Simulating dust monomer collisions: expansion of the JKR theory

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Collisional sticking is the first process of dust aggregate growth. However, some problems prevent the dust from growing. One of the serious problems is the fragmentation of dust aggregates. When the dust aggregates collide at high velocities, which is about several tens m/s, they are broken and become fragments. The maximum collisional velocity can reach 50 m/s without turbulence (e.g., Adachi et al. 1976; Weidenschilling & Cuzzi 1993). To discuss this problem, we should understand the critical collision velocity of fragmentation, and many numerical simulations of dust aggregate collisions (e.g., Wada et al. 2007, 2008, 2009, 2013; Suyama et al. 2008, 2012).

Dust aggregates are composed of many monomers, which are submicron-sized particles. Dust growth processes have been investigated by numerical simulation studies. Numerical simulations are *N*-body simulations and calculate interactions between monomers based on the JKR theory, which is one of the contact theories. However, the JKR theory doesn't consider molecular effects such as molecular motions and deformation of monomers. It is suggested that they lead to energy dissipation at collisions and promote coalescence (Krijt et al. 2013; Tanaka et al. 2012). Therefore, the monomer interaction should be investigated including molecular physics.

We used Molecular Dynamics (MD) simulation to analyze molecular motions and performed simulations of monomers' head-on collision. We focused on the coefficient of restitution *e* and investigated the dependence on monomer radius (10-100 nm), impact velocity (20-150 m/s), and temperature (0-80 K). We adopted the Lennard-Jones potential as the intermolecular interaction.

We showed that the coefficient of restitution of the MD results is smaller than that of the JKR theory. The energy dissipation due to molecular motion and deformation makes the coefficient of restitution small. First, we found the coefficient of restitution increases with monomer radius. It is considered that the ratio of contact radius to monomer radius decreases with increasing monomer radius and that it causes this radius-dependence. We also found that *e* decreases for the impact velocity larger than 50 m/s. The JKR theory cannot predict decreasing *e* because it doesn't include the effect of monomer deformation, which causes significant energy dissipation. Finally, we found that *e* decreases with higher temperatures. Decreasing *e* represents the increasing energy dissipation and we confirmed that the kinetic energy of monomers was converted to the potential energy and kinetic energy of molecular random motions. The JKR theory doesn't consider these effects.

Based on our MD results, we tried to expand the JKR theory. We referred to Krijt et al. (2013) to introduce the dissipative force. First, we showed that the Krijt model cannot fit the MD results. Then, we modified their model to be of the form compression length dependent. This model can reproduce the MD results at low impact velocity, although it has insufficient energy dissipation at high impact velocity. This is because their model doesn't include energy dissipation due to monomer deformation. We consider that another force is required to reproduce decreasing *e* at high impact velocity.

Our results show that the sticking probability in the MD simulation is larger than that of the JKR theory. Therefore, we can expect that dust aggregates can more easily grow by direct sticking even at high collision velocity and the growth rate becomes fast.