

Abstract Submitted
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Internal Strain in Nano-Diamond and Boron Nitride WILLIAM MATTSON, DONALD JOHNSON, US Army Research Laboratory — Nanodiamond surfaces undergo reconstruction imposing stress on nanoparticle (NP) core and possibly storing strain energy. The unique way in which these NPs store energy may lead to useful applications, but a greater understanding of strain energy storage/release is needed. In the current work, density functional theory methods are employed to predict structural properties and energetics of C (diamond) and cubic-BN NPs. The goal is to quantify NP core stress and its relationship to surface rearrangement, particle size, and material composition. Initial results suggest different chemical factors drive surface rearrangement, leading to compressive stress in C and tensile stress in BN.

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