Strong plastic deformation and softening of fast colliding Lennard-Jones nanoparticles by Molecular Dynamics simulations\textsuperscript{1}

YOICHI TAKATO, SURAJIT SEN, State University of New York at Buffalo, JEREMY LECHMAN, Sandia National Laboratories — We present a Molecular Dynamics study of the coefficient of restitution $e$ for colliding two equal sized nanoparticles. Nanoparticles often show distinctly different mechanical and dynamical properties than bulk materials. We investigate the collision velocity $v_{\text{coll}}$ and the nanoparticle size dependence of coefficient of restitution. We find that the size dependent yield velocity $v_Y$, a sharp crossover point between elastic collision and plastic collision, appears to approach the theoretical constant value for macroscopic spheres as the nanoparticle size grows. We also find that above $v_Y$, the coefficient of restitution $e \propto v_{\text{coll}}^{-\alpha}$, where $\alpha \approx 1$, which is distinct from the inelastic macroscopic sphere collision case, $\alpha = 1/4$. It indicates that nanoparticles colliding at high collision velocity are softened. We discuss possible insights of the size dependent yield velocity and the soft nanoparticles above $v_Y$.

\textsuperscript{1}US Army Research Office, Sandia National Laboratories