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Random Walk in 3D Model of Water Diffusion in the Human Mineralized Collagen Fibril

*Fabiano Bini*, Andra Pica', Andrea Marinozzi’, Franco Marinozzi1, Department of Mechanical and Aerospace Engineering, “Sapienza” University of Rome, Italy, ‘Orthopedics and Traumatology Area, “Campus Bio-Medico” University, Italy

At the nanoscale bone tissue is characterized by the mineralized collagen fibril (MCF), a recurring structure mainly composed of apatite mineral, tropocollagen molecules (TC) and water. The latter has a crucial role in bone mineralization. In this study, we aim to analyze the mass transport at the collagen-apatite level of porosity by means of a 3D random walk model. We considered a representative building block of the MCF according to [1-2]. We assumed a mineral volume fraction that represents an intermediate mineralized condition (32%vol). The geometrical dimensions of the nanocrystals and TC molecules are obtained from experimental data and used to model the building block. The diffusion coefficient is calculated from the mean square displacement of water molecules (MSD) according to the equation $D = \frac{\text{MSD}}{2nt}$, where $D$ is the diffusion coefficient, $n$ is the spatial dimension, i.e. $n=3$, $t$ is the time, and $nT$ – number of time steps [3]. The model provides a good prediction of the apparent diffusion coefficient, i.e. $D = 3.25 \times 10^{-10}$ m$^2$/s in agreement with previous results achieved from experimental [4] and computational investigations [2]. The 3D random walk model is a valuable tool for investigating the influence of the structural hindrance on the diffusivity since the structure of the building block is included in the diffusion model. Insights into MCF structure and properties enhance the understanding of bone mineralization and may improve the design of smart structural nanomaterials.


Disclosures: Fabiano Bini, None

P-316

The Interactive Effects of Dynamization Time and Degree on Bone Healing
*Ruisen Fu*, Bettina Willie*, Haisheng Yang*, Department of Biomedical Engineering, Beijing University of Technology, China, McGill University, Shriner’s Hospitals for Children, Canada

Introduction: Dynamization, reducing the fixation stiffness from a rigid to a more flexible condition, is widely used clinically to promote fracture healing. However, the most effective time to apply dynamization on healing outcomes remains controversial. Preclinical studies have demonstrated that dynamization with a degree of ~0.1 (the ratio of the flexible to rigid stiffness) at an early stage of healing (e.g. one week post-osteotomy) in rat femurs led to delayed healing (1-2). In contrast, a clinical study observed enhanced bone healing with early dynamization (3). It should be noted that the baseline fixation stiffness as well as the dynamization degree are different between those studies. Given the critical role of the fixation stiffness in determining the interfragmentary movement and thus regulating the healing process, it is important to understand how the degree and timing of dynamization interactively affects the healing process. Thus, the aim of the current study was to use finite element modeling to quantify the combined effect of degree and timing of dynamization on healing outcomes in an ovine model. Methods: Based on an ovine tibial fracture healing model which involves a fuzzy logic-based mecano-regulated tissue differentiation algorithm (4-5), we applied varied dynamization degrees (DC=0.1 to 1; 1 represents a rigid fixation) at 1, 2, 3, and 4 weeks (R1wF, R2wF, R3wF, R4wF) and computationally evaluated bone formation and biomechanical integrity during the healing process. Results: Our results demonstrated that early dynamization (at 1 and 2 weeks) significantly affected the healing process and outcomes (Fig. 1). However, the beneficial effect of early dynamization was dependent on the dynamization degree. Specifically, a higher dynamization degree (e.g. 0.1) led to a marked delay in bone formation and uncovered stiffness whereas moderate dynamization degrees (e.g. 0.3 or 0.5) significantly enhanced bone formation and biomechanical properties of the fractured bone (Fig. 1). Conclusions: Our results suggest that dynamization degree and timing interactively affects the healing process and therefore clinical application of dynamization should consider their interaction carefully to achieve a beneficial healing outcome.