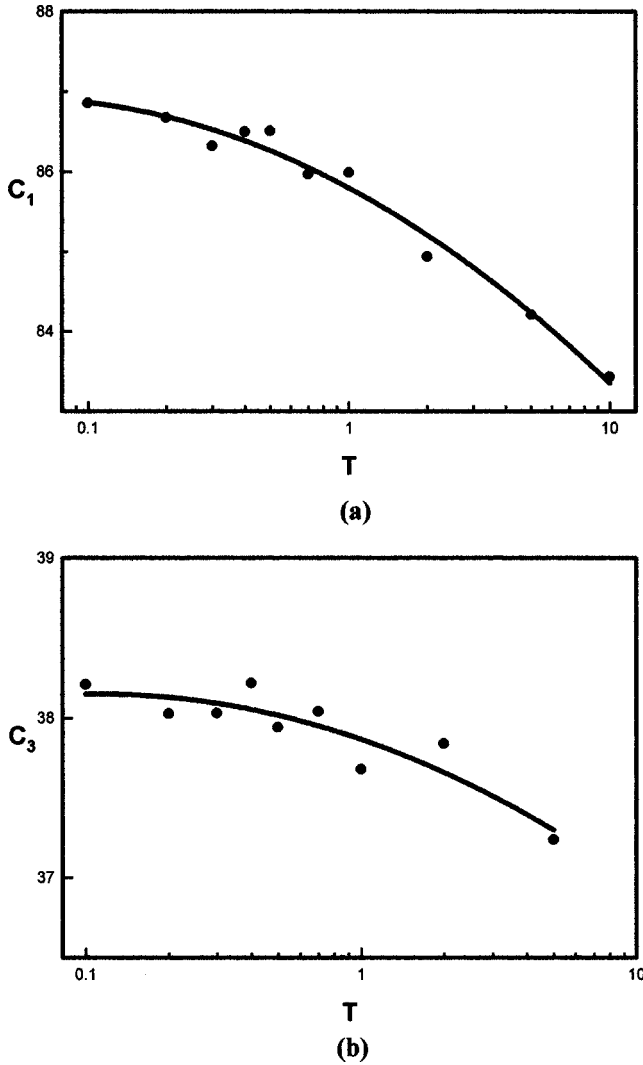


FIG. 10. Dependence of (a) the first sound speed and (b) the second sound speed on the temperature in the computational plane. The system pressure is 2000.

turbances in the longitudinal direction while the third portion of departure was due to the transverse velocity disturbances. These evidences conclude the energy carried by the first thermoelastic wave is mainly the elastic energy. Thus, a strong compressive stress wave is accompanied with it and it is more far from local thermal equilibrium. These three thermal waves decayed gradually as time evolved. The W_2 wave first became indistinguishable from the background, followed the W_3 wave, and finally the W_1 wave. The lifetime of the W_1 wave was about 500 ns, which was much longer than the lifetime of the same W_1 wave when induced by the pure, thermal impulse energy in Fig. 5.

In Fig. 5, the W_2 wave was invisible. To reexamine this fact, we applied a pure thermal impulse energy to promote solely the velocity distribution of v_z and v_x for atoms in the heated region. Results showed that only the W_1 and W_3 were detectable and no any visible the W_2 wave. The W_3 wave induced by an ideal thermal impulse energy was thermal equilibrium, which is different from the thermally nonequilibrium, thermoelastic, W_3 wave induced an ideal kinetic im-

pulse energy. That is why the wave forms of the W_3 in Fig. 5 and Fig. 6 are different. Figure 8 shows distributions of the same four quantities when the impulse energy was the superposition of thermal and kinetic, the type III. It is interesting to note the results shown in Fig. 8 are simply close to the superposition of Figs. 5 and 6. If C_1 , C_2 , and C_3 represent the wave speeds of W_1 , W_2 , and W_3 , respectively. Our computational results show the ratio of C_1 to C_2 was from 1.1 to 1.2, and the ratio of C_1 to C_3 was about 2.0 to 2.3. These results are close to wave speeds obtained from theoretical models and computational results.^{15,19}

