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Nonequilibrium gas flow in the transition regime: A molecular-dynamics study

D. K. Bhattacharya
IBM Corporation, Dept. 48B/MS 428, Neighborhood Road, Kingston, New York 12401

G. C. Lie*
Central Research and Development, Dow Corning Corporation, Midland, Michigan 48686
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The microscopic dynamics of nonequilibrium gas flows in the transition regime (Knudsen number ~ 1) is studied using novel molecular-dynamic (MD) simulations. The Knudsen number dependence of the shear viscosity, temperature jump, slip length, and the entropy production is investigated. It is shown that the assumption of local equilibrium breaks down in supersonic flows. A good agreement of the MD simulation results with available experiments and other theoretical studies is found.

I. INTRODUCTION

Experiments conducted by Somoluchowski[1] and Knudsen[2] at the turn of the century revealed that a class of nonequilibrium flow and heat transfer problems, in which the mean free path of gas particles is comparable with the geometric dimension of the flow system, cannot be described by continuum hydrodynamics. These flows, characterized by the Knudsen number $(K_n) \sim 1$, exhibit a velocity and temperature slip, and are encountered in diverse fields such as high-altitude aerodynamics, isotope separation techniques, aerosol dynamics, vacuum-pump operation, energy transfer in molecular collisions, and the attainment of millikelvin temperatures by flow cooling.[3] Despite numerous studies, the microscopic and macroscopic description of the transition regime flow phenomena remains an intriguing problem, requiring the extension of the methods of the kinetic theory of dilute gas and nonequilibrium thermodynamics.[4]

The search for a complete theory of transition regime gas flows has progressed along three different paths. The first approach, advanced by Grad, concerns itself with a new method for solving the Boltzmann equation. In his 13-moment method solution of the Boltzmann equation, Grad argues that the nonequilibrium transport phenomena of gas flows in the transition regime can be described by a set of generalized hydrodynamic equations, where the well-known Navier-Stokes and Fourier laws are replaced by a new set of constitutive equations incorporating the nonlocal heat and stress relaxation phenomena in addition to the dissipative effects arising from spatial nonuniformities of field quantities.[5] The full potential of the neoclassical hydrodynamics embedded in the 13-moment method has, however, not been realized, firstly because of the lack of appropriate boundary conditions needed to solve the heat and stress evolution equations, and secondly due to the recognition that unlike the Navier-Stokes equations, these new transport equations do not admit solutions for all flow parameters.[6] For example, in the particular case of a one-dimensional shock wave in a monoatomic gas, although the Navier-Stokes equations would admit a solution for all values of Mach number, the hydrodynamic theory based on Grad's equations would break down at a critical Mach number of ~ 1.65. Recently, in the framework of extended irreversible thermodynamics,[7] Grad's theory has been generalized to the nonlinear domain.[8] This theory predicts that in the transition regime the transport coefficients depend on the heat flux and shear stress which can give rise to sharp boundary layer at the wall. A second approach to the transition regime flow is due to Dorfmann and van Beijeren[4] and is based on the extended Boltzmann equation wherein the collision dynamics of gas-surface interaction is explicitly incorporated. In a somewhat different third approach, Wood has applied the mean-free-path theory as initiated by Maxwell and obtained an expression for the heat flux vector and pressure tensor valid for all values of the Knudsen number.[9] The merit of the mean-free-path theory is that it relies on the actual physical mechanism of transport and does not require a kinetic equation for the velocity distribution function. However, the conclusions derived in the framework of Wood's theory are likely to be rigorously valid only for the hard-sphere molecules for which the concept of a mean free path is unambiguously defined.

