# Growth of Cosmic Dust Aggregates and Reexamination of Particle Interaction Models

Hidekazu TANAKA,[1,*] Koji WADA,[2] Toru SUYAMA[3] and Satoshi OKUZUMI[4]

[1]*ILTS, Hokkaido University, Sapporo 060-0819, Japan*
[2]*PERC, Chiba Institute of Technology, Narashino 275-0016, Japan*
[3]*Nagano City Museum, Nagano 381-2212, Japan*
[4]*Department of Physics, Nagoya University, Nagoya 464-8602, Japan*

Dust growth is the first step of planet formation in protoplanetary disks. Dust growth also influences the temperature of protoplanetary disks. However, we still have a large uncertainty in the dust growth process. This uncertainty mainly comes from unknown factors in dust internal structure and collisional outcomes. The dust structure and the collisional outcome would be closely related with each other. In recent years, many theoretical studies on aggregate collisions and growth have been done. In the present paper, we introduce remarkable results in these theoretical studies, mainly focusing on numerical simulations of dust collisions by our group. In the numerical simulations of dust collisions, we adopt the interaction model between constituent particles of dust aggregates. We have started the rexamination of the particle interaction model, by performing molecular dymnamics simulation of particle collisions. We also report the preliminary results of our molecular dynamics simulations.

## §1. Introduction

Dust growth is important as the first step of the planet formation process. Since dust grains are the main source of the disk opacity, dust growth also influences the temperature of protoplanetary. Hence it is necessary to take into account dust growth in theoretical disk models and in data analysis of disk observations. Moreover, although many chemical reactions proceed on the surface of dust grains, dust growth reduces the total surface area of them. For these reasons, many authors have studied dust growth in protoplanetary disks.[1)−5)]

On the other hand, dust growth is not a simple process. In protoplanetary disks, dust grains would grow to aggregates composed of sub-micron particles. Such aggregates have various kinds of internal structure, depending on their growth mode. Collisional outcome of dust aggregates also has a large variety, depending on the impact velocity or the dust structure, as will be shown below. In the study of dust collisional growth, therefore, we have to know detail of the dust internal structure.

In the early stage of dust growth in protoplanetary disks, collision velocities between dust grains are extremely low ($< 1\,\mathrm{mm\ sec^{-1}}$) and collisions between comparable-size grains are dominant. In such a growth mode, dust aggregates are expected to resemble the BCCA clusters (ballistic cluster-cluster aggregation clusters).[10)] The BCCA clusters are formed by the sticking of two equal-sized clusters with no restructuring. Because the fractal dimension of their structure is $\simeq 2$, large BCCA clusters are very porous and have an extremely low bulk density (see

*) E-mail: hide@lowtem.hokudai.ac.jp

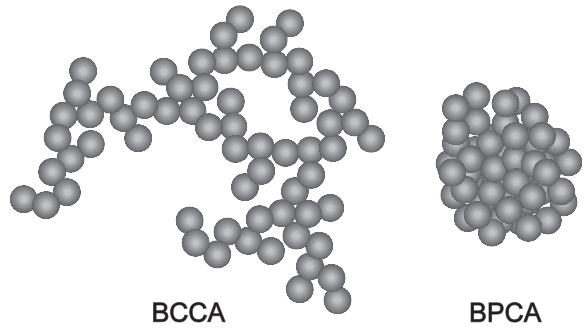


Fig. 1. Schematic examples of a BCCA cluster and a BPCA cluster. The BCCA clusters have a open and fluffy structure, whereas BPCA clusters have a relatively compact structure.

Fig. 1). Thus, dust aggregates have a very fluffy structure, at least, in the early growth stage.[6)−9)] Another simple example of aggregate models is the BPCA (ballistic particle-cluster aggregation).[10)] The BPCA clusters are made by depositions of single particles. Although BPCA clusters have a high porosity of 86%, BPCA clusters are much more compact than BCCA because the fractal dimension of BPCA cluster is 3. In the later growth stage, dust aggregates start to shrink due to collisional compression. Suyama et al.[7)] suggested from the collisional energy that shrinkage of fluffy aggregates would start when the aggregate size reaches centimeters in planet-forming regions. The bulk density of compressed aggregates is expected to be between those of BCCA and BPCA, but there still exists a large uncertainty in their bulk density. Because of this uncertainty in the aggregate internal structure, optical properties of dust aggregates remains unknown parameters, too.

