Modeling of the relation between degradation and mechanical properties of a collagen fibril: A precursor examination towards understanding cartilage health

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Collagen fibrils are a very important component in most of the connective tissue in humans. An important process associated with several physiological and pathological processes is the degradation of collagen. Degradation of collagen is usually mediated by Metallo-Matrix-Proteinases (MMPs). MMPs usually are involved in unfolding and cleavage of tropocollagen molecules of the fibril, but the effect on the mechanical properties of the fibrils is not well understood. In this work we use molecular dynamics simulations to study the influence of degradation on the mechanical properties of the collagen fibril. We applied tensile stress on different collagen fibrils with different percent of degradation. We compared the differences in the aggregate mechanical response for two degradation scenarios; non-enzymatic crosslink removal and surface degradation. The resulting simulations shows dramatic change in the fibril material properties with a small amount (% weigh) for both degradation processes. Our results indicated that surface degradation yielded a much larger change in the mechanical properties when compared to the crosslink removals. The associated change in fibril stiffness and yield response exhibited a highly nonlinear dependence on degradation rate. This suggests that the hierarchical structure of the fibril is a key component for the toughness and is very sensitive to cleavage. We also investigated the local stress inside the fibril through the tropocollagen bond length distribution. This distribution shows regions of local concentration of stress that are modified during degradation. The overall results are intended to provide a theoretical framework for the understanding the mechanical behavior of collagen fibrils under degradation and provide basis for the development of volumetric finite element for the macro-mechanics of cartilage.

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