In the absence of a well-accepted analytical method for solving the Boltzmann equation for the transition regime gas flows, the current approach is to solve the equation or its approximations numerically.[10] The most widely used algorithm is the one proposed by Bird.[11] In his direct-simulation Monte Carlo (DSMC) method, Bird simulates the physics of the transport process occurring in a rarefied hard-sphere gas by uncoupling molecular motions and intermolecular collisions over small time intervals and cell sizes. The DSMC algorithm of Bird is based on the Kac master equation and is computationally efficient. A slightly different DSMC method based on the Boltzmann equation has been proposed by Nanbu.[12] Meiburg has shown that the DSMC method does not conserve the angular momentum and hence may not ac-

curately describe a high-vorticity flow problem.[13] However, Nanbu, Watanabe, and Igarashi argued that if cell sizes are sufficiently small, then the angular momentum is almost conserved.[14] Moreover, since the vorticity is only related to the linear momentum which is conserved in the DSMC method, the method should be applicable for high-vorticity problems.[14]

The present paper outlines a new approach for studying the microscopic dynamics of nonequilibrium heat and momentum transport in the transition regime ($K_n \sim 1$). Using the molecular dynamics (MD) method,[15] we explicitly solve the dynamical equations of gas particles confined between two thermal walls. Two problems are considered. First we study the heat transfer in argon gas between parallel plates and compare our results with experiments and the analytical solutions of the linearized Boltzmann equation. Then we analyze the three-dimensional channel flow problem and report some new results on the velocity slip, and the distortion of the nonequilibrium velocity distribution function in a supersonic flow. The density variation of the shear viscosity in the channel flow is also examined and compared with the ones obtained using the DSMC method. Our MD computations indicate that the Maxwell model of slip phenomena breaks down in the transition regime and that the assumption of local equilibrium, which is central to the classical theory of irreversible thermodynamics, is not valid in supersonic transition regime flows. In Section II we outline the computational algorithm of our simulation. Section III discusses, and compares with other available experimental and theoretical data, results of the simulations of flow and heat transfer in a three-dimensional channel. Section IV is for final conclusions.

II. COMPUTATIONAL ALGORITHM

In our simulation, the dynamic evolution of fluid particles is studied using the molecular-dynamic method. A few thousand fluid particles are enclosed in a three-dimensional channel. The fluid particles interact via a truncated Lennard-Jones potential:[16]

$$V(r)=\begin{cases} 4\epsilon\left[\left[\frac{r}{\sigma}\right]^{-12}-\left[\frac{r}{\sigma}\right]^{-6}+\frac{1}{4}\right], & \forall r \le r_c = 2^{1/6}\sigma \\ 0, & \forall r > r_c \ . \end{cases} \tag{1}$$

This potential is short ranged; i.e., there is no interaction for any atomic pair that is more than r_c apart. The potential parameters are chosen to represent the argon gas. Thus we set $\sigma = 3.45$ Å and $\epsilon = 119.8 k_B$, where k_B is the Boltzmann constant. Newton's equations of motion are solved by a sixth-order Gear's predictor-corrector method.[17,18] Thus the evolution of the dynamical system is studied by analyzing the vector $\mathbf{r}_0$ which represents a set of particle positions and its five successive time derivatives.[18] Thermal walls placed in the direction perpendicular to the x axis act as heat reservoirs. When a particle hits one of the two walls, it gets thermalized and the particle is returned to the system immediately with a velocity chosen randomly from the Maxwell-Boltzmann distribution at the wall temperature T_w:

$$V_x = \sqrt{-2k_B T_w \ln(\xi_1)/m} \ , \tag{2}$$

$$V_y = \sqrt{-2k_B T_w \ln(\xi_2)/m}\ \sin\xi_3 \ , \tag{3}$$

$$V_z = \sqrt{-2k_B T_w \ln(\xi_2)/m}\ \cos\xi_3 \ , \tag{4}$$

where ξ_1, ξ_2, ξ_3 are random numbers between 0 and 1, and m the mass of the particle. The stochastic boundary conditions used here are analogs to the one proposed by Tenenbaum, Cicotti, and Gallico.[19] Periodic boundary conditions are employed in the y and z directions. The time step of the simulation was 10^{-14}sec. To maintain a nonequilibrium flow, an acceleration field of strength g is applied in the y direction (i.e., every particle is subject to a constant force mg in the y direction). By manipulating the strength of the acceleration field different flow regimes can be realized in the channel. An imposed acceleration field is analogous to a gravitational field. However, to establish an ordered flow profile in a channel of microscopic dimension the magnitude of the acceleration is orders of magnitude larger than the gravitational field. A limited number of experiments were also performed in the plane Couette flow geometry wherein the flow can be induced in the system by moving the upper plate. We have checked that various predictions of our simulations did not depend on the specific way that the flow was induced, but depended solely on the parameters such as the Knudsen number and the Mach number characterizing the flow system.