Recently, evolution of dust structure during dust growth has been examined by many authors.[6)−9),11)] To reveal such structural evolution, we need to know the outcome of dust collisions for wide ranges of parameters, i.e., the impact velocity, the dust material, the dust structure, etc. Dust collisional outcomes have been investigated with laboratory experiments[12)−16)] and with numerical simulations.[7),8),17)−23)] Progresses by these studies are described in §§2 and 3 in detail.

In the numerical $N$-body simulation for the collisional outcome between dust aggregates, we have to adopt an interaction model between the constituent particles of dust aggregates. In the interaction model used in the numerical simulations, the constituent particles are considered as adhesive elastic spheres. The adhesion force between them is described by the JKR theory.[24)] As for tangential resistive forces against sliding, rolling, or twisting motions, Dominik and Tielens developed a theoretical model.[17),25),26)] Although the energy dissipation is a key factor in the collisional outcome, the interaction models have a large uncertainty in the energy dissipation rate. Some laboratory experiments on interaction of constituent particles have done[12),27),28)] but they do not seem enough to fix the uncertainty in the theoretical interaction models.

As well as laboratory experiments, molecular dynamics (MD) simulation would be also a powerful approach to check of the interaction models. In the MD simulation, two (constituent) particles consist of a large number of molecules and the

interaction force between the particles are directly obtained. We have started such a MD simulation of particle collisions to re-examine the particle interaction models. Recently, many MD simulations of particle collisions have been done.[29)−33)] These studies, however, focus on nano-size particles, which consist of less than two thousand molecules. In this size range, the energy dissipation at particle collisions is significant and the interaction force would be strongly deviated from the macroscopic JKR model. Indeed, any quantitative comparisons with the JKR model are not tried in the previous studies. We performed MD simulations of particle collisions for larger particles with up to sub-micron size and compared the obtained interaction force with the models. The re-examination of the particle interaction models with MD simulations would be also useful in the field of granular physics. In §4, we describe detail of our MD simulation and show the preliminary results. Summary is given in the last section.

## §2. Studies on dust growth and structure in protoplanetary disks

Dust growth and structural evolution are governed by the interaction force between sub-micron constituent particles. The adhesion force between two particles in contact is originated from the van der Waals force for silicate particles (or the hydrogen bonds for icy ones). For sub-micron particles, the adhesion force is strong enough to bind them and to construct large aggregates.

The theoretical model of this kind of particle interaction has been developed by Johnson, Kendall, and Roberts.[24),34)] Their model is called the JKR theory and has been widely used in many fields of science and technology.[35)] According to the JKR theory, the critical velocity of two colliding sub-micron particles for sticking is $\sim$1 m/sec for silicate and $\sim$10 m/sec for ice. Dominik and Tielens further developed the interaction model, by taking into account resistive forces against sliding, rolling, and twisting motions between particles.[17),17),25)]

Using their particle interaction model, Dominik and Tielens examined collisional outcomes of dust aggregates through numerical simulations.[17)] They also made a simple recipe for collisional outcome, which determines conditions on the impact velocity for sticking or compression. According to their recipe, the critical velocity for sticking of two aggregates is comparable to the critical velocity for sticking of two constituent particles.

Laboratory experiments of aggregate collisions are energetically done in Germany.[12)−15),27),28)] These experimental results are almost consistent with the recipe by Dominik and Tielens though some bouncing events are also observed for relatively compact aggregates. Recently, Güttler et al. revised the recipe of collisional outcome, by compiling the experimental data of aggregate collisions.[16)] By the use of these recipes of collisional outcome, some authors start to examine internal structure of growing dust aggregates.[6),9)]

However, these outcome recipes do not seem accurate enough to be applied to dust growth in protoplanetary disks. Since dust aggregates are expected to have a highly fluffy structure like BCCA clusters in their early growth stage, we need accurate information for fluffy aggregates to simulate dust growth. Because of technical

difficulty, on the other hand, only a few laboratory collisional experiments have been done for highly fluffy aggregates. Most experiments have been done for aggregates with the volume filling factor larger than or comparable to 0.1. The recipe based on these laboratory experiments would have a poor accuracy on the collision between fluffy aggregates though it is useful for relatively compact aggregates. At present, we can examine the collisions between highly fluffy aggregates only with $N$-body numerical simulations.

## §3. Recent $N$-body simulations of dust aggregate collisions

Recently, some researchers performed $N$-body numerical simulations of dust aggregate collisions to reveal the collisional outcome for fluffy dust aggregates.[7),18)–23)] Here we introduce these results, focusing on results obtained by our group.

