Negative normal restitution coefficient for the oblique impact of nanoclusters

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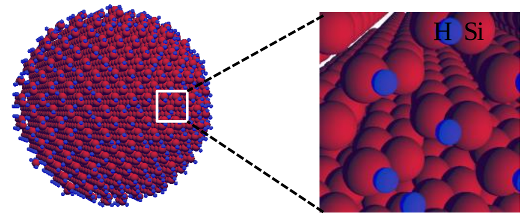
Introduction

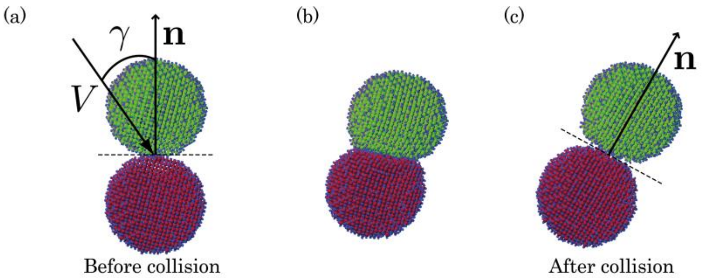
Restitution coefficient *e*, which represents the lost of energy at the impact, has been introduced so far for macroscopic bodies. However, the increasing interest to nano-particles raises an important question to what extent the macroscopic concepts are applicable and do they acquire new features in the nano-world. We have studied the oblique impact of nanoclusters numerically, and demonstrated the macroscopic collision model of adhesive dissipative particles well reproduces the observed behaviors of *e*.

Molecular Dynamics simulation

To demonstrate the oblique impact of nanoclusters, the molecular dynamics (MD) simulation is adopted. The H-passivated Si nanocluster, which is coated by hydrogen atoms to reduce the surface reactivity, is mimicked by the Tersoff potential.



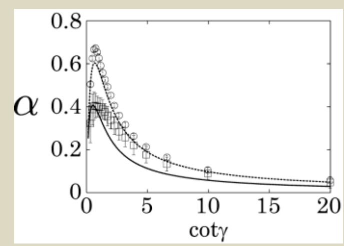
Oblique impact of H-passivated Si nanoclusters



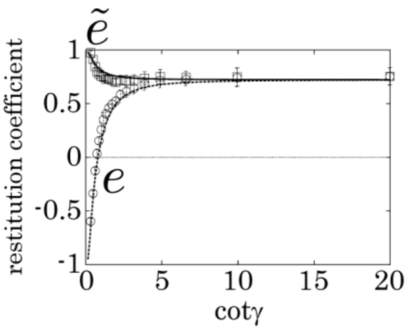
Due to the adhesive force between the colliding two nanoclusters, the duration time cannot be neglected. As a result, a reorientation of the contact plane is occurred. (Left) Dependence of the angular displacement

$$\cos\alpha = \mathbf{n}(0)\cdot\mathbf{n}(t_c)$$

on the incident angle γ.



Restitution coefficients for nanoclusters



Dependence of the normal restitution coefficient of nanoclusters. Here, *e* is defined by the usual manner as

$$e = -\frac{\mathbf{g}(t_c)\cdot\mathbf{n}(0)}{\mathbf{g}(0)\cdot\mathbf{n}(0)}$$

, where g is the relative velocity of colliding nano-clusters

$$\mathbf{g} = \mathbf{v}_{12} + \frac{d}{2}[\mathbf{n}\times\omega_{12}]$$

Because of the reorientation of the contact plane, *e* becomes negative if the angular displacement α is large. We introduce the modified definition of *e*

$$\tilde{e} = -\frac{\mathbf{g}(t_c)\cdot\mathbf{n}(t_c)}{\mathbf{g}(0)\cdot\mathbf{n}(0)}$$

, which is always positive.

Theoretical model for the oblique impact

The impact theory for viscoelastic adhesive particles is adopted to the normal force acting between two nanoclusters. It contains the Hertzian force, JKR force, and the dissipative force.

$$F_H - F_B = \frac{4a^3}{Dd} - \sqrt{\frac{6\pi\sigma}{D}}a^{3/2} \qquad F_D = \dot{a}\eta\left(\frac{12a^2}{Dd} - \frac{3}{2}\sqrt{\frac{6\pi\sigma}{D}}a^{1/2}\right)$$

Because of the reorientation of the contact plane, the inertial force should be considered, and the conversation of the angular momentum leads the equation of motion

$$\mu\frac{d'^2}{dt^2}\xi_n + F_H - F_B + F_D + \frac{\mu V^2 d^2}{(d-\xi_n)^3}\sin^2\gamma = 0$$

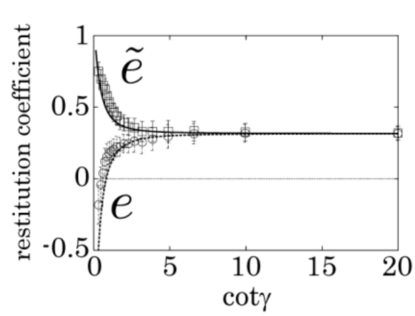
(The solid and broken lines in the figures are calculated from the solution of the above equation of motion.)

Simplified model - modified Lennard-Jones (LJ) nanoclusters

To demonstrate the oblique impact of nanoclusters by a simple model, we adopt modified LJ potential for the interaction between the atoms in the nanoclusters (where C=0.2).

$$\phi(r) = 4\varepsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - C\left(\frac{\sigma}{r}\right)^{6}\right\}$$

The results of the normal restitution coefficients are also well reproduced by the macroscopic theory, and negative restitution coefficient is also observed.



Discussion and Conclusion

There are some discrepancies in the time development of ξ (about 1.0~1.4 times smaller than the MD simulation results). However, we find the characteristics of the inelastic collision of nanoclusters are well explained by the macroscopic theory. We also conclude the anomalous behavior of the restitution coefficient, i.e. negative e, can be observed in the oblique impacts of adhesive macroscopic particles.

Reference Kuniyasu Saitoh, Anna Borova, Hisao Hayakawa, and Nikolai V. Brilliantov
"Negative normal restitution coefficient for nanocluster collisions", accepted to Phys. Rev. Lett. (2010)
arXiv:1005.5429 (2010)