The calculation of the interparticle interaction is the most time-consuming part of any molecular-dynamics algorithm. Since the interaction potential used in our simulation is short ranged, a "link-cell" method[18] was used for calculating the interaction forces among the fluid particles. In this approach, before starting the calculation of the interaction forces, we divide the simulation system into small cells such that each side of the cell is greater than the cutoff distance r_c. Each atom is assigned to a cell and is linked to two atoms in the same cell through pointers. That is, cell i first points to atom k, then points to the next atom in the same cell, m, which in turn points to the other atom n,....., etc. The calculation of the interaction forces proceeds in the following ways.

(1) We choose a cell and pick up the particle appearing in the headlist (which shows the first particle in the given cell). The interaction of this particle with all other particles occupying the same cell is calculated utilizing the linked list.

(2) The interaction of the chosen particle with the particles residing in the adjacent cells is calculated. A careful application of Newton's third law reduces the computations of the interaction force among the particles. However, this necessitates searching the adjacent cells in a particular order.

(3) After all possible interactions of the chosen particle (from a chosen cell) have been calculated, we move to the next particle (using a linked list) and then repeat the pre-

vious two steps. This process is repeated until all the particles in the chosen cells are exhausted.

(4) We now move to the next cell and repeat the procedure until all cells in the simulation system have been considered.

In the "link-cell" approach, the computational and the memory allocation requirements for evaluating the interaction forces scale roughly as N. This is very useful, and may become necessary, whenever the number of simulated particles is sufficiently large.

To make a connection with the continuum hydrodynamics and experiments we divide the simulation system into three-dimensional boxes and calculate the average values of the velocity, number density of particles, and the kinetic energy of fluid in each box at each time step. These average quantities are collected for a few thousand time steps, then new statistics are obtained by time-averaging the dynamical information contained in each box. In the transition regime, the dissipative effects become weaker as the Knudsen number is increased. Therefore, in order to correctly compute the steady-state flow properties, the simulations in some cases were conducted for one million time steps. The reported "macroscopic" velocities, densities, and temperatures were all collected by dividing the simulation box into cells of size 50:1:1 and averaging over 20 000 time steps. An initial stage of relaxation was first carried out for about 30 000 time steps and the statistics were collected for the next 700 000 time steps to obtain a total of 35 samples of velocities and densities. These samples are used to make sure that steady state has indeed been reached and to calculate the standard deviations of the reported macroscopic properties.

To realize such a long simulation as required by infrequent collisions of a dilute gas system, we have used the parallel processing facilities available in an IBM 3090/400 computer. The structure of the parallel algorithm is as follow. If the number of available processors in the system is k, then in the predictor (or corrector) step the total number of molecules is divided into k different segments and each processor is assigned the computation of a given segment. In this step there is no overlap between the computations undertaken by the processors. For calculating the interaction force between the fluid particles, the total volume of the fluid system is divided into k parts, and each processor is assigned the computation of the interaction forces of the fluid particles occupying the volume segment assigned to the processor. Since the fluid particles in the boundary of the chosen volume segment can also interact with the fluid particles which belong to the other processor, a certain amount of the information has to be exchanged between the processors. Using four processors it was possible to speed up the computation by 3.6 times. Here we might add that the molecular-dynamics algorithm, as the one discussed here, can also be efficiently implemented in a massively parallel computer system, using special hardware.[20]

Preliminary results on the molecular-dynamic simulation of nonequilibrium flow and heat transfer in a very dilute gas have been reported earlier in a letter.[21] These simulations examined the flow behavior in a two-dimensional geometry, in the slip flow regime ($K_n \sim 0.1$). The consistency of the molecular-dynamics results with the experiments of Kundt and Warburg and the solution of the linearized Boltzmann equation was given. The present paper investigates the three-dimensional nonequilibrium flow in the transition regime ($K_n \sim 1$). Several new results such as the deformation of the nonequilibrium velocity distribution function in supersonic flows, temperature rise at the wall due to viscous heating, and the consistency of the MD simulation and the DSMC method are discussed.