### 3.1. *Compression of dust aggregates at collisions*

Wada et al. newly developed an $N$-body simulation code to calculate collisions of large aggregates made of up to a few ten thousands of constituent particles and performed numerous runs of collision simulation to survey the wide parameter range of the collisional outcome.[18),19)] They examined collisions between two equal-sized BCCA clusters and developed an empirical compression model from their numerical results. Figure 2 shows the numerical results on aggregate compression and their compression model. At low-velocity collisions, aggregates just stick to each other and compression does not occur. At collisions with higher velocities, the resultant aggregates are compressed and their size gradually decreases as the impact energy increases. The dependence of the size of the resultant aggregates on the impact energy is given by the power-law function with the exponent $-0.1$. It is also found that the compressed aggregates have a fractal dimension of 2.5, which explains the fact that even the compressed aggregates are much more porous than BPCA clusters with a fractal dimension of 3. The fractal dimension of 2.5 of the compressed aggregates is also consistent with their empirical compression model. Such a low fractal dimension of the compressed aggregates was not expected in the previous studies.

Although Wada et al. examined the compression of BCCA clusters in a single collision, dust aggregates would be gradually compressed by successive collisions in realistic systems. In order to examine such a gradual compression process during dust growth, Suyama et al.[7)] performed $N$-body simulations of sequential collisions of aggregates. In this simulation of sequential collisions, the resultant aggregate and its copy are used as the initial aggregates at the next collision. By repeating $N$-body calculations of aggregate collisions with a constant impact velocity, they simulated gradual compression of aggregates and examined the density evolution during aggregate growth. Figure 3 shows the results of the sequential collision simulation for various impact velocities and rolling energies. As they grow, the aggregates are compressed and have larger bulk densities than BCCA clusters. However, their bulk densities keep decreasing. It was also found that the fractal dimension of the resultant aggregates is 2.5, which is consistent with Wada et al. This low fractal dimension explains the decrease in the bulk density of resultant aggregates. Suyama et

