Abstract Submitted
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High-Velocity Collisions of Nanoparticles DONALD JOHNSON[1], WILLIAM MATTSON, Army Research Laboratory — Nanoparticles (NPs) are a unique class of material with highly functionalizable surfaces and exciting applications. With a large surface-to-volume ratio and potentially high surface tension, shocked nanoparticles might display unique materials behavior. Using density functional theory, we have simulated high-velocity NP collisions under a variety of conditions. NPs composed of diamond-C, cubic-BN, and diamond-Si were considered with particle sizes up to 3.5 nm diameter. Some simulations involved NPs that were destabilized by incorporating internal strain. Normal, spherical NPs were carved out of bulk crystals and structurally optimized while the NPs with internal strain were constructed as a dense core (compressive strain) encompassed by a thin shell (tensile strain). Both on-axis and off-axis collisions were simulated at various speeds. The amount of internal strain was adjusted by varying the compression ratio of the inner core. Collision dynamics, shock propagation, and fragmentation will be presented and analyzed. The effect of material properties, internal strain, and collision velocity on the final temperature of the fragments will be discussed.

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