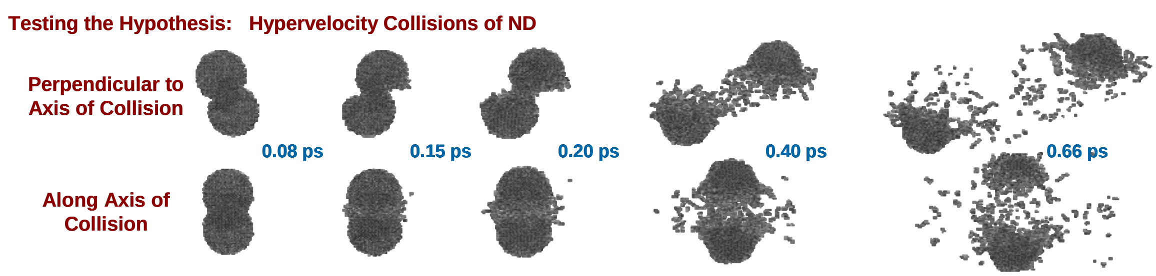
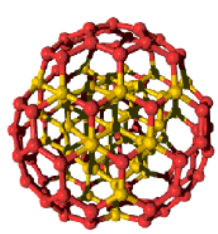
Detonation Nanodiamonds as an Advanced Energy Source

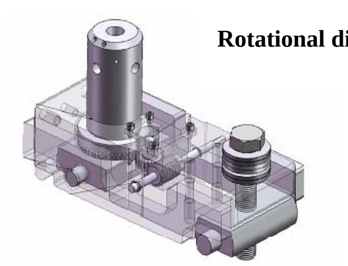
Many simple, stable materials exist which can transition to lower energy states through a solid-solid phase transition. Such transitions are so slow that no useful work is obtained from the corresponding energy release, but in principle, energy can be stored in the intermolecular bonds and rapidly liberated during a phase transition, a phenomenon termed Structural Bond Energy Release (SBER). The Army Research Laboratory is investigating the SBER potential of detonation nanodiamonds (ND) as a viable source for next generation energetic materials. The strained fullerene-type surface of ND leads to compression of the diamond core and causes subtle change in the bonding structure. Quantum mechanical density functional calculations were used to characterize the behavior of two bare, reconstructed ND impacted at 20km/sec. A series of sequential snapshots during this trajectory show that the ND comminutes into mono and multi-atomic fragments moving at high velocities and that these fragments are highly reactive. Such high-velocity reactive particles, when encountering atmospheric gases would result in combustion, thus providing significant energy release. Unlike the idealized ND explored by our computational studies, real ND is a composite structure comprised of a diamond core and an amorphous carbon outer shell. The amorphous carbon shell hinders the initiation of SBER in ND under normal experimental conditions. However, experimental static high-pressure experiments of ND indicate the amorphous carbon shell thins as pressure increases, and greater exposure to the diamond core occurs. To date, these experimental measurements have provided evidence of only slow transitions, but future experiments will focus on combining high-pressure with high-shear/strain conditions, which will substantially lower the transition barrier, using the ARL designed rotational diamond anvil cell. We expect that further theoretical and experimental investigations into the surface morphology and requirements to initiate SBER will allow for a fundamental understanding of the conditions in which rapid release of this energy can be used.



Structure of ND



Rotational diamond anvil cell



Reference/Publication

Mattson, W.D., R. Balu, B.M. Rice, J.A. Ciezak, Exploring structural bond energy release in nanodiamonds using quantum molecular dynamics and static high pressure, *Proceedings of Army Science Conference*, 2008.

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