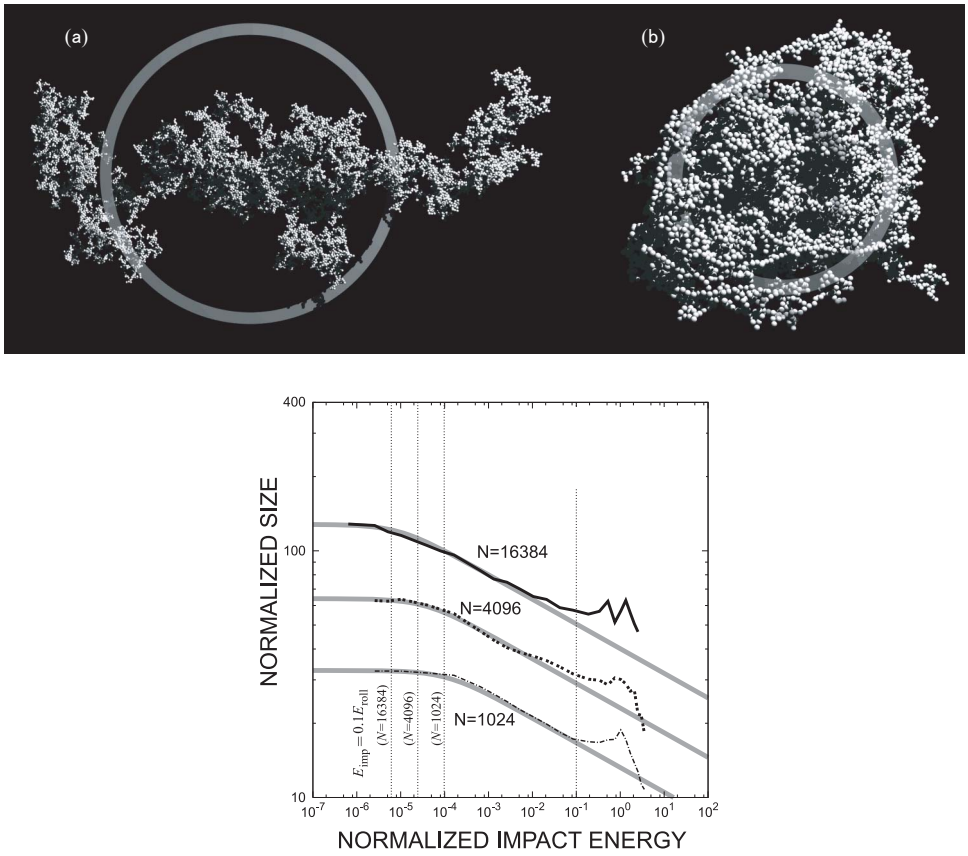


Fig. 2. Results of $N$-body simulations on aggregate compression at collisions (This figure is reproduced based on Figs. 3 and 12 of Wada et al.[19] by permission of the AAS). Top: Examples of collisional outcomes; (a) a hit-and-stick case with the impact velocity of 0.024 m s$^{-1}$ and (b) a maximum compression case with the impact velocity of 13 m s$^{-1}$. Initial colliding aggregates are equal-sized icy BCCA clusters. Both resultant aggregates are composed of 16,384 ice particles of 0.1 $\mu$ m radius. The gray rings indicate the gyration radii of the aggregates. Bottom: Impact velocity dependence of the size of resultant aggregates for various aggregate masses. Gray lines are drawn by their compression model. Model lines reproduces numerical results very well.

al. also derived an empirical formula describing the density evolution of aggregates. Applying this formula to dust growth in protoplanetary disks, they suggested that meter-sized dust aggregates have an extremely low density of $10^{-4}$ g/cm$^3$. If such extremely-low-density aggregates are formed, it would significantly influence their motion, growth process, and optical properties of protoplanetary disks. Recently, Suyama et al. constructed the outcome model based on their numerical results for fluffy aggregates.[23] Using this outcome model, Okuzumi et al. performed numerical simulations of dust growth in protoplanetary disks.[11] Their growth model for fluffy dust aggregates suggests the possibility to overcome the difficulties in planetesimal formation.

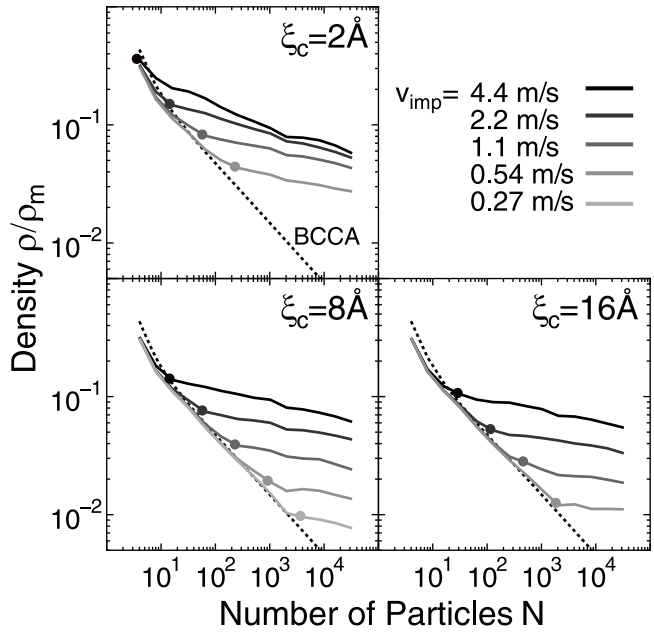


Fig. 3. Compression of icy aggregates during their growth (reproduced based on Fig. 5 of Suyama et al.[7] by permission of the AAS). The bulk densities of resultant aggregates in subsequent collisions are shown. The horizontal axis is the number of constituent particles in the resultant aggregates, which is proportional to the aggregate masses. The impact velocity and the rolling energy between two constituent particles are parameters; the rolling energy is proportional to the critical rolling displacement $\xi_c$. They performed 13 runs for various values of these parameters. The dotted lines shows the bulk density of BCCA clusters which experience no restructuring. Deviations from the BCCA line indicates the occurrence of compression at collisions. In spite of the compression, the bulk densities of growing aggregates keep on decreasing in all cases.

