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► To cite this version:

Abdelwahed Barkaoui, Ridha Hamblí, Awad Bettamer. Biomechanical role of collagen cross-links in bone strength: finite element study. ASBMR 2011, Sep 2011, San Diego, California, United States. hal-00654926

HAL Id: hal-00654926

<https://hal.science/hal-00654926>

Submitted on 23 Dec 2011

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Biomechanical role of collagen cross-links in bone strength: finite element study.

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Introduction:

Bone contains exclusively genetic Type I collagen. These collagens are identical sequences of amino acids that form the tropocollagen molecules linked by cross-links found at the end of each tropocollagen molecules. Collagen cross-linking, a major post-translational modification of collagen, plays important roles in the biological and biomechanical features of bone. The aim of this work is to use a 3D nano-scale finite element model of a sub structure in collagen fibril called mineralized collagen microfibril and to investigate the important roles of cross-links in the expression of bone strength and its capacity and ability to absorb energy. Studies *in vitro* and *in vivo* have reported that increases in cross-linking are associated with enhancement of some mechanical properties (strength and stiffness) and reductions of others (energy absorption). These experimental data are limited in their ability to define individual biomechanical effects of altered cross-linking. In the present work the study of the effect of cross-links is more realistic that's because the proposed finite element model success to combines the collagen, mineral and cross-links furthermore been able to varying the mechanical and geometry properties of each phase and to visualize their influence on corresponding equivalent properties of the collagen microfibril.

Materials and Methods

A 3D finite element model of collagen microfibril with symmetric and periodic boundary conditions is considered here, with an array of 5 TC cross-linked together, the all is put into a mineral matrix. A parametric study was performed in order to investigate the influence of varying number of cross-links on the mechanical behaviour of the microfibril. This Finite element model was coupled to a UMAT and optimization algorithm to calculate the equivalent proprieties of microfibrils. From a FE point of view, spring elements can be used to model connections between two different regions to couple a force with a relative displacement representing the elasticity of the physical connecting constituents (physical cross links).

Results:

In this study results were obtained under tensile loading with symmetric and periodic boundary conditions. These results show that the number of cross-link has a most influence on the increase in the elastic and failure proprieties. at constant Young's modulus, if the number of cross-link (N) increase the bone material will be more stronger, however when $N > 20$ fracture stress does not depend on the cross-link number and it remains at constant value "plateau value", same observation has been also found by Markus J.Buehler [1] in his molecular multi-scale study. Where it is found that fracture stress depend on the cross-link density" β " only when $\beta < 25$. This plateau can be explained by the fact that whenever the number of cross link increases their stiffness increases up a threshold value hence the behaviour of all collagen-cross-links becomes insensitive to the number (N), this explanation is demonstrated by an analytical calculation.

References:

- [1] Markus J.Buehler, Nanomechanics of collagen fibrils under varying cross-links densities: atomistic and continuum studies, journal of the mechanical behavior of biomedical materials 1(2008) 59-67.