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Rotation of hard particles in a soft matrix

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ABSTRACT

Soft–hard materials integration is ubiquitous in biological materials and structures in nature and has also attracted growing attention in the bio-inspired design of advanced functional materials, structures and devices. Due to the distinct difference in their mechanical properties, the rotation of hard phases in soft matrixes upon deformation has been acknowledged, yet is lack of theory in mechanics. In this work, we propose a theoretical mechanics framework that can describe the rotation of hard particles in a soft matrix. The rotation of multiple arbitrarily shaped, located and oriented particles with perfectly bonded interfaces in an elastic soft matrix subjected to a far-field tensile loading is established and analytical solutions are derived by using complex potentials and conformal mapping methods. Strong couplings and competitions of the rotation of hard particles among each other are discussed by investigating numbers, relative locations and orientations of particles in the matrix at different loading directions. Extensive finite element analyses are performed to validate theoretical solutions and good agreement of both rotation and stress field between them are achieved. Possible extensions of the present theory to non-rigid particles, viscoelastic matrix and imperfect bonding are also discussed. Finally, by taking advantage of the rotation of hard particles, we exemplify an application in a conceptual design of soft-hard material integrated phononic crystal and demonstrate that phononic band gaps can be successfully tuned with a high accuracy through the mechanical tension-induced rotation of hard particles. The present theory established herein is expected to be of immediate interests to the design of soft–hard materials integration based functional materials, structures and devices with tunable performance via mechanical rotation of hard phases.

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1. Introduction

Soft and hard materials have been seamlessly integrated in biological materials and structures in nature such as the soft organic biopolymer-hard inorganic aragonite integrated structure in mollusk shells (Li, et al., 2004; López & Meyers, 2016; Meyers, et al., 2013; Wang, et al., 2001), the soft proteins and hard mineralized chitin fibrils in the exoskeleton of crustaceans like lobster and crab (Chen, et al., 2008; Fabritius et al., 2012; Fabritius, et al., 2009; Naleway, et al., 2016; Yang et al., 2013), and the soft collagen matrix-hard hydroxyapatite crystal in the bone structures of human body (Gao, 2006; Jäger & Fratzl, 2000; Rho, et al., 1998; Weiner and Wagner, 1998). The inherent physical distinction of these soft and hard phases has led to fundamental differences in their mechanical behavior (Barthelat & Espinosa, 2007; Espinosa, et al., 2009; Meyers, et al., 2008a; Tai et al., 2007). For example, the elastic modulus of the hard aragonite tablets in nacre is three orders of magnitude

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higher than that of the soft organic phase (Barthelat, et al., 2006; Katti, et al., 2001). Nevertheless, such dramatic mismatch in mechanics is harnessed very well in biological structures through elegant and facile integrated organizations such as hierarchical or multi-scale structures and leads to extraordinary mechanical performance as a whole. For example, using computational and nanoscale experimental techniques, Yao et al. unraveled a unusual protection mechanism to external attacks in a deep-sea gastropod *cransomallon squamiferum* that consists of soft–hard interlayered structures (Yao et al., 2010), where the hard layer provides defense against fractures, and the soft layer assists energy dissipation to arrest cracks. Besides, the simultaneous achievement of both high strength and strong toughness of nacre is attributed to the brick-and-mortar arrangement of stiff aragonite bricks and soft protein layers (Li et al., 2004; Meyers, et al., 2008b; Sun & Bhushan, 2012), and have also been confirmed through numerical simulations (Ni, et al., 2015; Pro et al., 2015). For another typical soft–hard integrated biological structure, bone, both computational simulations and nanoscale experiments found that its ductility, toughness and energy dissipation are promoted by nanoscale heterogeneity (Tai et al., 2007). Besides, the staggered structure of the soft and hard phases at the nanoscale in bones leads to a fast attenuation of stress waves (Qwamizadeh, et al., 2015).

Inspired by the soft–hard materials integration in these biological structures, man-made materials and structures have been designed to achieve high mechanical performance (Naleway, et al., 2015; Tang, et al., 2003; Wang, et al., 2016; Wegst, et al., 2015). For example, inspired by layered structures of soft–hard materials integration in nacre, nanocomposites have been designed and prove a ~50% improvement in energy dissipation in comparison with that in individual bulk either hard or soft materials (Espinosa et al., 2011). Staggered mineral platelets and polymer microframes, as another nacre-inspired composite materials, have also been investigated and show that such structured arrangements significantly enhance the post-yield lateral expansion and improve plastic dissipation capability (Wang & Boyce, 2010). In addition to inspirations from nacre, by mimicking the nanocomposite structures in the exoskeleton of crustaceans, Liu incorporated halloysite nanotubes into chitosan, constructed biocompatible composite films and found enhancement of tensile modulus and strength (Liu, et al., 2012). Furthermore, utilizing mechanical mismatch in the soft–hard materials integration, laminated structures have been designed to prevent from fracture and catastrophic damage (Yao, et al., 2015).

