Continuum models for nanoparticle-wall collisions

A.P. Weber[1], C. Schöner[2], M. Gensch[1], A. Werner[1], T. Pöschel[2]

[1]Institute of Particle Technology, Technical University of Clausthal, 38678 Clausthal-Zellerfeld, Germany
[2]Institute for Multiscale Simulation, Friedrich-Alexander University, Erlangen-Nuremberg, Germany
Keywords: nanoparticle, mechanical properties, rebound, coefficient of restitution
Presenting author email: alfred.weber@mvt.tu-clausthal.de

While nanoparticles properties such as optical, electronic and magnetic behavior have been studied extensively, their mechanical behavior has been investigated only for quasi-static stressing. Little is known about their mechanical properties at high shear rates such as encountered during high velocity impaction. Most of the knowledge for such stressing is based on Molecular Dynamics (MD) simulations.
In contrast to the significant number of MD simulations of nanoparticles hardly any experimental data are available. Recent experiments have investigated the critical velocity, which is the minimum impact velocity for a particle to bounce, as a function of the particle size (Rennecke and Weber, 2013). There seems to be a transition from the micrometer range down to the nanometer range. While the extrapolation of the critical velocities, as measured in the micrometer range, to the nanoparticle sizes would predict critical velocities of several thousands of m/s, the observed critical velocities of nanoparticles are orders of magnitude lower. This raises the question if there is a transition in the mechanical material properties when reaching the nanorange.

From a more general point of view, but with significant practical implications, it is of interest to elaborate how far simple continuum mechanics can be applied for nanoparticles.

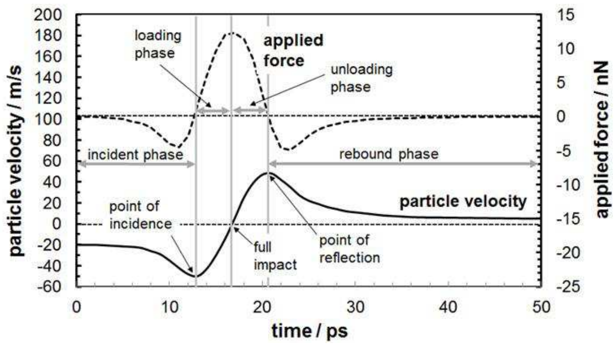

Fig.1. MD simulation of the temporal evolution of particle velocity and applied force for the different phases of a particle-wall collision: incident phase (approach), contact phase (loading/unloading) and rebound phase.

Therefore, a novel approach is taken here to combine molecular dynamics (MD) simulations with nanoparticle impaction experiments to supply the first comprehensive picture of the physics behind the collision of a single dense spherical particle with a wall. While physical parameters before and after the collision are measured by modified single stage low pressure impaction (e.g. impact velocity, bounce velocity, charge transferred to the particle), the details of particle compression (e.g. acceleration due to adhesion forces, applied force and resulting contact area) are retrieved from molecular dynamics simulation (cf. Fig.1).

In Fig.2 the relationship between maximum applied force F_{max} and the Hertz parameter a^3/R (with R=particle radius) as obtained from MD calculations for Ag nanoparticles impaction on a hard target (e.g. mica) is shown.

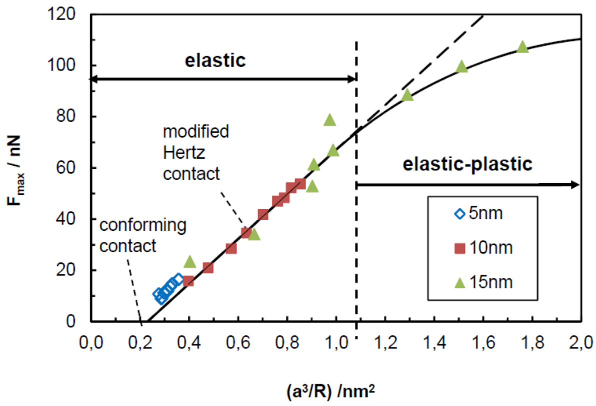

Fig.2. Maximum force vs. Hertz parameter for Ag nanoparticles impacting on a mica target

For the weakly attractive potential between the particle and the target surface a contact area is already formed without an external applied force. Therefore, the Hertz theory has to be modified to account for the nanoparticle deformation behavior (conforming contact). For larger impaction velocities the contact becomes increasingly plastic as also observed in the charge transferred to the particles.

However, the Young modulus obtained from Fig.2 is close to the bulk value of the bulk Pt, while the experimental results point towards a significantly enhanced yield pressure which increases with decreasing particle size. In conclusion, continuum models can be used to describe the particle behavior when appropriate material parameters are used.

This work was supported by the German Research Foundation (DFG) under grantWE 2331/12-2.

Rennecke, S and Weber, A.P.; (2013) *J. Aerosol Sci.* **58**, 135-147