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The bouncing threshold in silica nanograin collisions

Maureen L. Nietiadi,[a] Philipp Umstätter,[a] Tiffany Tjong,[b] Yudi Rosandi,[b] Emmanuel N. Millán,[c] Eduardo M. Bringa[c] and Herbert M. Urbassek *[a]

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Using molecular dynamics simulations, we study collisions between amorphous silica nanoparticles. Our silica model contains uncontaminated surfaces, that is, the effect of surface hydroxylation or of adsorbed water layers is excluded. For central collisions, we characterize the boundary between sticking and bouncing collisions as a function of impact velocity and particle size and quantify the coefficient of restitution. We show that the traditional Johnson–Kendall–Roberts (JKR) model provides a valid description of the ingoing trajectory of two grains up to the moment of maximum compression. The distance of closest approach is slightly underestimated by the JKR model, due to the appearance of plasticity in the grains, which shows up in the form of localized shear transformation zones. The JKR model strongly underestimates the contact radius and the collision duration during the outgoing trajectory, evidencing that the breaking of covalent bonds during grain separation is not well described by this model. The adhesive neck formed between the two grains finally collapses while creating narrow filaments joining the grains, which eventually tear.

I. Introduction

Collisions of dust grains are ubiquitous in astrophysics, occurring in diverse places such as protoplanetary disks[1,2] and the dust tails of comets.[3,4] While the grain composition may vary, grains are typically classified as silica and ice grains. Dust particles have a complex structure; they are aggregates of small grains with sizes <1 μm.[5] The collision of dust particles is studied theoretically by means of granular-mechanics codes, which treat each grain as an entity with only a few degrees of freedom (translation, rotation).[6–8] In these codes, a variety of physical forces and torques must be taken into account, which describe the details of attractive, repulsive, dissipative and frictional interactions. These forces are often modeled by laws and parameters based on macroscopic concepts.[9] It remains unclear to what extent they apply to the collision of micro- or nanoscopic grains.

Molecular dynamics simulations may be used to test the assumptions underlying the granular-mechanics models. Such simulations have been carried out, in particular, for energetic grain collisions.[10,11] But they can also analyze the behavior at smaller collision velocities, and thus determine the sticking and bouncing behavior. Only a few such simulations have been reported, and mostly for generic interaction potentials such as the Lennard-Jones potential.[12–14] The sticking process is relevant for understanding the evolution of dust growth, since only sticking collisions will lead to grain agglomeration.[9]

An important exception is provided by the work of Sun *et al.*[15] who studied the collision of silica nanospheres (radii of 4 nm and below) using a non-reactive force field. This force field models the interatomic bonding and the van-der-Waals attraction between atoms, but does not allow for bonds to break and new bonds to form. This study showed that the collision of silica grains can be well described by the Johnson–Kendall–Roberts (JKR)[16] theory of adhesive contacts; in particular, the force-displacement curves and the contact radii are well reproduced.

However, more energetic collisions may lead to close encounters of the two grains where bonds may dissociate and new bonds may form. In particular, at the high pressures present in the compression phase, strong bonds may form between the two grains; such effects could not be considered in the previous study.[15]

In the present paper, we want to understand specifically the collisional behavior of silica grains. To this end, we use amorphous silica particles colliding at relatively small velocities, where their interaction is described by either sticking or bouncing. We compare the collision results with the available macroscopic JKR model. In addition, we characterize the changes induced in the material by the collision.

[a] *Fachbereich Physik und Forschungszentrum OPTIMAS, Universität Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany. E-mail: urbassek@rhrk.uni-kl.de; Web: http://www.physik.uni-kl.de/urbassek/*

[b] *Department of Geophysics, Universitas Padjadjaran, Jatinangor, Sumedang 45363, Indonesia*

[c] *CONICET and Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Cuyo, Mendoza, 5500, Argentina*