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Determination of Activation Energy for Thermal Decomposition of Selected Soft Tissues Components

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Abstract : Tendons are the biological soft tissue structures composed of collagen, proteoglycan, glycoproteins, water and cells of extracellular matrix (ECM). Tendons, which primary function is to transfer force generated by the muscles to the bones causing joints movement, are exposed to many micro and macro damages. In fact, tendons and ligaments trauma are one of the most numerous injuries of human musculoskeletal system, causing for many people (particularly for athletes and physically active people), recurring disorders, chronic pain or even inability of movement. The number of tendons reconstruction and transplantation procedures is increasing every year. Therefore, studies on soft tissues storage conditions (influencing i.e. tissue aging) seem to be an extremely important issue. In this study, an atomic-scale investigation on the kinetics of decomposition of two selected tendon components – collagen type I (which forms a 60-85% of a tendon dry mass) and elastin protein (which combine with ECM creates elastic fibers of connective tissues) is presented. A molecular model of collagen and elastin was developed based on crystal structure of triple-helical collagen-like 1QSU peptide and P15502 human elastin protein, respectively. Each model employed 4 linear strands collagen/elastin strands per unit cell, distributed in 2x2 matrix arrangement, placed in simulation box filled with water molecules. A decomposition phenomena was simulated with molecular dynamics (MD) method using ReaxFF force field and periodic boundary conditions. A set of NVT-MD runs was performed for 1000K temperature range in order to obtained temperature-depended rate of production of decomposition by-products. Based on calculated reaction rates activation energies and pre-exponential factors, required to formulate Arrhenius equations describing kinetics of decomposition of tested soft tissue components, were calculated. Moreover, by adjusting a model developed for collagen, system scalability and correct implementation of the periodic boundary conditions were evaluated. An obtained results provide a deeper insight into decomposition of selected tendon components. A developed methodology may also be easily transferred to other connective tissue elements and therefore might be used for further studies on soft tissues aging.

Keywords : decomposition, molecular dynamics, soft tissue, tendons
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