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# MS 59 - Soft Biological Tissue: Microstructure-Based Modeling and Simulation - Coarse-grained Steered Molecular Dynamcis Simulations of Collagen Fibrils

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Collagen fibrils are the main building constituent of bone as well as of other human tissues. Their specific staggered building pattern with cross-links connecting tropocollagen molecules to a fibril provides them with astonishing mechanical properties: high elasticity, large strength and a substantial energy dissipation during deformation. It has been observed that the augmented glycation level in diabetic patients triggers an increased formation of random non-enzymatic cross-links, so-called Advanced-Glycation-Endproducts (AGEs) between tropocollagen molecules in bone, but also in soft tissues with a long half-life of collagen. The increased occurance of AGEs again correlates with an increased fracture risk in diabetic bone and deterioration of mechanical properties in collageneous tissues. Since the shearing of collagen gives bone its plasticity and toughness, any restriction of this might make bone more brittle. However, it is unknown how AGE accumulation affects collagen sliding mechanisms and damage.
Here, we study the mechanisms leading to inferior bone quality in diabetic patients using a computational bottom-up approach. In a first step, we implemented a computational 3D coarse-grained model of a collagen fibril segment presenting five repeating gap- and overlap zones, the typical basic building unit of collagen fibrils, based on *Depalle et al.* [1]. Longitudinal tensile tests applying Steered Molecular Dynamics are performed on this collagen segment until fracture, gradually increasing the amount of random cross-links in order to investigate the influence of the density of AGEs on the mechanical behaviour. We observe three different regimes in the stress-strain curves, depending on amount of cross-links. Further, the plastic work to fracture decreases with an increasing cross-link density. The next step is to identify the location where the fibril ruptures, whether it is cross-links or tropocollagen molecules and whether this is dependent on the AGE cross-linking.

## REFERENCES

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