MICROCRACK NUCLEATION AND FRACTURE IN BONE ULTRASTRUCTURE: A COMPUTATIONAL STUDY

Hamid Alijani (1), Ted J.Vaughan (1)

1. Biomedical Engineering and Biomechanics Research Centre, School of Engineering, College of Science and Engineering, University of Galway, Galway, Ireland.

Introduction

Bone is a natural biological composite material that demonstrates outstanding mechanical properties, which is mainly due to the intricate arrangement of its constituents across seven hierarchical levels [1]. At the macro-level, two types of bone can be identified: a dense cortical shell and spongy trabecular core, both of which comprise of lamellar bone at ultrastructural level. Much work has been done to understand structure-property relationships for the elastic behaviour of the tissue. For example, A power law equation ($E \propto \rho^{\alpha}$) can relate elastic modulus (E) to density (ρ) at the macrostructural level, but for the tissue level (mm scale), more complicated models are needed to account for structure and density [2], [3]. However, beyond the elastic regime (e.g. fracture behaviour), these relationships tend to break down and we need more involved models at each structural level to predict bone biomechanics. The objective of this study is to investigate the fracture behaviour of lamellar bone, focusing on the onset and evolution of microcracks in the bone ultrastructure.

Methods

Two-dimensional geometries of the bone ultrastructure were created in in finite element package ABAQUS comprising of cylindrical mineralised collagen fibrils (MCFs) embedded through an extra-fibrillar matrix (Figure 1). Between the minerals (transversely anisotropic elastic material [4]) and around the MCFs there are interphase regions filled with non-collagenous proteins (NCPs) that mediate bonding mineral-mineral and mineral-MCFs respectively. The MCFs were modelled as transversely anisotropic elastic-linear plastic material [5] through Hill48 plastic potential [6]. The interphases between the material components were considered to have the same material properties with an exception of fracture strength and were described through a phase-field damage model, which was implemented through a UMAT subroutine in the Abaqus finite element package. This method is capable of capturing the onset and propagation of microcracks and takes a non-local order parameter ϕ to describe the material condition with $\phi = 0$ for intact material and $\phi = 1$ describing fully broken material. The created model of tissue with and without a notch were then stretched to study the onset and evolution of microcracks, respectively. Meanwhile, a parametric study was carried out by varying the MCFs volume fraction as well as the interphase strength ratios to capture their role in bone biomechanics.

Results and Discussion

It was found that microcracks emerged from mineral rich area of the extra-fibrillar space under both transverse and axial loading, when the interphase strength of MCFs was higher than the interphase between minerals ($\sigma_{\text{interphaseMCF}} > \sigma_{\text{interphaseHA}}$). On the other hand, once $\sigma_{\text{interphaseMCF}} < \sigma_{\text{interphaseHA}}$, the microcracks showed no preference between the interphase regions under uniaxial loading. Simulating crack propagation in notched specimens demonstrated that MCFs do not affect the crack path at low MCF volume fractions. However, at the high volume fractions, it was found that MCFs could either facilitate cracking when $\sigma_{\text{interphaseMCF}} < \sigma_{\text{interphaseHA}}$ or act as a barrier to crack propagation when $\sigma_{\text{interphaseMCF}} > \sigma_{\text{interphaseHA}}$ (see Figure 1b). This implies that indeed the interphase region filled with NCPs dictates the failure behaviour of tissue under transverse loading at physiological $\text{Vf}_{\text{MCF}} = 50\%$. Under axial loading, we saw that their effect is less pronounced (Figure 1a).

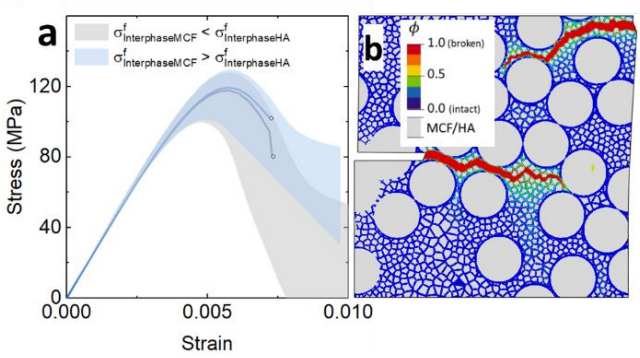

Figure 1: (a) tissue effective properties under axial loading with different interphase strengths. (b) order parameter distribution for tissue under transverse loading when $\sigma_{interphaseMCF} > \sigma_{interphaseHA}$.

References

1. Launey et al., Annual Review of Materials Research. 2010.
2. Nobakhti et al., Curr. Osteoporos. Rep. 16:404-410, 2018.
3. Alijani et al., J. Mech. Behav. Biomed. Mater. 129: 105139, 2022.
4. Lin et al., J. Phys. Chem. C. 120, 9: 4975–4992, 2016.
5. Buehler et al., Nanotechnology. 18, 29, 2007.
6. Yan et al., J. Manuf. Process. 20, 46–53, 2015.

Acknowledgements

This work was supported by the European Research Council (ERC) under the grant agreement No. 804108.