

Research Topic : MD Simulations of Nanoparticle-Substrate Adhesion
Duration : 2006-Present
Sponsor(s) : Intel Corp. and CAMP
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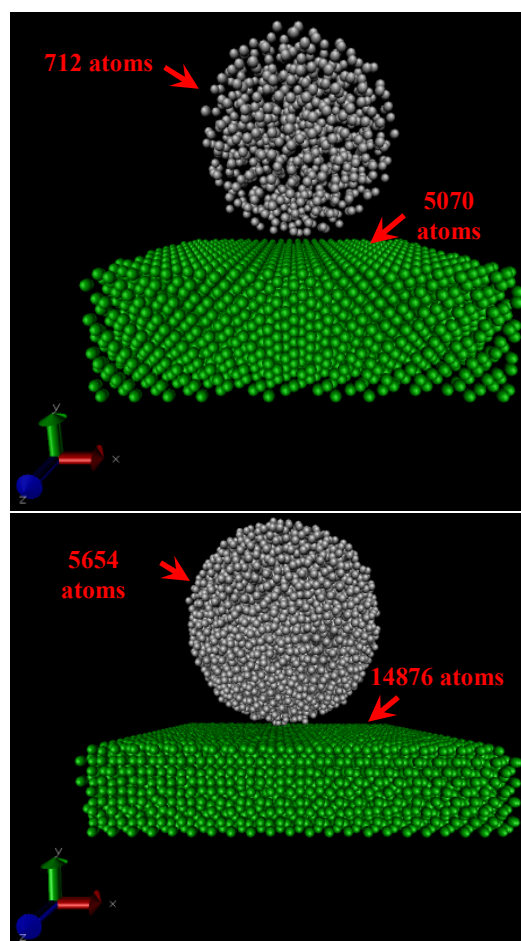
Synopsis of Research and Sponsored Projects

A Molecular Dynamics (MD) simulation study is initiated to gain fundamental understanding of rolling and sliding elasto-adhesion interactions between a spherical nanoparticle and a substrate. This study is needed to understand the modes of particle removal and detachment for cleaning of semiconductor substrates, MEMS, the strength and stability of network of adhered round objects in a diverse spectrum of applications (e.g. particles, powders, blood cells and nanotubes) on micro/nano-scale.

In current simulations, the adhesion between the particle and the substrate due to the Van der Waals forces was modeled by the Lennard-Jones (LJ) 12-6 potential. The particle was pushed towards the substrate (vertically downwards) to obtain the force of interaction between the particle and the substrate. The temperature of the substrate atoms was regulated by periodically scaling to mimic the bulk substrate effect. The total force-displacement curves of the particle in the cases of particle being pushed normally towards the substrate and the particle pushed tangentially, while in adhesion with substrate, were obtained. The minimization parameters were selected such that the adhesion force between the particle and the substrate stays within the limits of adhesion force estimated from the JKR and the DMT theory, as given by the adhesion map.

The simulations were carried out with a 4.2 nm and 7.8 nm silicon particle on a silicon substrate. It was observed that the force required to slide the 4.2 nm particle is lower than rolling. While the forces required to slide and roll a 7.8 nm particle is of the same order. The rolling resistance moment calculated from the slope of the force-displacement curve obtained in the simulations was found to be in good agreement with the theoretical predictions based on a two-dimensional adhesion theory.

Simulations were extended to investigate the removal mechanism for ellipsoidal and irregular particles as these are the very common native particle defects on the semiconductor substrates. In case of the ellipsoidal particle rolling mode is dominant. When an irregular particle in contact with the substrate at two points was subjected to lateral force, the rolling mode was initiated and it resulted in lift-off of the particle from the substrate as most of the particle lost contact with the substrate during rolling.



Recent Publications

M. D. Murthy Peri, C. Cetinkaya, *Molecular Dynamics Simulations of Nanoparticle-Substrate Adhesion Interactions*, Submitted for publication in the Applied Physics Letters.