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Michele Marino, Giuseppe Vairo



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# Influence of inter-molecular interactions on the elasto-damage mechanics of collagen fibrils: a bottom-up approach towards macroscopic tissue modeling

Michele Marino\*, Giuseppe Vairo\*

*Department of Civil Engineering and Computer Science Engineering (DICII), Università degli Studi di Roma "Tor Vergata", via del Politecnico 1, 00133 Roma - Italy*

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## Abstract

In this paper, a novel modeling approach for describing the elasto-damage mechanical response of collagen fibrils is proposed. The model is developed by adopting a multiscale rationale that allows to consistently account for nanoscale mechanisms and to introduce model parameters with a clear biophysical/biochemical meaning. A detailed description of nanoscale inter-molecular interactions is considered, highlighting their great influence on fibril mechanical response. The model is successfully validated by comparisons with available data based on molecular dynamics simulations. Proposed results proves model capability to reproduce many well-established features of fibril mechanics, fully in agreement with available experimental evidence.

### *Keywords:*

Collagen fibrils, multiscale modeling, molecular inter-strand delamination, inter-molecular slip-pulse mechanism, constrained variational formulation

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\*Corresponding author. Phone: +39 06 7259 7016.

*Email addresses:* [m.marino@ing.uniroma2.it](mailto:m.marino@ing.uniroma2.it) (Michele Marino),  
[vairo@ing.uniroma2.it](mailto:vairo@ing.uniroma2.it) (Giuseppe Vairo)

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