The effect of thermal fluctuation on impacts of nanoclusters

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Recently, theorists have developed several theoretical results known as the fluctuation theorem (FT), which has been numerically and experimentally tested.[1] FT estimates the probability of emergence of the negative entropy production in tiny objects subject to large thermal fluctuation.

We have performed a molecular dynamics simulation of collision of nanoclusters and investigated the relation between FT and impact phenomena of argon clusters. We have arranged two identical nanoclusters, each of which is consisted of 682 argon atoms governed by the Lennard-Jones potential(Fig. 1). Initially, the configuration of atoms of a cluster has a FCC structure. We define the initial temperature of the clusters by the variance of the normal distribution for the initial velocities of atoms. After equilibrating the clusters to an arbitrary temperature, we have made the two clusters collide head-on with the initial velocities smaller than the thermal velocity of the system. We assume the interaction between the two clusters as the repulsive part of the Lennard-Jones potential. By changing the set of initial velocities of all the atoms and the initial orientation of the cluster, we have carried out 1000 simulations per initial condition and averaged the results.

From our simulation, it became clear that the relation between the relative colliding speed \( v \) and the restitution coefficient \( e \) obeys \( a - e \propto v^{1/5} \), where \( a \) is a parameter larger than unity when the initial temperature ranges from \( T = 0.01E/k_B \) to \( T = 0.03E/k_B \). Here, \( E \) and \( k_B \) are

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the scaling unit of energy and the Boltzmann constant, respectively. When \( a \) is equal to 1, this relation becomes the quasistatic theory of low-speed impact of elastic materials.\[2\] In addition, it became clear that the frequency distribution of the restitution coefficient has the Gaussian form when \( v = 0.02\sqrt{E/\overline{m}} \), where \( \overline{m} \) is the mass of an atom.

We also have investigated the relation between our numerical results and FT for impact problems. In order to do that, at first, we have obtained the probability function of \( \epsilon \), \( P(\epsilon) \), where \( \epsilon = 1 - e^2 \). After equilibrating the rebounded clusters, we made the clusters collide again with the rebounded speed to measure the restitution coefficient of the time reversal trajectory, \( \bar{e} \), and obtained the probability distribution \( \tilde{P}(\bar{e}) \), where \( \bar{e} = 1 - \bar{e}^2 \). According to FT for impact problems, the connection between \( P \) and \( \tilde{P} \) becomes

\[
\exp(\beta W)P(\epsilon) = \tilde{P}(\bar{e}),
\]

where \( \beta \) is the inverse temperature and \( W \) is the energy loss of the center of mass. In our simulation, when the initial temperature is \( T = 0.02E/k_B \), it became clear that the connection between \( P(\epsilon) \) and \( \tilde{P}(\bar{e}) \) shows a good agreement with the above expression.

参考文献
