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Crack propagation in bone at the microscale: effect of the interfibrillar glue molecules with sacrificial bonds and hidden length

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ABSTRACT

Sacrificial bonds and hidden length (SBHL) in structural molecules provide a mechanism for energy dissipation at the nanoscale. It is hypothesized that their presence leads to greater fracture toughness than what is observed in synthetic materials without such features. Here, we investigate this hypothesis using a simplified model of a mineralized collagen fibril sliding on a polymeric interface with SBHL systems. A 1D coarse-grained nonlinear spring-mass system is used to model the fibril. Rate-and-displacement constitutive equations are used to describe the mechanical properties of the polymeric system. The model quantifies how the interface toughness increases as a function of polymer density and number of sacrificial bonds. Other characteristics of the SBHL system, such as the length of hidden loops and the strength of the bonds, are found to influence the results. The model also gives insight into the variations in the mechanical behavior in response to physiological changes, such as the degree of mineralization of the collagen fibril and polymer density in the interfibrillar matrix. The model results provide constraints relevant for biomimetic material design and multiscale modeling of fracture in human bone.

*Introduction: I*n this article, we focus on the mechanical response of a single mineralized collagen fibril sliding on a polymeric layer that includes SBHL systems [1]. The fibril utilizes the breakage of sacrificial bonds and the release of hidden length to dissipate energy while being stretched. This process introduces a microscopic mechanism for fracture resistance [2].The mechanical behavior of the polymer backbone is described by the worm-like chain model [e1]. The existence of SBHL systems is incorporated in this model by introducing a dynamical variable: the available length [3], which is the difference between the polymer contour length and the sum of the unfolded length of the hidden loops. The rate dependence of the SBHL system is modeled using the transition state theory [4,5]. In this article we will implement the rate and displacement model developed by Lieou et al. [5] as the constitutive law for the polymeric layer with SBHL system. We developed a coarse grained model for the mineralized collagen fibril with polymeric glue. The system is integrated in the quasistatic limit which is proved to be equivalent to dynamic analysis in our study and is appropriate for exploring nucleation characteristics and stable crack growth speeds. Many cohesive law formulations exist in mechanics literature and some of them have been used in the context of multiscale modeling of bone fracture [e.g., Ref. 6 and references therein]. Our approach is different in the sense that the cohesive law is derived based on physical principles. The constitutive law parameters (such as peak force, maximum elongation, and fracture energy) vary in response to variations in the internal variables (e.g., polymer density and number of sacrificial bonds) in a self-consistent way. Hence, the proposed approach has a more predictive power and is capable of integrating small scale physics in multiscale simulations without prior assumptions on the specific shape of the cohesive law.

*Results and discussion: O*ur numerical results show that the sacrificial bonds and hidden length system generally increases energy dissipation and resists crack propagation. The presence of SBHL system increases the system toughness (~8.5%), increases the critical crack size that has to be reached before dynamic instability is triggered (~10%), and it also reduces the stable crack growth speed (~5%). The exact numbers depend on the assumptions of model and simulations.

We have also shown that the increase in the polymer density leads to an increase in energy dissipation, peak resistance force, and ductility. Because the number of polymers produced by the osteocytes may decrease as the individual ages [7], this investigation reveals that a possible mechanism for bone toughness degradation with age, other than loss of bone density, is the reduction in polymer density. The degree of mineralization of the collagen fibril is another factor controlling the fracture properties of bone. We have found that within the elastic regime of the fibril, the average crack propagation speed along the interface increases as the percentage of mineralization increases. On the other hand, for unmineralized fibrils and high polymer density the system fails by strain localization within the fibril rather than by slip along the interface. This mode of failure is brittle and prevents the full utilization of the SBHL system. With aging, the degree of mineralization is reduced [9, 10, 11] and this may be another mechanism for frequent bone fractures in the elderly.

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REFERENCES

[1] Thompson, JB. Kindt, JH. Drake, B. Hansma, HG. Morse, DE., et al., Bone indentation recovery time correlates with bond reforming time. *Nature*. 2001, 414, 773–775.

[2] Fantner, GE. Hassenkam, T. Kindt, JH. Weaver, JC. Birkedal, H., Sacrificial bonds and hidden length dissipate energy as mineralized fibrils separate during bone fracture. *Nature Materials.* 2005, 4, 612–616.

[3] Elbanna, AE. Carlson, JM, Dynamics of polymer molecules with sacrificial bond and hidden length systems: towards a physically-based mesoscopic constitutive law. *PLoS ONE*. 2013, 8(4), e56118. DOI:10.1371/journal.pone.0056118.

[4] Bell, G.I., Models for the specific adhesion of cells to cells. *Science.* 1978. 200, 618.

[5] Lieou, C.K., Elbanna, A.E., Carlson, J.M. Sacrificial bonds and hidden length in biomaterials: a kinetic constitutive description of strength and toughness in bone. *Physical Review E*. 2013, 88(1), 012703.

[6] Buehler, M., Molecular nanomechanics of nascent bone: fibrillar toughening by mineralization. *Nanotechnology.* 2007, 18, 295102.

[7] Ural, A. Mischinski, S., Multiscale modeling of bone fracture using cohesive finite elements. *Engineering Fracture Mechanics*. 2013, 103, 141–152.

[8] Hansma, P.K., Fantner, G.E., Kindt, J.H., Thurner, P.J., Schitter, G., et al. Sacrificial bonds in the interfibrillar matrix of bone. *J. Musculoskelet Neuronal Interact*. 2005, 5(4), 313–315.

[9] Nallaa, RK, Kruzica, JJ, Kinney, JH, Ritchie, RO. Effect of aging on the toughness of human cortical bone: evaluation by R-curves. *Bone*. 2004, 35, 1240–1246.

[10] Koester, K.J., Barth, H.D., Ritchie, R.O. Effect of aging on the transverse toughness of human cortical bone: evaluation by R-curves. *Journal of the Mechanical Behavior of Biomedical Material*. 2013, 4, 1504–1513.

[11] Nair, A.K., Gautieri, A., Chang, S.W., Buehler, M. Molecular mechanics of mineralized collagen fibrils in bone. *Nature Communications*. 2013, 4, 1724.