MECHANICAL CHARACTERIZATION OF MINERALIZED COLLAGEN FIBRIL USING MULTISCALE ASYMPTOTIC HOMOGENIZATION

By

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This work is dedicated to My Mother, Father and Teachers.

CERTIFICATE

This is to certify that the thesis entitled "**Mechanical Characterization of Mineralized Collagen Fibril using Multiscale Asymptotic Homogenization**" being submitted by **Abhilash Awasthi** is the report of bonafide research work carried by him under our supervision. This thesis has bean prepared in conformity with the rules and regulations of INDIAN INSTITUTE OF TECHNOLOGY MANDI. We further certify that the thesis has attained a standard required for the award of a Master of Science (by Research) degree of the Institute. The research reported and the results presented in the thesis have not been submitted, in part or full to any other institute or university for the award of any other degree or diploma.

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Abstract

The nanostructure of bone consists of two hierarchical levels called as 1) Mineralized Collagen Fibril (MCF), and 2) Microfibril. At both levels, the nanostructure contains different volume fractions and arrangements of highly tough collagen and highly stiff mineral phases which yields unique properties like lightweight, high strength, stiffness, and toughness.

A finite element (FE) model has been developed, where the inclusions are considered as one-dimensional embedded elements and matrix is modeled with two-dimensional plane stress continuum elements. Two-scale asymptotic homogenization approach has been used to derive the mechanical properties of MCF. In addition to this, the effect of uncertainties associated with geometric and material parameters of mineral and collagen phases has also been considered directly in the FE mesh. Different realizations of MCF are generated using in-house MATLAB code and Monte-Carlo type simulations are performed to obtain the characteristic elastic modulus and strength of MCF. The results are found to be in good agreement with experiments and molecular dynamics simulations. The present model has closely predicted the local distribution of stresses and strains with a significant reduction in the computational cost.

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