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A hierarchical lattice spring model to simulate the mechanics of 2-D materials-based composites

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It is known that structural biological materials such as bone or dentin show unprecedented damage tolerance, toughness, and strength. The common feature of these materials is their hierarchical heterogeneous structure, which contributes to increased energy dissipation before failure occurring at different scale levels. These structural properties are the key to achieve superior nanocomposites. Here, we develop a numerical model in order to simulate the mechanisms involved in damage progression and energy dissipation at different size scales in composites, which depend both on the heterogeneity of the material (defects or reinforcements) and on the type of hierarchical structure. Both these aspects have been incorporated into a 2-D model based on a Hierarchical Lattice Spring Model approach, accounting for geometrical non-linearities and including statistically based fracture phenomena. The model has been validated by comparing numerical results to linear elastic fracture mechanics predictions as well as to finite elements simulations, and then employed to study how hierarchical structural aspects influence composite material (mainly 2d, e.g., graphene based) properties, which is the main novel feature of the approach. Results obtained with the numerical code highlight the dependence of stress distributions (and therefore crack propagation) on matrix properties and reinforcement dispersion, geometry, and properties, and how the redistribution of stresses after the failure of sacrificial elements is directly involved in the damage tolerance of the material.

Keywords: hierarchical lattice spring model, numerical modeling, fracture mechanics, composite materials, hierarchy

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Introduction

Biological materials often display mechanical properties that differ from traditional engineering materials in that they are capable of simultaneously optimizing competing properties, such as stiffness and density or strength and toughness (Gao et al., 2003; Meyers et al., 2008; Giesa et al., 2011; Ritchie, 2011). The optimization mechanisms found in biomaterials can usually be traced back to their internal structure, which includes various characteristic features, principally heterogeneity and a hierarchical arrangement of microstructural and base components (Zhang et al., 2011; Bosia et al., 2012; Meyers et al., 2013). The challenge in recent years has therefore been to fully understand the mechanisms responsible for such outstanding properties and to replicate them in synthetic materials (Munch et al., 2008; Pugno et al., 2012; Wegst et al., 2015). Composite materials already base their lightweight and directional strengthening properties to the combination of materials with