### 3.2. *Critical impact velocity for dust growth*

Wada et al.[20] examined disruption at collisions between compressed aggregates. As compressed aggregates, they adopted icy BPCA clusters. With their simulation of aggregate collisions, they clarified the maximum impact velocity which marginally allows aggregate to grow. Figure 4 shows the averaged masses of the largest resultant aggregate after the disruptive collisions with various impact velocities. The averaging are done for the impact parameter at collisions. At low-velocity collisions, disruption hardly occur and aggregates grow almost perfectly. At high-velocity collisions, on the other hand, significant disruption reduces the resultant aggregate mass below the initial mass. The critical velocity for growth is $\sim 60$ m s$^{-1}$ ($= 216$ km hour$^{-1}$) for icy aggregates composed of constituent particles of 0.1 $\mu$m radius. The critical energy is scaled with the binding energy of two constituent particles in contact ($E_{\rm break}$). The above high critical velocity is originated from the strong binding force between sub-micron icy particles. For silicate aggregates or for aggregates composed of larger particles, we obtain a lower critical velocity than the above because of smaller binding energies in those cases. In protoplanetary disks, the collision velocity reaches several tens m/sec. This critical velocity indicates that icy planetesimals are able to form

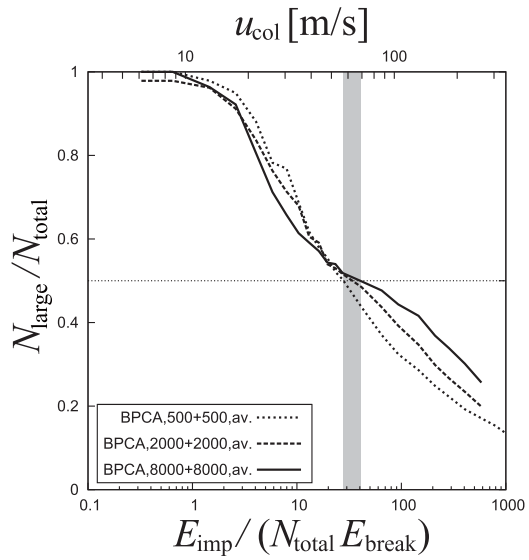


Fig. 4. Averaged masses of the largest resultant aggregate after the disruptive collisions (reproduced based on Fig. 11 of Wada et al.[20] by permission of the AAS). The horizontal axis is the impact velocity at each collision. Outcomes strongly depend on the impact parameter at each collision. Nine runs are performed for various impact parameters at each impact velocity and the averaged masses are obtained from results of these runs. The averaged masses (the vertical axis) are normalized by the total mass of the system, which is the twice of the mass of an initial aggregate. Numerical simulations are done for various initial aggregate masses, too.

through direct dust growth.

In these simulations of aggregate collisions, they examined only collisions of equal-sized aggregates. The effect of the mass ratio between two colliding aggregates should be examined in future researches. The constituent particles are also assumed to be of equal size in the simulations. The size distribution of the monomer particles would affect the collisional outcomes.

The most important assumption in the $N$-body simulation would be the interaction models of constituent particles. As seen above, the binding energy between two constituent particle and the rolling energy are key parameters in disruption and restructuring at collisions, respectively. In the next section, we show our re-examination on the particle interaction models with molecular dynamics simulations.

## §4. Re-examination on the particle interaction model with MD simulation

In order to check the particle interaction models adopted in the numerical simulation of dust aggregate collisions, we have started molecular dynamics simulation of particle collisions. In the MD simulation, two (constituent) particles consist of a large number of molecules. The interaction force between the particles are directly obtained from the simulation and can be compared with the theoretical models. Here we show preliminary results of our molecular dynamics simulation.

