Molecular dynamics simulations of rolling motions between two contacting dust monomers

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The first step of planet formation is the dust growth due to collisional sticking. It is considered that the dust is an aggregate composed of monomers, whose size is submicron. The aggregates collisions have been investigated by powder simulations (e.g., Wada et al., 2013; Hasegawa et al., 2021), which calculate the interactions between the monomers in contact when calculating the monomer motion. In the powder simulations, a physical model is used that gives the interactions between the elastic spheres to the monomer interactions (Johnson et al., 1987). However, the physical model assumes elastic spheres and therefore does not include viscous effects. It has been suggested that this viscous effect is due to the molecular motion, and such a microscopic effect is considered to be particularly well represented at submicron sizes (Tanaka et al. 2012). Therefore, the physical model needs to be revised for accurate powder simulations.

We use molecular dynamics (MD) simulations, a method of studying the physical processes of a system by solving for the molecular motion. In the previous Cosmic Dust meeting, we showed the MD simulations of head-on collisions and the normal forces. This presentation will focus on rolling motion. Roling motion significantly affect the collision results since it causes the most energy dissipation in aggregate collisions among four interactions. In the model of rolling motion, there is an important physical parameter called the critical displacement, which gives the threshold of displacement at which the two spheres begin to roll. However, the value of the critical displacement is not yet agreed upon: 0.2 nm theoretically (Dominik & Tielens, 1995), 3.2 nm experimentally (Heim et al., 1999), and 0.8 nm used in powder simulations. This study investigates the value of the critical displacement.

In MD simulations, we treat monomers consisting of 0.1 - 100 million molecules. For initial conditions, two monomers are prepared in contact and given opposite angular velocities of spin rotation about a certain tangential direction to the contact surface. We check that the angular velocity decreases with time due to a resistive torque and quantify the magnitude of the resistive torque by comparing the MD simulations to the model. In particular, we analyze the critical displacement from the magnitude of the resistive torque and show that its magnitude is about 0.2 nm, which is consistent with the value predicted by theory and smaller than the value used in previous powder simulations. This suggests that the monomers are more likely to roll among themselves than in previous studies, indicating that the compressive strength of the aggregates is lower. Therefore, it is conceivable that the dust density could be greater than previously thought, e.g., due to ram pressure due to the low compressive strength. We will present the above results.