Impact properties and related scalings of single layer graphene, hexagonal boron nitride, and hybrid multilayer 2D nanoarmors

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Abstract

Impact properties of single layer graphene and hexagonal boron nitride (BN) 2D nanoarmors have been quantified under C_{60} fullerene hypervelocity impact via Density Functional Tight Binding (DFTB) simulations [1]. For the first time the phenomenon is approached at this level of atomistic modeling accuracy beyond classical molecular dynamics (MD) [2]. Ballistic curves for the two materials, discriminating between projectile penetration and bouncing regimes, were reconstructed. Specific energy absorption (energy absorbed per layer) scalings [3,4] with variable number of layers and spacing were studied, both for homogeneous and hybrid (graphene + BN) multilayers. A surprisingly synergetic interaction between layers emerges not recorded at the micro- and macroscale for graphene armors [5], suggesting a transition in the impact behavior from macro- to nanoscale as atomic interactions become preponderant over mechanics. Results are rationalized via a mechanical impact model [3]. On the basis of the atomistic results, a Finite Element (FEM) continuum model is also proposed for the simulation of impact behavior of composites and larger armor systems at the upper scales. The result may be of importance in the design of graphene- and other 2D materials-based nanocomposites for enhanced crashworthy structures.

References

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