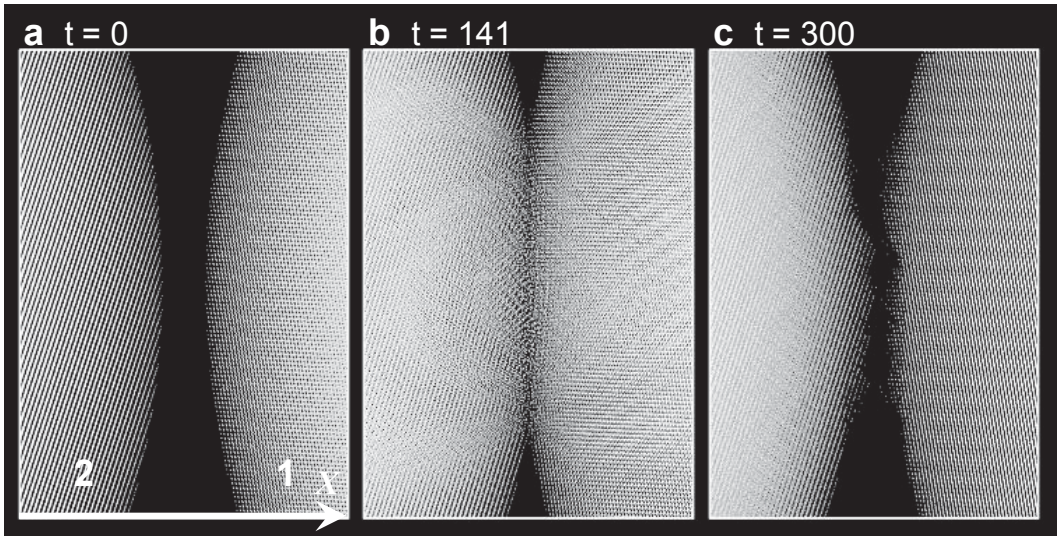


Fig. 5. Snapshots of a head-on cluster collision with the impact velocity of 0.06 for clusters composed of approximately six million LJ molecules.

### 4.1. *Numerical procedure of the MD simulation*

In our MD simulation, we consider collisions of two particles made of Lennard-Jones type molecules. The interaction potential between two Lennard-Jones molecules, $u_{LJ}(r)$, is given by

$$u_{\rm LJ}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right], \tag{4·1}$$

where $\sigma$ and $\epsilon$ are the parameters of length and energy of the potential, which are set to be the unit length and energy, respectively, in our MD simulation. The mass unit $m$ is the mass of a molecule. For argon system, the units are given by $\epsilon/k = 119.8$ K (where $k$ is the Boltzmann constant), $\sigma = 0.3405$ nm, and $m = 6.634 \times 10^{-23}$ g. To save computational time, we truncate the interaction potential at a cutoff distance $r_{\rm c} = 5\sigma$. The collision of two spherical particles is simulated, by calculating motions of constituted molecules interact with each other. Motions of the molecules are integrated with the leap-frog integrator. The time step is set to be $0.01\tau$, where the time unit $\tau$ $(= m\sigma^2/\epsilon)$ is 2.16 ps for argon system.

As the initial particles, we adopt face-centered-cubic crystalline clusters with the lattice constant of $1.091\sigma$. The spherical cluster is obtained by simply cutting out from a large crystal. The initial temperature of the particles are set to be very low. Since we use particles with no lattice defect and a low temperature, the dissipation process is relatively hard to occur in our MD simulations. Hence our MD simulations give a minimum energy dissipation rate at particle collisions. We consider only collisions of two equal-sized clusters in our simulation. The crystalline directions of the initial clusters are chosen randomly.

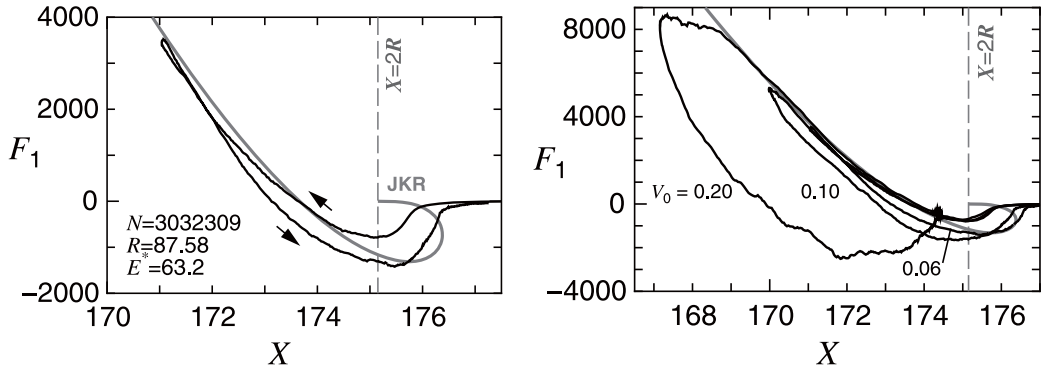


Fig. 6. The interaction force between two particles as a function of the distance between their centers of mass. Left: The typical case with the impact velocity of 0.06 is displayed. The gray line represents the prediction by the JKR theory. For $X > 2R$, the JKR prediction has two branches; the lower branch corresponds to the stable deformation of two elastic particles, whereas the upper is unstable. The maximum adhesive force in the unloading phase agrees well with the model. Right: The cases with various impact velocities of 0.06–0.20 are shown. For the impact velocity of 0.20, two clusters do not rebound but stick while they rebound in other cases.

