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Letter

Local buckling analysis of biological nanocomposites based on a beam-spring model

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ABSTRACT

Biological materials such as bone, tooth, and nacre are load-bearing nanocomposites composed of mineral and protein. Since the mineral crystals often have slender geometry, the nanocomposites are susceptible to buckle under the compressive load. In this paper, we analyze the local buckling behaviors of the nanocomposite structure of the biological materials using a beam-spring model by which we can consider plenty of mineral crystals and their interaction in our analysis compared with existing studies. We show that there is a transition of the buckling behaviors from a local buckling mode to a global one when we continuously increase the aspect ratio of mineral, leading to an increase of the buckling strength which levels off to the strength of the composites reinforced with continuous crystals. We find that the contact condition at the mineral tips has a striking effect on the local buckling mode at small aspect ratio, but the effect diminishes when the aspect ratio is large. Our analyses also show that the staggered arrangement of mineral plays a central role in the stability of the biological nanocomposites.

Materials scientists have arrived at a consensus that biological nanocomposites, such as bone, tooth, nacre have superior mechanical properties due to the exquisite design of their microstructure from nano to macroscale [1–6]. It was shown that there is a convergent nanocomposite structure consisting of mineral crystals and protein where the minerals often have large aspect ratio and staggered arrangement in the protein matrix [1,7–11]. A multitude of studies showed that this nanocomposite structure plays a central role in the mechanical properties from stiffness to strength and fracture toughness [12–17], which provided valuable insights into the mechanical principles of the design of biological nanocomposites.

However, the mechanical behaviors of biological materials under compressive load have not yet been understood. Because the mineral crystals have high aspect ratio, and protein is up to three orders of magnitude softer than mineral, the nanocomposite structures are susceptible to buckle under compression. Therefore, it is interesting to ask the question how the biological materials deal with the possible buckling problem. Ji et al. [18] studied the buckling behaviors of a single mineral in the nanocomposites with the assumption that its neighboring minerals remain unbuckled, i.e., the interaction between minerals are not considered, which leads to a higher buckling mode. Su et al. [19] studied the buckling behaviors of two neighboring minerals in a periodic unit by considering the coordination among the adjacent mineral crystals. The symmetric and anti-symmetric buckling modes were identified by using the perturbation method, and corresponding buckling strength for each mode was derived. They showed that the anti-symmetric mode often happens at small aspect ratio, but the symmetric mode at high aspect ratio, and their buckling strength both asymptotically approached to that of the continuous fiber reinforced composites predicted by the Rosen model [20,21].

Those previous studies generally limited their analysis within a periodic unit, and the interaction among minerals beyond the unit is not considered. However, the buckling behaviors of composite structure at larger scale with many minerals should be much different. In this paper, we develop a simple beam-spring model, with which the buckling behaviors of a system with plenty of minerals can be analyzed, where the mineral is modeled by Euler beam while the matrix by distributed elastic spring. We focus on the effect of aspect ratio of minerals and the contact condition at the mineral tips on the buckling behaviors of the biocomposites.

It is arduous to analyze the buckling behaviors of the composite structure with many mineral crystals even using numerical method. An obstacle of such analysis is that massive elements must be used to discretize the mineral and protein system in order to get accurate buckling modes and strength using conventional

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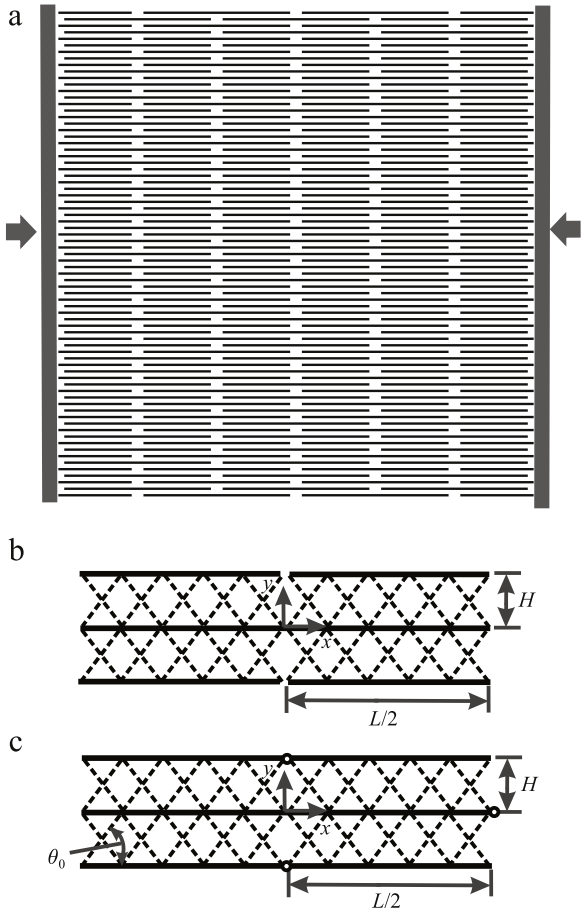

Fig. 1. The beam-spring model of the nanocomposite structure of biological materials. (a) Finite element method (FEM) model of the nanocomposite in which the minerals are staggered in the protein matrix. Rigid body plates are used to apply compressive loads at the left and right boundaries; (b) Free-staggered model of the periodic unit, where there is no contact at the mineral tips; (c) Pinned-staggered model of the periodic unit, where there is point contact at the mineral tips modeled by pinned joints.