In addition to the improvement of mechanical applications such as strength and toughness, soft–hard materials integration has also been utilized in the design of multifunctional electronic devices to achieve good flexibility and stretchability (Libanori et al., 2012). For example, Lacour et al. integrated stiff subcircuit islands on an elastomeric substrate and demonstrated a fundamental architecture for use in stretchable electronics (Lacour, et al., 2006). Skin-like electronics system has also been designed (Gao et al., 2014; Kim et al., 2011a; Xu et al., 2015; Xu et al., 2013; Xu et al., 2014), where the soft elastomeric substrate is employed to accommodate the large deformation, and the hard metal circuits are integrated to achieve functionalities. As another examples, integrating hard particles into soft elastomeric matrixes has been utilized to obtain magneto-active elastomers (Castañeda & Galipeau, 2011; Danas, et al., 2012; Tian, et al., 2011) and phononic metamaterials (Liu et al., 2000; Wang, et al., 2004; Wu et al., 2014; Yang, et al., 2008).

The unique properties of soft–hard integrated natural or man-made materials, structures and devices are closely underpinned by the soft–hard interactions, where the rotation of hard phases in a soft matrix has been considered to be very critical and plays a significant role in the entire mechanical properties and functionalities. For instance, the rotation of fibers in soft collagenous tissues is considered to account for the anisotropic and nonlinear stress–strain behavior of the tissues upon deformation (Lanir, 1979). In situ experimental observations show a clear rotation of the hard aragonite nanograins (nanoparticles) in the soft organic biopolymer in nacre under tension (Li, et al., 2006). This rotation is also considered as a primary deformation mechanism that leads to extraordinary toughness and energy dissipation (Ortiz & Boyce, 2008; Sun & Bhushan, 2012). Similar rotation phenomena have also been found in synthetic polymer materials and are closely associated with their unusual mechanical properties. For example, a prodigious negative Poisson's ratio as large as -12 has been achieved in a biocompatible polytetrafluoroethylene due to the rotation of hard nodal particles in the soft fibril network (Caddock & Evans, 1989). Moreover, for polymeric elastomer containing a low concentration of hard segments, in situ mechanical and X-ray measurements indicate that the hard segments rotate toward the stretching direction to accommodate an extraordinarily high strains up to 500% (Yeh, et al., 2003). The rotation of the hard phases or particles in composite materials has proved to significantly affect functionalities either globally or locally such as conductivity (Kushch & Knyazeva, 2016), acoustic band structures (Goffaux & Vigneron, 2001; Susa, 2002; Wu & Chen, 2007) and surface morphologies (Guttag & Boyce, 2015). In the soft–hard materials integrated electronic devices, the rotation of hard subcircuit islands and metal wires has been utilized to mitigate the strain and improve the overall stretchability of the devices (Lu & Yang, 2015; Zhang et al., 2015). From fundamental mechanics point of view, the rotation of hard materials in soft matrixes is led by their mechanical deformation mismatch, and strongly depends on the geometric shape, fraction of hard materials and orientations of external loadings, yet a theoretical framework in mechanics is lacking.

In this paper, we will establish a mechanics theory to quantitatively describe the rotation of arbitrarily shaped, located and oriented hard particles in a soft elastic matrix subjected to a far-field tensile stress. These particles are assumed to be rigid and perfectly bonded with the soft matrix. This study is purely mechanical and is conducted within the framework of continuum mechanics in a two-dimensional plane. The details of theoretical framework of the rotation of hard particles are presented in Section 2 by considering geometric nonlinearity on the basis of the complex variable method and superposition principle. An explicit theoretical formulation and solution to the rotation of a single arbitrarily shaped particle in the matrix is provided in Section 3. Numerical modeling and finite element analysis (FEA) simulations are performed to validate theoretical analysis in Section 4. Then, we exemplify an application of mechanical tension-induced rotation of a periodic hard particle in soft–hard materials integrated metamaterials to tune phononic band gaps in Section 5. In Section 6, we

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