### 4.2. *Results*

We first show a typical case where the number of molecules in each cluster $N$ is about three million (the exact number is 3,032,309) and their diameter is 175.2 in the LJ unit (59.6 nm for argon system). Figure 5 shows the snapshots of a head-on collision between two particles. The initial relative velocity is set to be 0.06 (in the LJ unit). In the snapshots, the sphere on the right hand size is the cluster 1 while the cluster 2 is the left one. With the repulsive force between the two clusters, they stop at the time of the maximum compression ($t = 140$) and start to move to the opposite direction. In this simulation, the connection between the particles is cut and they rebound.

In the MD simulation, we observe the motions of the centers of mass of each particles. Using the velocity evolution of their centers of mass, we calculate the accelerations of each particle and, then, also obtain the interaction force between the particles. The left panel of Fig. 6 shows the force on the particle 1 as a function of the distance between the centers of mass of two particles, $X$. The fitting line by the JKR formula is also plotted. In the JKR formula, the surface tension is set to be 3.2, which is approximately equal to the value for the amorphous of LJ solid at very low temperature.[36] The reduced Young modulus is set to be 63.2.

The theoretical models approximately reproduce this numerical result. The maximum adhesive force in the unloading phase agrees well with the models. However, a hysteresis exists between the loading and unloading phases. The hysteresis is related to the energy dissipation. The JKR theory predicts the deviation in the radial distance between the points of the contact and the disconnect of two spheres. Such a deviation between the contact and the disconnect is also seen in the left panel of Fig. 6. On the other hand, the hysteresis during the contact (i.e., $X < 2R$) is not

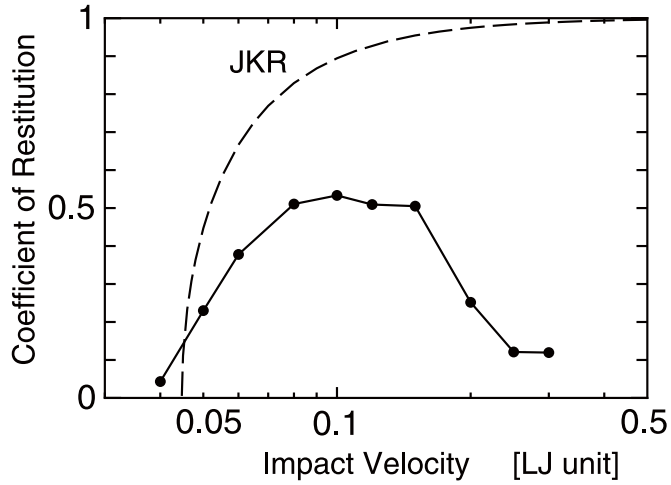


Fig. 7. The mean coefficient of restitution for various impact velocities. The broken line shows the prediction by the JKR theory. In MD simulations, stronger energy dissipation is observed than the JKR prediction.

explained by the JKR theory. Performing the runs with various impact velocities, we examined the dependence on the impact velocity. The results are shown in the right panel of Fig. 6. Higher impact velocities cause stronger hysteresis (and stronger energy dissipation).

At each simulation of particle collisions, we obtained the final rebounding velocities of two particles and also the coefficients of restitution. Figure 7 shows the coefficients of restitution as a function of the impact velocity. The particle interaction force and the coefficients of restitution is dependent on the contact surface of two particles. Changing the initial directions of two particles, we performed ten runs of collision simulation for each impact velocity and obtained the mean value of the coefficients of restitution. The mean values are plotted in Fig. 7. For the comparison, the prediction by JKR theory is also plotted. The obtained dissipated energies at each collision are larger than the predictions by the JKR theory. Especially, for high impact velocities larger than 0.1, the deviation is significant. For such high velocity impacts, we observed plastic deformation in particles after collisions. This would be the origin of the large energy dissipation.

We also performed similar simulations of particle collisions with the impact velocity of 0.06 for various particle size. Figure 8 shows the results on the interaction forces for various cluster sizes. Although hysteresis in the interaction force exists for all sizes, the hysteresis is relatively weaker for larger clusters. The deviation from the theoretical models has the same size dependence. The maximum adhesive forces in the unloading phase is well reproduced by the theoretical models in all sizes.

