

Catastrophic phenomena that afflict millions of lives all have mostly one common underlying theme: the breakdown of the basic constituents leading to the failure of its overall structure and intended function. The failure and deformation of engineering materials has been studied extensively with significant impact on our world. However, the mechanisms of failure in biological systems are not well understood, thus presenting an opportunity to generate novel concepts to initiate a new paradigm of materials science.

Here we undertake a systematic bottom-up analysis of the structure and properties of protein materials (PMs), illustrated by studies of intermediate filaments (IFs) in the cytoskeleton of eukaryotic cells.

We review and extend a mathematical model, which allows us to describe the mechanical strength properties of PMs in dependence of the hierarchical geometrical architecture. This model enables us to identify structure-property links and to predict the behavior of highly diverse protein structures.

We validate and apply this theory in atomistic simulation studies of the fundamental fracture behavior of alpha-helix (AH) based protein domains, with and without structural defects occurring at different length and time scales. Further, we show by using a fully atomistic-informed coarse-grained multi-scale model of an alpha-helical network, that the particular architecture of IF protein networks leads to intrinsic flaw-tolerant behavior.

We conclude this Thesis by discussing the role of nanostructured hierarchies and reviewing the key findings in light of materials science concepts. Our analysis suggests that the hierarchical, nanostructured design enables PMs to unify seemingly contradicting material properties with high potential for various new bioinspired material concepts.