STAGGERING AND HIERARCHY SELECTED BY LOAD-BEARING BIOLOGICAL MATERIALS FOR MAXIMAL TOUGHNESS

Zuoqi Zhang[*a)], Bin Liu[**], Yongwei Zhang[*], Huajian Gao[***] & Keh-Chih Hwang[**]
[*]*Institute of High Performance Computing, A*STAR, Singapore, 138632, Singapore*
[**]*Department of Engineering Mechanics, Tsinghua University, Beijing, 100084, China*
[***]*School of Engineering, Brown University, Providence, RI 02912, USA*

Summary Load-bearing biological materials such as shell, mineralized tendon and bone generically exhibit staggered structure at nanoscale, while show 2-7 levels of structural hierarchy from nanoscale, to micro-scale and macro-scale. Through these fabulous structures, the biological materials achieve overall good performances from brittle minerals and soft proteins. Two key questions remain unanswered or answered not enough are: why staggered structures are selected by nature and what determines the number of hierarchical levels in these materials. To address the first question, we developed a universal framework to characterize the mechanical properties of various microstructures, and showed that staggered structures can provide superior overall properties. For the second question, we developed a quasi-self-similar hierarchical model to show that, depending on the mineral content, there exists an optimal hierarchy for maximal toughness of biocomposites. These studies are helpful to understand the structure-property relationship in biocomposites and design bio-inspired green (environment-friendly) materials.

BACKGROUNDS AND MOTIVATIONS

Fig. 1 shows a typical structure of bone, with the staggering structure [1] and 7 levels of hierarchy [2]. Through this fabulous structure, bone achieves superior mechanical properties from brittle mineral and soft protein. Mechanics and materials scientists have been trying to understand the structure-property relationship and also trying to develop bio-mimetic materials. However, two questions are still not well answered. The first one is, why the staggering structure is adopted by nature. The second one is why there are just several levels of hierarchy (e.g., 7 for bone).

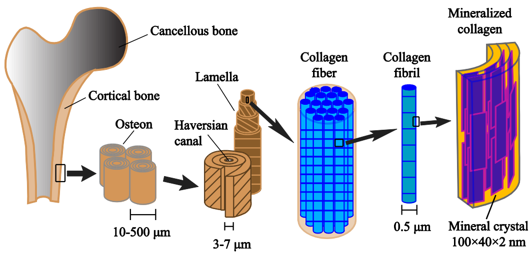

Fig. 1. A typical structure of bone

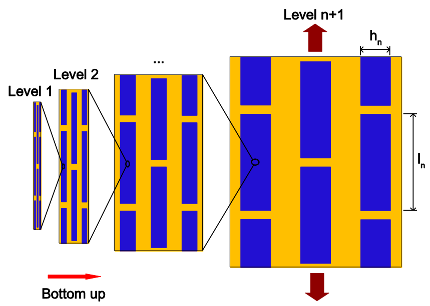

Fig. 2. A quasi-self-similar model for hierarchical biological materials

A UNIVERSIAL FRAMEWORK FOR STAGGERED STRUCTURES

Actually, we can see different staggering structures in bone and shell. In bone, it is stairwise, while in shell somehow random. Previously, Ji and Gao proposed tension-shear chain model [1]. In their model, mineral just sustain tensile force while protein just bear shear force, so that the staggering composite is simplified into a one-dimension chain. Adopting the basic spirit of tension-shear chain model and the principle of minimum complimentary energy, we developed a universal framework for arbitrary platelet distributions [3]. The effects of platelet distribution are incorporated into four dimensionless factors, β_1, β_2, β_3 and β_4. The Young's modulus can be expressed in terms of β_1 and β_2

$$E = \frac{1}{\dfrac{\beta_1}{\phi E_m} + \dfrac{\beta_2 (1-\phi)}{\phi^2 \rho^2 G_p}}, \tag{1}$$

and therefore β_1 and β_2 are named stiffness distribution factors. Note that ϕ, ρ and E_m are the volume fraction, aspect ratio and Young's modulus of mineral platelets, respectively, while G_p denotes the shear modulus of the protein matrix. The strength depends on β_3 and β_4 as

[a)] Corresponding author. Email: zhangzq@ihpc.a-star.edu.sg.