III. RESULTS AND DISCUSSION

In the first simulation, designed to understand the heat transfer process in a very dilute gas, the dynamics of 8000 particles was studied. The thermal walls were 564 Å apart and kept at 288 and 368 K, respectively. The Knudsen number

$$K_n = \frac{\lambda}{L} = \frac{1}{(\sqrt{2}\pi n \sigma^2 L)} , \tag{5}$$

where λ is the mean free path of the gas particle as given by simple kinetic theory, n the number density, σ the Lennard-Jones parameter signifying the particle diameter, and L the length of the simulation cube, for the flow system was 0.758. The statistical error in the calculated density profile is less than 3%. Figure 1 compares the density profile obtained through the MD approach with the moment method solution of the linearized Boltzmann equation by Gross and Ziering[22] and the experimental measurements by Tegan and Springer.[23] Even though the Knudsen number in the MD simulation and the experiment is the same, it should be noted that they are achieved in two different ways: In the simulation the gas is *dilute* and the flow system has a microscopic dimension (5.64×10^{-6} cm), whereas in the experiment the size of

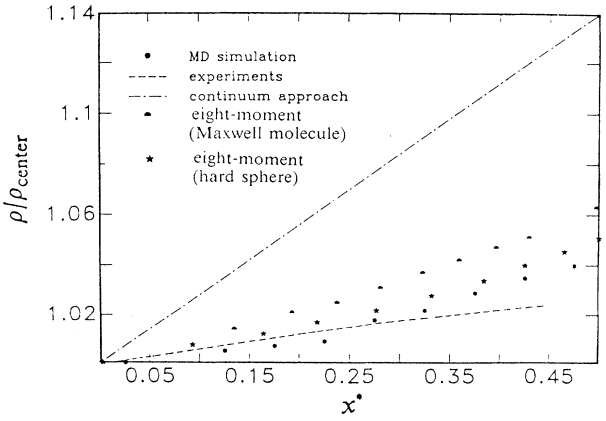

FIG. 1. Comparison of the different density profiles for fluids confined between two parallel thermal walls at $K_n = 0.758$. x^* is a scaled coordinate across the system ($\equiv x/L$) with the origin at the center of the system.

the flow system has a macroscopic dimension (0.13 cm) and the gas density is in the *rarefied* regime. The good agreement among the simulation, the experimental, and the theoretical results indicates that the underlying dynamics of the nonequilibrium heat transport phenomena studied in the former two methods is the same as the one embodied in the Boltzmann equation.

We now turn our attention to analyzing the velocity slip in the channel flow. We have studied seven different flow configurations, as shown in Table I. An acceleration field of strength $g=1\times10^{14}$ cm/sec^2 was applied in the $-y$ direction which produces subsonic flows (Mach number varies from 0.5 to 0.99). The Knudsen numbers characterizing these flows are in the transition regime. The thermal walls were kept at 300 K. The velocity slip at the wall increases with an increasing Knudsen number. However, at all levels of the Knudsen number, the measured velocity profiles agree remarably well with the solution of the Navier-Stokes equation with the velocity slip condition. According to Maxwell's theory of slip phenomena,[24] for a small Knudsen number, the dimensionless slip length,[21]

$$l_s=\frac{v_w}{L(dv/dx)_w} \tag{6}$$

is proportional to the Knudsen number. Here v_w is the slip velocity at the wall, and is determined by calculating the velocity of the fluid in the statistical cell adjacent to the wall. Our earlier simulation had confirmed that Maxwell theory is indeed true as long as the Knudsen number is in the slip flow regime ($K_n<0.05$).[21] However, as is shown in Fig. 2, in the transition regime the slip length scales as the log of K_n. This result also indicates that the recently proposed velocity slip model by Coron,[25] using the Chapman-Enskog solution, would break down in the transition regime.

