Super-elastic collisions in a thermally activated system

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分子動力学法に基づいた、少数原子から成るクラスターモデルの衝突シミュレーションを行った。その結果、2個の同質なクラスター同士を系の熱速度よりも小さい相対速度で正面衝突させると、反発係数が1以上になるようなイベントを多数観測することがわかった。また、衝突速度と反発係数の関係はマクロな物質同士の低速衝突の衝突則として知られる準静理論に近い傾向を示すことがわかった。更にクラスター同士を低速で正面衝突させたときの巨視的なエネルギーロスの確率分布に基づいて、衝突問題における揺らぎの定理との比較を行なった。

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 to observe the negative entropy production in small systems subject to large thermal fluctuation.

We have performed molecular dynamics simulations of collisions of Lennard-Jones clusters and investigated the relation between FT and impact phenomena of small clusters. Our model is composed of two identical clusters, each of which is consisted of 682 "atoms" bounded together by the Lennard-Jones potential(Fig. 1). We assume the interaction between the two clusters as the repulsive part of the Lennard-Jones potential. Initially, the configuration of "atoms" of one cluster has a FCC structure. The initial velocities of the "atoms" obey Maxwell-Boltzmann distribution, the variance of which corresponds to initial temperature of the system. Sample average is taken over different sets of the initial velocities for "atoms". After equilibrating the clusters to an arbitrary temperature, we make the two clusters collide against each other with the initial velocities smaller than the thermal velocity of the system.

From our simulation, we found that the relation between the relative colliding speed v and the restitution coefficient e obeys $a - e \propto v^{1/5}$. Here a is a constant larger than unity when the initial temperature ranges from $T = 0.01\epsilon$ to $T = 0.03\epsilon$, where ϵ is the scaling unit of energy. When a is equal to 1, this relation becomes the quasistatic theory of low-speed impact of elastic materials.[2] We have also made the two clusters pressed against each other to obtain the relation
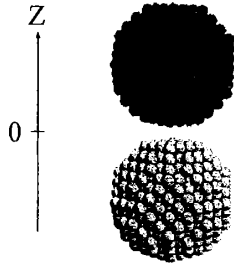
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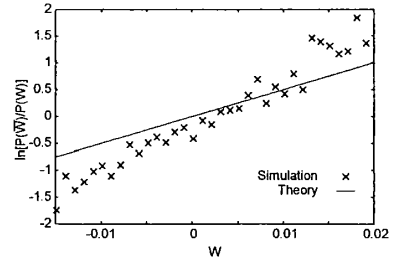Figure 1: Numerical model of clusters

Figure 2: Comparison between numerical results and fluctuation relation

between deformation and compressive force. We found that the relation can be described by three-dimensional Hertztan contact theory.

We have also investigated the relation between our numerical results and fluctuation relation for impact phenomena which is based on FT. In this simulation, at first, we obtain the probability function of $P(W)$ during a collision, where W is a macroscopic energy loss. After equilibrating the rebounded clusters, we reverse the rebound velocity to make the clusters collide again and measure the probability distribution function $P(\bar{W})$ of the time reversal trajectory. According to the fluctuation relation, the connection between $P(W)$ and $P(\bar{W})$ may be decsribed as

$$\exp(\beta W)P(W) = P(\bar{W}), \tag{1}$$

where β is the inverse temperature. Figure 2 shows that the connection between $P(W)$ and $P(\bar{W})$ in our simulation shows a good agreement with eq.(1). [3]

References

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