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PULLING RATE DEPENDEANCE OF THE NANOMECHANICS OF SINGLE TROPOCOLLAGEN MOLECULES

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ABSTRACT

Collagen is the most important structural protein in vertebrates and is responsible for the integrity of many tissues like bone, teeth, cartilage and tendons. The mechanical properties of these tissues are primarily determined by their hierarchical arrangement and the role of the collagen matrix in their structures. The lowest hierarchical level of collagenous tissues is formed by the tropocollagen triple helix. Both experimental [1-4] and simulation [5-7] approaches have been used in the analysis of the mechanical properties. However, the range of results for Young's modulus is quite broad, spanning from 0.35 to 18.8 GPa.

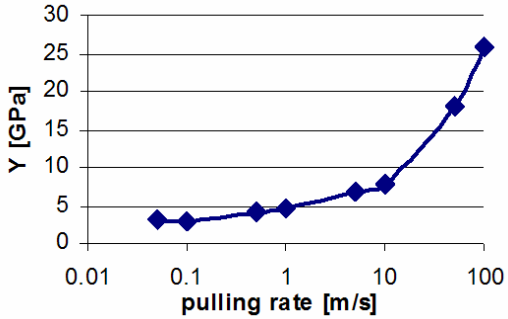

Fig. 1 *– Young modulus as a function of loading rate. For pulling rates lower than 10 m/s the estimated Young modulus falls in the range found with experimental techniques.*

The goal of the work presented here is to establish a clear understanding of the influence of the pulling rate on Young's modulus *Y* of individual tropocollagen molecules. Using Steered Molecular Dynamics (SMD) simulations we stretch a collagen peptide model sequence $[(\text{Gly-Pro-Hyp})_{10}]_3$ up to 10%, for pulling rates ranging from 0.05 to 100 m/s. Our results clearly demonstrate a strong influence of the loading velocity on the observed mechanical properties (Fig. 1). In particular, three regions in the *Y* vs. pulling rate plot could be defined: (i) a flat regime for velocities up to 1 m/s, where Young's modulus is almost constant, with *Y* values ranging from 3.1 to 4.6 GPa, (ii) a heel region from 1 to ~20 m/s and finally (iii) a steep increase of *Y* for pulling rates > ~20 m/s. Most importantly, Young's modulus converges to values of

approximately 3.5 GPa which is in the range obtained with experimental techniques.

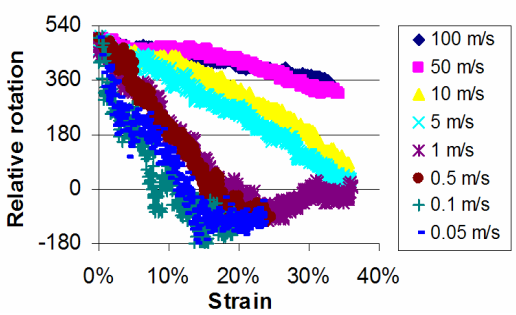

***Fig. 2** – End-to-end rotation as a function of strain. The end to end rotation has been calculated taking in consideration the first and last C_α of each chain.*

The analysis of the simulation trajectory shows that the collagen molecule unfolds in three different ways depending on loading rate, enlightened by the relative rotation of the peptide ends as a function of strain (Fig. 2). These different behaviours match the regions in the *Y* vs. pulling rate relationship as shown in Fig. 1. For low pulling rates, the triple helix completely uncoils at 10-20% strain, then undergoes some recoiling in the opposite direction and finally straighten for strain > 30%, where the backbone begins to be stretched. For intermediate rates (the heel region in *Y* vs. pulling rate plot) the molecule unfolds linearly with strain up to 35% strain. Finally, at higher velocities the triple helix fails to unfold, thus leading to higher mechanical properties.

In summary, we show that collagen mechanical properties are rate sensitive, but converge to a constant, finite value for pulling rates below 1 m/s. Furthermore, we show that the collagen triple helix undergoes different uncoiling mechanisms depending on the loading rate. Future work will include the analysis of pathological mutations influence on structure and properties of collagen, and the investigation of higher hierarchical level, such as the microfibril.

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