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A MULTISCALE MODEL INVESTIGATING THE ROLES OF MINEARLISED COLLAGEN FIBRILS AND THE EXTRA-FIBRILLAR MATRIX ON BONE BIOMECHANICS

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Summary: Bone is a naturally occurring composite material whose constituent phases are hierarchically organized to provide a highly optimized structure that exhibits high stiffness and excellent resistance to fracture. At the sub-tissue level, lamellar bone represents a fundamental structural unit of the tissue and it consists of mineralized collagen fibrils (MCFs) embedded within an extra-fibrillar matrix comprised of hydroxyapatite minerals distributed throughout a matrix of non-collagenous proteins. While both intra- and extra-fibrillar phases provide a critical contribution to tissue-level behaviour, the mechanical implications of their structural arrangement and in particular the relative distribution of HA minerals between both phases, remains poorly understood. This study presents a multiscale computational framework that uses both finite element analysis and steered molecular dynamics to investigate the role of the MCFs and extra-fibrillar phases on the mechanical properties of bone tissue. At the nano-scale, representative volume elements (RVEs) of both MCFs and the extra-fibrillar matrix were developed within a finite element framework, and a homogenisation strategy was used to determine the effective elastic properties of each phase. At the sub-micron level, a RVE of lamellar bone that accounted for newly reported patterns of mineral platelets encircling mineralised collagen fibrils was used to predict the effective response of lamellar bone tissue, with material properties established from the previous length scale. The results demonstrated that the overall mineral content in the tissue is the biggest contributor to the effective elastic properties of lamellar bone. While this is perhaps unsurprising, importantly, it was demonstrated that the extra-fibrillar matrix (and mineral therein) is the phase that makes the primary contribution to the elastic response of the tissue. On the other hand, the predicted elastic properties of MCFs were much lower than the extra-fibrillar matrix, indicating that intra-fibrillar mineralisation only provided a modest contribution to the stiffness of bone tissue. To explore the role of MCFs in more detail, a steered molecular dynamics (SMD) framework was used to simulate tensile deformation until failure using LAMMPS software. A staggered MCF model was assumed, which had length and radius of 335 and 10nm, respectively. In this model, we considered mineral volume fractions of 5% and 35%, distributed in either intra-fibrillar or extra-fibrillar patterns. Interestingly, this study revealed that HA minerals themselves contribute to strain-hardening behaviour of MCFs, by resisting the characteristic sliding behaviour between adjacent collagen molecules. We also uncovered characteristic behaviour of mineralised collagen fibrils, whereby their tensile behaviour showed three distinct phases: (i) under initial elastic loading, the residual stress is released and shear loading between adjacent collagen takes place followed by (ii) sliding of adjacent collagen molecules and (iii) work-hardening mediated by HA minerals until eventual failure by breaking the collagen molecules. In terms of failure, it was found that the Ultimate Tensile Strength (UTS) of the MCF reached its maximum amount as mineral become more uniformly distributed in the intra-extrafibrillar region, but this coincided with a reduction in elastic modulus of the MCF.