INVESTIGATION OF THE IMPACT OF NANOSCALE GEOMETRY ON THE MECHANICAL PROPERTIES OF HYDROXYAPATITE PLATELETS

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Introduction

The increase in bone fracture risk with age is generally explained by a loss of bone mass and an alteration in the skeletal architecture, but those effects contribute to only 75% of the increased risk of fracture. Recent studies have shown how changes in bone tissue mechanical properties could be a reasonable explanation for the remaining part of the age-related fracture risk increase [1]. Previous computational studies already associated properties of hydroxyapatite platelets with mechanical properties of bone nanocomposites. It has been observed, for example, that the size of hydroxyapatite crystals can influence the crack propagation at the nanoscale level [2], and that the nanosize confinement of HAP crystals controls the mechanical properties of the collagen-hydroxyapatite interface [3]. From an experimental point of view, whether and how the crystal platelets change with age is an open and still debated issue. Measurements of HAP platelets dimensions have been performed on mice [4] and human [5][6] bone samples using X-ray diffraction, Fourier-transform infrared spectroscopy (FTIR) and electron microscopy, without establishing a unique correlation between their dimensions and age, both because of limitation of indirect measurement techniques (in which size changes could be a hypothesis, but not the only factor that plays a role) and because of the very small number of bone samples usually considered in each study. In our work we systematically investigate, through computer simulations, what is the effect of hydroxyapatite platelets' size on their mechanical properties, to test the effect of aging on this crucial bone component.

Methods

We perform full atomistic molecular dynamics (MD) simulations of hydroxyapatite nanocrystals using the Interface Force Field (IFF) as an effective potential [7]. We study variations in hydroxyapatite platelets size in all the crystallographic directions *a*,*b*, and *c*. In particular we consider three different samples: 'small' (200Åx100Åx20Å),'medium' (500Åx250Åx50Å), and 'large' (1500Åx800Åx100Å), based on experimental measurements in the literature. To assess hydroxyapatite single crystal mechanical properties, we perform uniaxial tension and compression tests along all three spatial directions, obtaining stress-strain curves and studying the maps of the per-atom stresses.

Results

In the following we show a preliminary result with the comparison of the stress-strain curves for platelets of different sizes (Fig. 1) and of the mechanical properties we computed for them (Tab. 1).

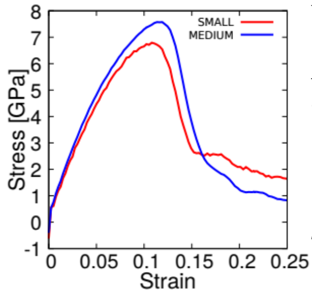

Figure 1: Stress-strain curves obtained from uniaxial tension test in the y direction for the 'small' platelet (red) and for the 'medium' one (blue).

Platelet Size [Å^3]	Elastic Modulus [GPa]	Ultimate strength [GPa]
200x100x20	137.809	6.792
500x250x50	128.724	7.573

Table 1: Mechanical parameters of platelets of different sizes

Discussion

Our preliminary results highlight a difference in term of mechanical response to loading due to the HAP size, both in term of ultimate strength and post fracture behavior. So far, extensive MD simulations are running on the HPC-Franklin facility at IIT, to obtain more systematic results for platelets of different size. Our comparison could clarify the issue of how HAP platelets change with age, on the basis of mechanical considerations. Our fundamental approach could advance the knowledge of age-releated bone diseases and may open new routes for targeted intervention based on a deeper mechanical knowledge of the bone at a nanoscale level.

References

1. D. B. Burr, Bone, 85:93-120,2019.
2. F. Libonati et al., Journal of the mechanical behavior of biomedical materials 184:191-20,2013.
3. Z. Qin et al, Langmuir, 1982:1992-28.4,2012
4. O.Akkus et al., Bone, 34.3:443-453,2004
5. M. Rubin et al., Bone, 33.3:270-282, 2003
6. B. Foley et al., Crystals, 10.10:859, 2020
7. T. Lin et al., The Journal of Physical Chemistry C, 120.9:4975-4992, 2016

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