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Title:	Optimal Protein Sequence Design Mitigates Mechanical Failure in Silk β -Sheet Nanocrystals
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Keywords:	silk β -sheet nanocrystals stick-slip dynamics tensile strength toughness
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Abstract:	<p>The excellent mechanical strength and toughness of spider silk are well characterized experimentally and understood atomistically using computational simulations. However, little attention has been focused on understanding whether the amino acid sequence of β-sheet nanocrystals, which is the key to rendering strength to silk fiber, is optimally chosen to mitigate molecular-scale failure mechanisms. To investigate this, we modeled β-sheet nanocrystals of various representative small/polar/hydrophobic amino acid repeats for determining the sequence motif having superior nanomechanical tensile strength and toughness. The constant velocity pulling of the central β-strand in the nanocrystal, using steered molecular dynamics, showed that homopolymers of small amino acid (alanine/alanine-glycine) sequence motifs, occurring in natural silk fibroin, have better nanomechanical properties than other modeled structures. Further, we analyzed the hydrogen bond (HB) and β-strand pull dynamics of modeled nanocrystals to understand the variation in their rupture mechanisms and explore sequence-dependent mitigating factors contributing to their superior mechanical properties. Surprisingly, the enhanced side-chain interactions in homopoly-polar/hydrophobic amino acid models are unable to augment backbone HB cooperativity to increase mechanical strength. Our analyses suggest that nanocrystals of pristine silk sequences most likely achieve superior mechanical strength by optimizing side-chain interaction, packing, and main-chain HB interactions. Thus, this study suggests that the nanocrystal β-sheet sequence plays a crucial role in determining the nanomechanical properties of silk, and the evolutionary process has optimized it in natural silk. This study provides insight into the molecular design principle of silk with implications in the genetically modified artificial synthesis of silk-like biomaterials.</p>
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