To analyze the effect of viscous heating on the velocity slip at $K_n=2.79$, we increased the strength of the acceleration field and studied flows at Mach number (M) of 1.68, 2.76, and 4.05. It was found that the velocity slip is proportional to the square root of the average gas temperature, while the velocity difference between the center and the wall scales as the acceleration field, as predicted by the Navier-Stokes equations.

In the framework of linear irreversible thermodynamics,[26,27] the linear transport equations are derived on the assumption of local equilibrium. The assumption of local equilibrium implies that even though the dissipative system is globally in a nonequilibrium state, the irreversible system can be partitioned into small cells which remain in a state of thermodynamic equilibrium such that the nonequilibrium entropy change is governed by the Gibbs equation. Since except for a *small* region very close to the wall, the temperatures are almost constant across the channel, we might anticipate that the velocity distribution is sufficiently close to the local Maxwellian distribution in our channel flows. This is indeed the case for subsonic flows as shown in Fig. 3. However in supersonic flows, also shown in Fig. 3, the presence of a high shear significantly distorts the shape of the velocity distribution

TABLE I. Parameters used in the molecular-dynamics simulation of three-dimensional channel flow (the total number of particles is 4096).

Run number	Length of box (Å)	K_n	λ/σ
1	208.44	0.20	12.24
2	300.63	0.42	37.08
3	392.31	0.72	82.95
4	459.53	1.00	134.95
5	559.66	1.48	243.25
6	647.69	1.98	376.63
7	767.92	2.79	629.22

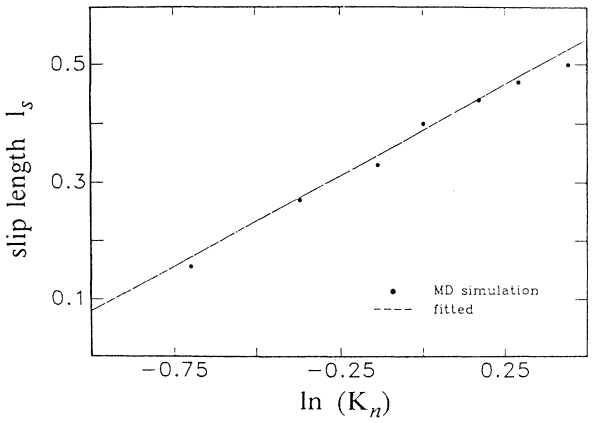

FIG. 2. The variation of slip length with the Knudsen number obtained from MD simulations.

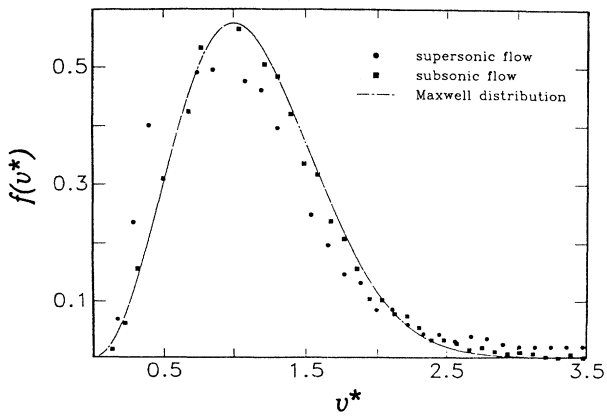

FIG. 3. Nonequilibrium velocity distribution functions at $K_n=2.79$ for a subsonic flow ($M=0.99$) and a supersonic ($M=4.05$) flow. The solid line represents the equilibrium Maxwell velocity distribution function. v^* is a scaled dimensionless velocity defined as $v/\sqrt{2k_BT/m}$. T for the subsonic and the supersonic flows are 423.68 and 1731.74 K, respectively.

function, and a deviation from the local Maxwellian distribution function is observed.