$$\sigma_{critical}=\begin{cases}\phi\tau^{p}_{critical}\cdot\dfrac{1}{\beta_4}\rho & \rho\le\rho_{critical}\\ \phi\sigma^{m}_{critical}\cdot\dfrac{1}{\beta_3} & \rho>\rho_{critical}\end{cases}, \tag{2}$$

and thus β_3 and β_4 are named strength distribution factors. In Eq. (2), $\rho_{critical}=\beta_4\sigma^{m}_{critical}/\beta_3\tau^{p}_{critical}$ is the critical aspect ratio, $\sigma^{m}_{critical}$ is the normal strength of the mineral platelets, and $\tau^{p}_{critical}$ is the shear strength of the protein matrix. Combining Eqs. (1) and (2), the failure strain and energy storage capacity can be got as below

$$\varepsilon_{critical}=\sigma_{critical}/E, \tag{3}$$

$$w_{critical}=\sigma^{2}_{critical}/(2E). \tag{4}$$

Here, energy storage capacity is an index related to toughness, indicating how much energy can be dissipated during composite failure.

The distribution factors can be analytically derived for various structures, for example, continuous layering, regular staggering, stair-wise staggering, and random staggering, so that the advantages and disadvantages of these structures can be easily obtained through comparing these factors. For details, see the reference [3]. Comparative study indicates that staggering structures are superior in stiffness, strength, ductility and rupture toughness, which may provide a possible answer to the first question aforementioned, why the staggering structure is widely adopted by nature.

A QUASI-SELF-SIMILAR MODEL FOR HIERARCHICAL BIOLOGICAL MATERIALS

Structural hierarchy is a universal strategy for biological materials to achieve their specific properties and functions. For instance, bone has 7 levels of hierarchy, mineralized tendon fiber has 4 levels, and shell has 2-3 levels. Especially, the mineralized tendon fiber, the structures in different level are well-ordered and somehow similar. Here, a quasi-self-similar model was developed for these hierarchical materials [4]. In the two-dimension model, every level has hard inclusion aligned in a staggered pattern in soft matrix; the aspect ratio of hard inclusion varies from level to level; and the structure level *n* serves as hard inclusion in level *n*+1. The principles of design observed in load-bearing biological materials are adopted: 1. Principles of flaw tolerance [1] which indicates that material strength would become insensitive to pre-existing cracks when the platelet thickness is smaller than a critical size; 2. Principle of equal strength and efficient stress-transfer; equal strength is to make hard phase and soft phase reach their strength simultaneously so that both of them are utilized efficiently; efficient stress-transfer is a well-known concept from composites science; 3. Limited selection of constituent materials which is a fact recognized from experimental observations; it is well known that bone-like materials consist of mainly mineral crystals and type I collagen; for example, type I collagen occupies about 90 percent of all proteins in bone. With the mechanical parameters and volume fractions of constituent materials given, an *N*-level hierarchical composite can be designed according to these principles. Furthermore, the stiffness, strength, fracture toughness and flaw-tolerant size of the hierarchical composites can be plotted against the level number *N* of structural hierarchy. For details, see the reference [4].

Our results suggest that there is an optimal level number *N* for maximum toughness of the hierarchical composites. The predictions by the quasi-self-similar model for mineralized tendon, bone and shell are all in good agreement with experimental observations. The level number of hierarchy is selected by load-bearing biological materials for maximum toughness, which suggests an answer to the second question aforementioned, why there are just several levels of hierarchy in biological materials.

CONCLUSIONS

The main results of the above studies can be summarized as follows:

1. A universal framework was developed for arbitrary staggered platelet distributions; comparative studies show staggering structures could achieve overall excellent mechanical properties;
2. A quasi-self-similar model was proposed to study load-bearing biological materials; optimal hierarchies are predicted for maximum toughness, and agree well with experimental observations;
3. Our models and conclusions here are helpful to understand structure-property relationship in biological materials, and also helpful to design bio-inspired “green materials” (high- efficiency, degradable, environment friendly, etc.).

References

[1]. Ji, B., Gao, H.: Mechanical properties of nanostructure of biological materials. J. Mech. Phys. Solids **52**: 1963-1990, 2004.
[2]. Rho J-Y, Kuhn-Spearing L., Zioupos P.: Mechanical properties and the hierarchical structure of bone. Med Eng Phys **20**:92-102, 1998.
[3]. Zhang Z. Q., Liu B., Huang Y., Hwang K. C., Gao H. J.: Mechanical properties of unidirectional nanocomposites with non-uniformly or randomly staggered platelet distribution. J Mech Phys Solids, **58**: 1646-1660, 2010.
[4]. Zhang Z. Q., Zhang Y. W., Gao H. J.: On optimal hierarchy of load-bearing biological materials. Proc R Soc B, **278**: 529-525, 2011.