From the wave form of temperature waves, especially when the imposed energy including kinetic energy shown in Figs. 6 and Fig. 8, double peaks, similar to an “M,” are observed. This is due to the heated region was at $z=0$ on which an adiabatic boundary condition was imposed. To get rid of the effect of adiabatic boundary conditions on the wave phenomena at early stage after imposing an energy impulse, cases with the heated region moved to the center plane at $z=\frac{1}{2}L_z$ were also studied. Figures 9(a) and 9(b) present distributions of several quantities at two times 2.4 and 4.8 when a type I impulse energy was imposed. From the left to the right, the first panel shows stress and H function and the second panel is for temperature and total energy. The total and kinetic energy of each individual atom are presented in the third panel and fourth panel, respectively. Total energy of each atom is given as $e_i = \frac{1}{2}v_i^2 + \frac{1}{2}\sum_{j(\neq i)}u(r_{ij})$. It was found that the W_1 wave was generated first, then the W_3 wave, and both waves were separated into two similar waves that propagated in the opposite directions. From the third panel, it is found that atoms with the highest level of energy are concentrated on the two W_1 waves. For those atoms with relatively higher energy and contained by the two W_1 waves distribute likely along the ripples formed by interference of waves. Because the imposed energy is pure thermal, the interference of waves are from a series of point sources, initially located in the slender heated region at $z=1/2L_z$, that propagated the imposed disturbances radially and isotropically. From the fourth panel, the higher kinetic energy atoms are, however, contained mainly by the wave fronts of the two W_3 waves and distribute more randomly. The main advantage of putting the heat region close to the adiabatic boundary condition at $z=0$ is the spatial enlargement of the wave form that helps the observation of wave phenomena.

Except for the wave forms, wave speeds and the existing time of wave, the characteristics of the waves at system pressures of 200 and 2000 were similar. When the system pressure was reduced to 10, our computations showed only the W_1 wave was detectable when the imposed energy was pure thermal. The disappearance of the second-sound wave was due to occurrence of local melting in the heated region. In a solid the principal generating mechanism for the second sound is the lattice vibration. For the existence of a liquid region, there is an alternative mechanism of energy transfer—motion of atoms. The motion of atoms weakens the lattice vibration, and results in disappearance of the second-sound wave. From the macroscopic viewpoint, part of the imposed energy was stored in atomic potential among the liquid atoms, the so-called melting energy, before being

transported away through the second thermal wave. The influence of the local melting on the W_1 wave is relatively smaller because this wave is generated mainly due to the suddenly expansion in the heated region, and once generated, it propagates away before the melting occurs. It is the thermal fluctuating energy that destroys the bonding energy among atoms and results in reducing in lattice vibrations.

Figure 10 shows the dependence of the wave speeds C_1 and C_3 on temperature at the system pressure of 2000. Figure 10(a) indicates that C_1 decreases monotonously with temperature. Because the nature of the W_1 wave is more similar to an elastic wave, the density has the principal responsibility for the wave speed. Higher density implies shorter distance between pair atoms, which, according to Eq. (1), results in stronger atomic interactions. Thus for the Lennard-Jones system, the first sound speed is positive proportion to the density. The declining of the C_1 with temperature is due to the decreasing in density as the temperature increases. The variation of the C_3 with temperature is presented in Fig. 10(b). In analogy to the second sound to the phonon gas, the phenomenon of the second sound is the collective mode representing a propagating energy fluctuation in the hydrodynamic regime. Previous theoretical and experimental studies^{3,22} also showed that the speed of the second sound decreases monotonically as the temperature increases. Our simulation results verify this trend.

IV. CONCLUSIONS

The thermoelastic waves propagating on the $\langle 111 \rangle$ plane in a solid produced by imposing a strong impulse energy has been studied by molecular dynamics simulation. The solid is assumed to be composed of the fcc lattice particles having the Lennard-Jones (12-6) interaction potentials. Three types of impulse energy, including the thermal energy, the ideal kinetic energy, and superposition of the thermal and kinetic energies are employed to investigate origins and characteristics of the propagating waves. The system pressure is set from $O(10)$ to $O(10^3)$ and the system temperature runs from

very low to the margin of liquid phase at the corresponding pressure. Computational results are obtained by executing the law of motion for 32 080 atoms constituting the computational plane. Time history of the propagating thermoelastic waves and the distributions of the kinetic energy, temperature, Boltzmann's H function as well as the stress in the computational plane are presented and discussed. Dependences of the wave speeds upon pressure and temperature are also given. The results of this investigation show the following.

(1) Three thermoelastic waves, namely, W_1 , W_2 , and W_3 , are induced by applying an ideal kinetic impulse energy. But only the W_1 and W_3 are detectable if the impulse energy is an ideal thermal.

(2) The W_1 wave, caused by suddenly expansion as the impulse energy applied, is the first-sound wave. Due to intercoupling of thermal and elastic energies, it is a nonequilibrium thermoelastic wave, but intrinsically more similar to an elastic wave.

(3) The occurrence of the W_2 wave is due to the strong, longitudinal velocity disturbances. It is invisible if the impulse energy is an ideal thermal.

(4) If induced by an ideal thermal impulse energy, the W_3 wave is the so-called second-sound wave. However, the W_3 wave is another nonequilibrium thermoelastic wave if it is induced by a kinetic impulse energy.

(5) A compressive stress wave accompanies the W_1 wave to move while the thermoelastic waves of W_2 and W_3 are accompanied by expansive stress waves. For a second-sound wave, it is stress free.

(6) The monotonically decreasing of the second-sound speed with increasing temperature is verified by molecular dynamics simulation.

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