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High-Velocity Collisions of Nanoparticles DONALD JOHNSON, WILLIAM MATTSON, Army Research Laboratory — Nanoparticles (NPs) are interesting materials with exciting applications due to their large surface-to-volume ratio and functionalizable surfaces. The large surface area and potentially high surface tension might result in unique materials behavior when subject to shock loading. Using density functional theory, we have simulated high-velocity NP collisions producing high-pressure, high-temperature, and extreme shock 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. 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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