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A Computational Framework for Load Mediated Patellar Ligaments Damage at the Tropocollagen Level

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Abstract : In various sport and recreational activities, the patellofemoral joint undergoes large forces and moments while accommodating the significant knee joint movement. In doing so, this joint is commonly the source of anterior knee pain related to instability in normal patellar tracking and excessive pressure syndrome. One well-observed explanation of the instability of the normal patellar tracking is the patellofemoral ligaments and patellar tendon damage. Improved knowledge of the damage mechanism mediating ligaments and tendon injuries can be a great help not only in rehabilitation and prevention procedures but also in the design of better reconstruction systems in the management of knee joint disorders. This damage mechanism, specifically due to excessive mechanical loading, has been linked to the micro level of the fibred structure precisely to the tropocollagen molecules and their connection density. We argue defining a clear frame starting from the bottom (micro level) to up (macro level) in the hierarchies of the soft tissue may elucidate the essential underpinning on the state of the ligaments damage. To do so, in this study a multiscale fibril reinforced hyper elastoplastic Finite Element model that accounts for the synergy between molecular and continuum syntheses was developed to determine the short-term stresses/strains patellofemoral ligaments and tendon response. The plasticity of the proposed model is associated only with the uniaxial deformation of the collagen fibril. The yield strength of the fibril is a function of the cross-link density between tropocollagen molecules, defined here by a density function. This function obtained through a Coarse-graining procedure linking nanoscale collagen features and the tissue level materials properties using molecular dynamics simulations. The hierarchies of the soft tissues were implemented using the rule of mixtures. Thereafter, the model was calibrated using a statistical calibration procedure. The model then implemented into a real structure of patellofemoral ligaments and patellar tendon (OpenKnee) and simulated under realistic loading conditions. With the calibrated material parameters the calculated axial stress lies well with the experimental measurement with a coefficient of determination (R2) equal to 0.91 and 0.92 for the patellofemoral ligaments and the patellar tendon respectively. The 'best' prediction of the yielding strength and strain as compared with the reported experimental data yielded when the cross-link density between the tropocollagen molecule of the fibril equal to 5.5 ± 0.5 (patellofemoral ligaments) and 12 (patellar tendon). Damage initiation of the patellofemoral ligaments was located at the femoral insertions while the damage of the patellar tendon happened in the middle of the structure. These predicted finding showed a meaningful correlation between the cross-link density of the tropocollagen molecules and the stiffness of the connective tissues of the extensor mechanism. Also, damage initiation and propagation were documented with this model, which were in satisfactory agreement with earlier observation. To the best of our knowledge, this is the first attempt to model ligaments from the bottom up, predicted depending to the tropocollagen cross-link density. This approach appears more meaningful towards a realistic simulation of a damaging process or repair attempt compared with certain published studies.

Keywords : tropocollagen, multiscale model, fibrils, knee ligaments
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