Liu and Lees have proposed a method for solving the transition regime gas flow problem, which consists in expressing the nonequilibrium distribution function as a superposition of two Maxwellians.[28] It was noticed that the theory of Liu and Lees breaks down above a critical Mach number, which for the Couette flow geometry is approximately 3.1. In view of our simulation, it is clear that the limitation of the theory of Liu and Lees lies in the fact that it fails to represent the nonequilibrium effects in the velocity distribution function encountered in supersonic flows.

To analyze the organization of the dissipation in the system, we have calculated the Rayleigh-Onsager dissipation function,[26] which in the framework of the linear irreversible thermodynamics represents the entropy production in the system. Consistent with the experiments of Sody and Berry,[29] we found that the dissipation in the system decreases monotonically with decreasing density, and that most of the dissipation takes place in a thin boundary layer, the thickness of which decreases with the increasing Knudsen number.

We have also studied the variation of the shear viscosity of argon with the Knudsen number. The viscosity has been calculated at the center of the channel from the measured velocity profile.[16,21] In the limit of a very low Knudsen number ($K_n=0.05$), we have calculated the shear viscosity at 316.7 K with 8000 particles and found the result, $\eta=(2.70\pm0.05)\times10^{-4}$ g/(cm sec), in good agreement with the analytical result of 2.58×10^{-4} g/(cm sec) obtained for hard-sphere particles at the same temperature.[30] Using the DSMC method Lengrand and Fadili have calculated the shear viscosity for the variable hard-sphere model.[31] Figure 4 shows the Knudsen number dependence of the shear viscosity, obtained using the MD and DSMC methods. Both simulations predict that the shear viscosity of the argon gas decreases with the Knudsen number. The difference between the two simulations is mainly due to the difference in the interaction potentials. The importance of the potential should diminish as the gas gets more rarefied. Thus the two methods should give the same viscosity in the limit of a high Knudsen number. Figure 4 seems to indicate that this is indeed the case.

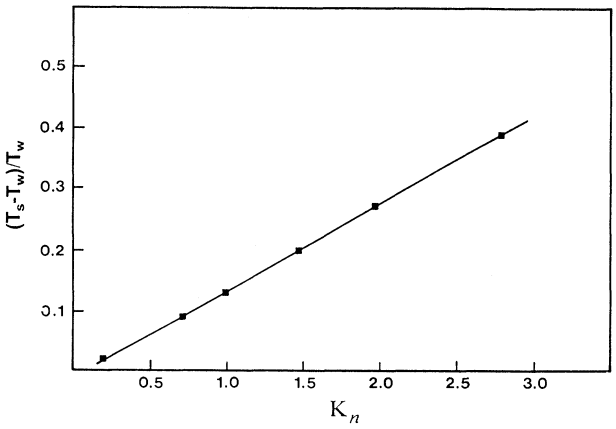

FIG. 5. The variation of the temperature jump $(T_s-T_w)/T_w$ with the Knudsen number in subsonic flows. The wall temperature is represented by T_w, while T_s denotes the temperature of the fluid next to the wall.

One of the objectives of the simulation of the transition regime gas flow problem was to analyze how the temperature jump at the channel wall depends on the Knudsen number and the speed of the flow. As is well known when a high-speed space vehicle (such as a space shuttle) reenters the atmosphere it experiences a severe thermal stress due to viscous heating.[32] To design an appropriate thermal protection system one needs an accurate estimate of the heating load at the surface. In Fig. 5 we have shown how the temperature jump varies with the Knudsen number. It appears that in the transition regime the

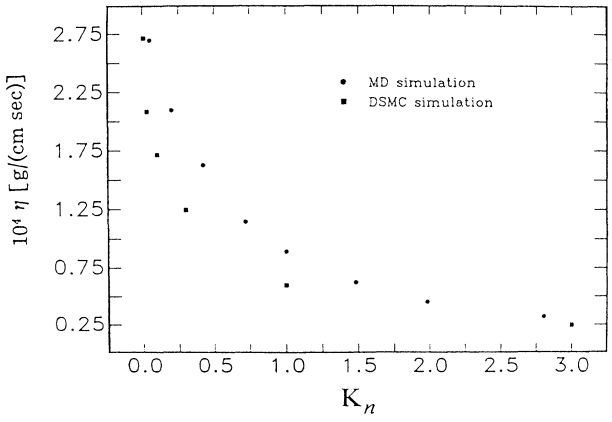

FIG. 4. Comparison of the Knudsen number dependence of the shear viscosity.

