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Molecular Dynamics Simulations of the Nanoparticle-Substrate Collisions[1] TRAIAN DUMITRICA, PAOLO VALENTINI, Department of Mechanical Engineering, University of Minnesota — Nanoparticle impact allows for the production of high quality thin films. To elucidate the microscopic details of nanoparticle-surface collisions in the low energy range (up to 1 eV/atom) of interest for the hypersonic plasma deposition technology, we have performed molecular dynamics simulations employing incident silicon particles of different sizes that are focused onto a silicon substrate. Our simulations offer a detailed microscopic picture of the dynamics of the collision process, including the energy conversion and redistribution, the local heating and melting, and the nanoparticle-surface bonding. Interestingly, beyond an impacting velocity threshold our simulations identified a soft landing regime mediated by a structural phase transition occurring in the nanoparticle. More insight into the pressure-induced structural phase transition was obtained by separate nanomechanical studies for the response of silicon nanoparticles to compression.

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