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**Bottom-up study of flaw tolerance properties of protein networks**[1] ZHAO QIN, MARKUS BUEHLER, Massachusetts Institute of Technology, LAMM TEAM — We study the material properties of an intermediate filament proten network by computational modeling using a bottom-up approach. We start with an atomic model of each filament's and obtain the mechanical behavior of them. We then use these parameters in setting up a mesoscale model of the network material at scales of micrometers. Using this multi-scale method, we report a detailed analysis of the associated deformation and failure mechanisms of this hierarchical material. Our modeling reveals that a structure transition that occurs at the proteins' secondary structure level is crucial for the networks' flaw tolerance property, which implies that the material retains its mechanical function despite the existence of large defects. We also examine the effect of crosslink strength on the failure properties. We discover that relatively weaker crosslinks lead to a more flaw tolerant network that is 23% stronger. This unexpected behavior is caused by that the crosslink strength functions as a switch to alter the failure mechanism. Weak crosslinks are able to efficiently diffuse the stress around the crack tip, making the crack more difficult to propagate. We compare our results to that of elastic and softening materials and find that the effect of crosslink strength is much smaller in those systems. These findings imply that the mechanical properties of both the filaments and interfaces among filaments are critical for bioinspired material designs, challenging the conventional paradigm in engineering design.

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