The hysteresis in the interaction force observed in our MD simulations would be modeled, by introducing an additional frictional force. If this additional frictional force between constituent particles is included in $N$-body simulation of aggregate collisions, it would increase the growth efficiency because of additional energy dissipation. For the modeling of the frictional force, we need detail investigation with

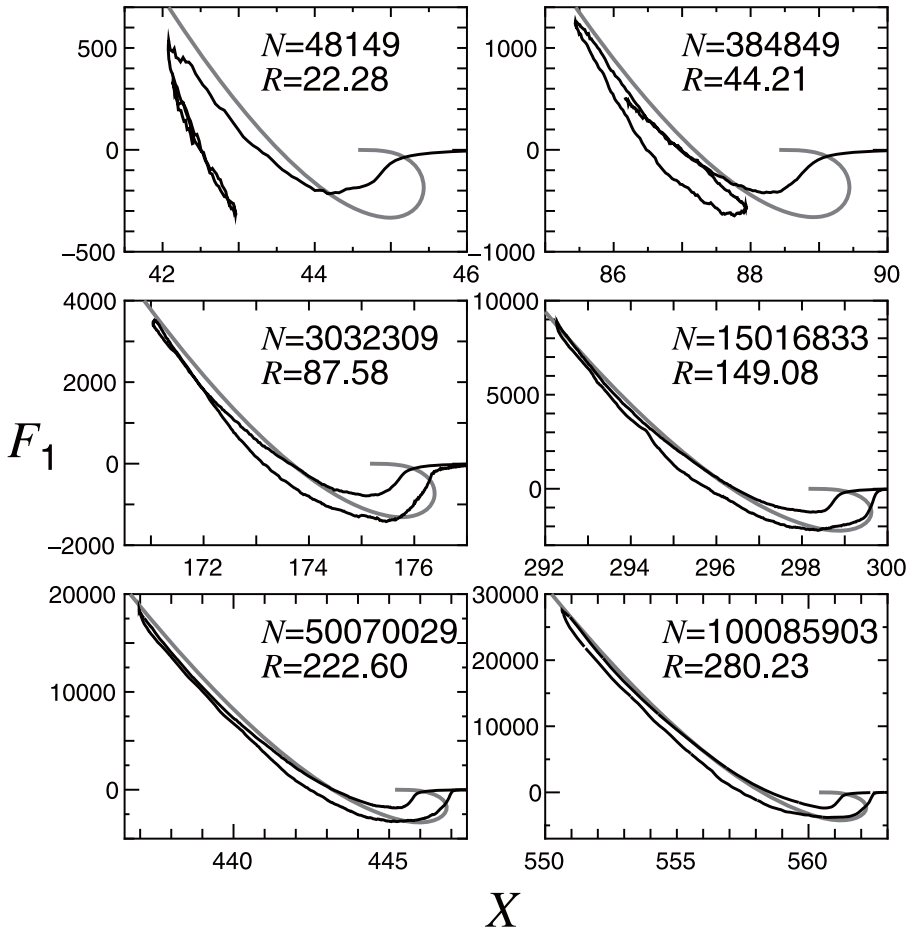


Fig. 8. Same as Fig. 6 but for various cluster sizes. The impact velocity is 0.06 in all of these runs. The gray line represents the predictions by JKR theory.

more simulation runs. We will try it in the future work. The resistive forces against sliding, rolling, or twisting motions are also able to be examined with MD simulations, by setting the initial motions of two particles properly. Such MD simulations will be done at the next step.

## §5. Summary

Summary of the present paper is listed below.

1. Dust growth is an important factor in planet formation process. To study dust growth, on the other hand, we need detail and accurate information on internal structure of dust aggregates and their collisional outcome.
2. In protoplanetary disks, dust aggregates have a highly fluffy structure like BCCA, at least, in the early growth stage. The $N$-body simulation is a powerful approach to reveal the collisional outcome for highly fluffy aggregates. The

$N$-body simulation of aggregate collisions showed that dust aggregates remain highly fluffy during their growth in spite of collisional compression and also that the critical velocity required for disruption is so high ($\sim 60$ m s$^{-1}$ for icy aggregates) that icy dust aggregates would safely grow in protoplanetary disks. These results in dust growth tend to resolve the difficulties in planetesimal formation process.

3. The most important assumption in the $N$-body simulation of aggregate collisions is the interaction model for constituent particles of dust aggregates. We have started to check the particle interaction models, by performing molecular dynamics simulation of particle collisions, in which each particle consist of a large number of Lennard-Jones type molecules. According to the results of our MD simulation, the adhesion force between particles almost agrees with the JKR theory. We also found an additional energy dissipation during particle collisions, which was not predicted by the JKR theory. Resistive forces against sliding, rolling, or twisting motions between particles can be also tested with similar MD simulations.

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