2D or 3D elements, which, however, brings unfordable computing workload. In order to address this difficulty, here we introduce the beam-spring model, in which the mineral is modeled by Euler beam while the matrix is simplified by distributed elastic springs between minerals. Fig. 1(a) depicts the model of the nanocomposite structure based on the beam-spring model. The mineral is arranged in a staggered manner, while the springs are arranged in a X-type pattern, as shown in Fig. 1(b) and 1(c). In addition, we consider two kinds of contact conditions between mineral tips along the longitudinal direction of mineral—one is no contact between the tips under the compressive load (Fig. 1(b)), while the other is point contact between the tips (Fig. 1(c)) modeled by a pinned joint. There are up to 3640 minerals in the whole system. A homemade FORTRAN program is used to create nodes and elements and a MATLAB program to build the connection of springs with minerals and assemble the whole system, and then create the input file for ABAQUS program. In order to apply uniform compressive load, a rigid plate is placed at each loading boundary at the left and right, while the top and bottom ones are maintained as straight lines by using the "coupled degrees of freedom" method (Fig. 1(a)).

The effective Young's modulus E_P and shear modulus G_P of protein as function of spring constant K can be derived as (see the Supporting Materials (Appendix A) for detailed derivations),

$$\begin{cases} E_P = K\rho_x H, \\ G_P = K\rho_x H\cos^2\theta_0 = E_P\cos^2\theta_0, \end{cases} \tag{1}$$

where ρ_x is the number density of springs along the beam length. Considering Poisson's ratio of protein is almost equal to 0.5, we get $\theta_0 = 54.7^o$ (the angle between right slanting spring and the positive direction of x axis), and $H = h_P$ is the thickness of protein layer.

The effective Young's modulus of the nanocomposite structure is then derived using the tension-shear chain model as [8,10]

$$\frac{1}{E} = \frac{4(1-\Phi)}{K\rho_x H\cos^2\theta_0\Phi^2\rho^2} + \frac{1}{\Phi E_M} \tag{2}$$

where $\rho = \frac{L}{h_M}$, E_M, Φ are the aspect ratio, Young's modulus, and volume fraction of mineral, respectively, in which L and h_M are the length and thickness of mineral crystals, respectively. We verified that the predictions of Eq. (2) agree well with our FEM calculations, which suggests that our beam-spring model can well describe the mechanics of the nanocomposite structure.

We first analyzed the buckling behaviors of the nanocomposite structure for the non-contact condition at the mineral tips (free-staggered model) at different aspect ratios of mineral. We found that the buckling mode was largely dependent on the aspect ratio, as shown in Fig. 2. When the aspect ratio was small (i.e., $\rho = 5$), the mineral crystals were prone to have rigid body rotation without bending, while the protein had both shear and tensile/compressive deformation. Note that the nanocomposite exhibited a typical local buckling mode with a periodic pattern along both horizontal and vertical direction; when the aspect ratio was increased to $\rho = 10$, the mineral crystals then had both rigid body rotation and bending deformation, and protein undertook both shear and tensile deformation; if the aspect ratio was further increased to $\rho = 30$, mineral crystal had more bending but less rigid body rotation, and protein undertook more shear deformation with slight lateral stretching at the end of minerals; finally, minerals undertook pure bending and protein had pure shearing when the aspect ratio was increased to as high as $\rho = 50$, at which the buckling mode approached to that of Rosen's model, a global shear buckling mode [20].

In the Rosen buckling mode, the continuous fibers undertake pure bending deformation, while soft matrix has pure shear deformation. The buckling strength of this buckling mode is given by Rosen's model as [19]

$$\sigma_c = E_P\left[\frac{1}{2(1+\upsilon_P)(1-\Phi)} + \frac{\pi^2\Phi\kappa}{3\rho^2}\right], \tag{3}$$

where υ_P is Poisson's ratio of protein, and $\kappa = \frac{E_M}{E_P}$. The critical buckling strength predicted by the beam-spring model based FEM simulations is close to that of Eq. (3), which again validates the beam-spring model.

We then analyzed the buckling behaviors of the nanocomposites with point contact condition (pinned-staggered model) at different aspect ratios, as illustrated in Fig. 3. We see that at the small aspect ratio ($\rho = 5$), the buckling deformation severely localized at the loading boundaries and degraded towards the center of the materials, which is different from the behaviors of the free-staggered model. The mineral crystals near the loading boundary were prone to have rigid body rotation without bending, while the minerals away from the boundary hardly deformed; when the aspect ratio was increased to $\rho = 10$, the material started to exhibit a feature of global buckling, and the mineral crystals undertook both rigid body rotation and bending deformation, while protein had both shear and tensile deformation; when the aspect ratio was further increased to $\rho = 30$ and up, the buckling mode exhibited a pure shearing mode, approaching to that of Rosen's model.

Our results showed that the aspect ratio of minerals plays a paramount role in the buckling behaviors of nanocomposite structure where the mineral are laid in a staggered manner in