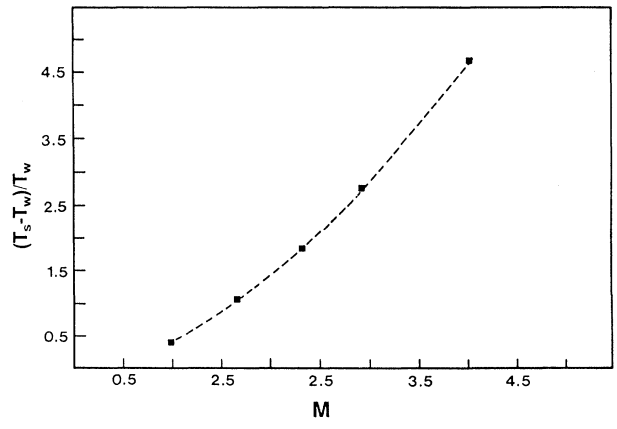

FIG. 6. The variation of the temperature jump $(T_s-T_w)/T_w$ with the Mach number at a Knudsen number $K_n=2.78$.

temperature jump at the wall varies linearly with the Knudsen number. This result is consistent with the one obtained by Cuda and Moss with the DSMC method.[33] Figure 6 shows the Mach number dependence of the temperature jump at a $K_n = 2.78$. It is evident that at a high Mach number viscous heating contributes to considerable thermal stress at the surface of a supersonic vehicle. Since continuum hydrodynamics does not provide any information on the temperature jump, our results outline the importance of molecular-dynamic simulations in studying the viscous heating problem in high-altitude aerodynamics.

IV. CONCLUSION

The flow behavior in the transition regime depends on the Knudsen number. The Knudsen number is the ratio of the mean free path of the gas particle to the characteristic length of the flow system. The Knudsen number can be large if the mean free path of the gas particle is large or if the characteristic length of the flow system is sufficiently small. The first situation is encountered in dealing with high-altitude flow problems. Much of the current interest in studies of the nonequilibrium transport in the transition regime stems from its advanced applications in space engineering, in particular the design of aeroassisted orbital transfer vehicles that achieve payload economy by passing through the Earth's atmosphere to change orbit and hypersonic aircrafts that may require propulsion by supersonic ramjets.[3,32] Transition regime flow phenomena can also be encountered in the identification and the analysis of the small particle transport mechanism in combustion environments which is an essential element in understanding particulate depositing rate.[34] Another example of transition regime transport phenomena arising from the second situation is the problem of the removal of heat from the integrated chips used in supercomputers. In general, these flows cannot be studied in the framework of continuum hydrodynamics. A particularly interesting evidence of this was recently shown by Rosner.[35] While analyzing film growth by vapor transport in a microgravity environment, he found that the familiar Stokes-Fourier-Ficks laws governing the evolution of fluxes of momentum, energy, and mass are inadequate even when the Knudsen number is as small as 10^{-3}. Advances in computer technology have offered a unique opportunity to address these flow problems at a molecular level. In the present paper we have shown that nonequilibrium flow problems in the transition regimes can be studied using molecular dynamics. We note that unlike the DSMC or the lattice gas dynamics method,[36] the MD method discussed in this study does not make any further approximation in the collision dynamics of fluid particles besides a simple potential form (which in principle can be made as realistic as it can). The latter can therefore be used to investigate some fundamental problems of the transition regime flow, such as the effect of the molecular constitution and the physical state of the thermal walls on the structure of the nonequilibrium Knudsen layer. It may also enable one to study complex nonequilibrium flow problems in a polyatomic fluid, in particular to analyze the effect of interatomic potential on the rotation-translational energy transfer, which is presently studied within the DSMC method using very simple models.[37] We are currently investigating these problems.

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*Permanent address: IBM, 2125 Ridgewood Dr., Midland, MI 48640.

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