Nonlinear behavior of silk minimizes damage and begets spider web robustness from the molecules up

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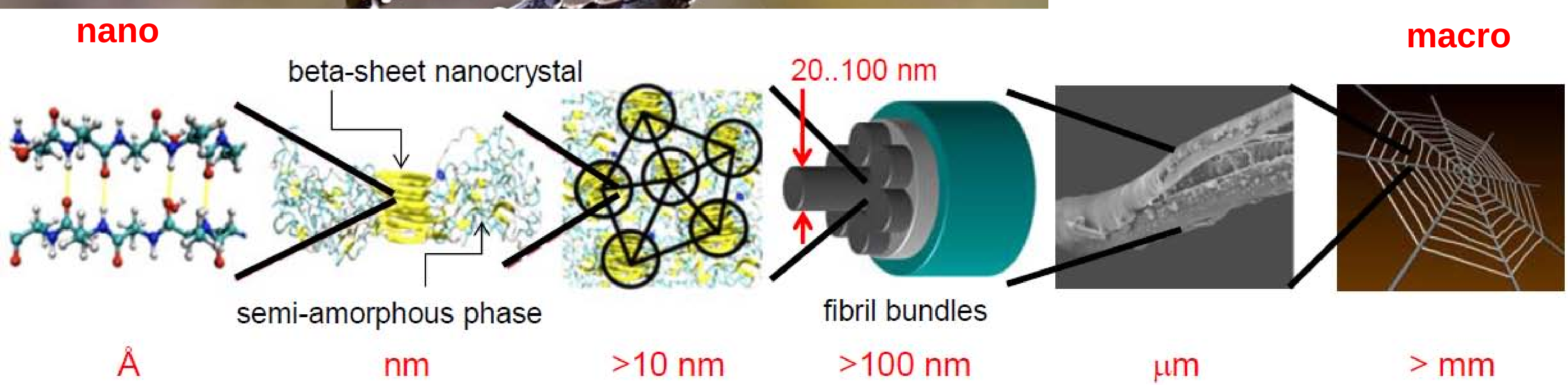
Massachusetts Institute of Technology

Steel: strength ~1 GPa
strong bonds

Spider silk: strength ~1-2 GPa & 60% strain @ failure
weak bonds

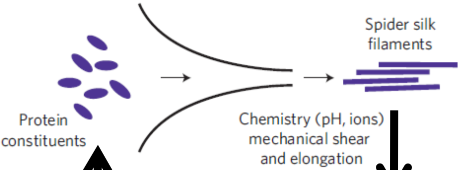
Made @ room temperature via self-assembly

Natural construction material



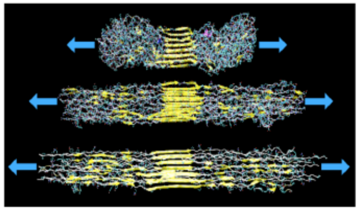
Mechanics of web from molecular principles

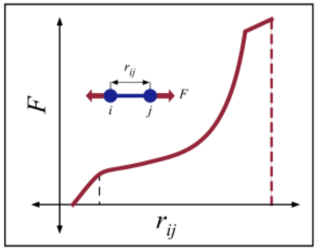
Silk structure identified using statistical methods (replica exchange MD)
Scheibel *et al.*



genetic information

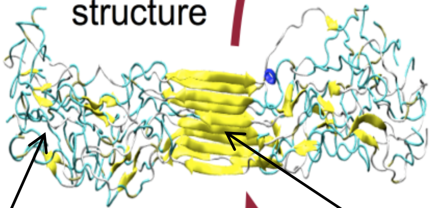
Nanomechanics characterization





Constitutive behavior (derived from molecular principles, w/ mechanisms: **Unfolding, slip, failure**)

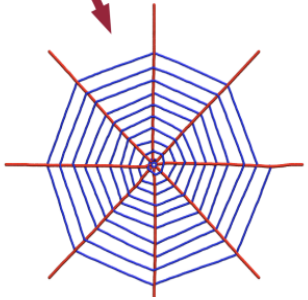
Full atomistic structure



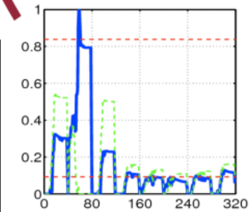
3_1-helices (semi amorphous)

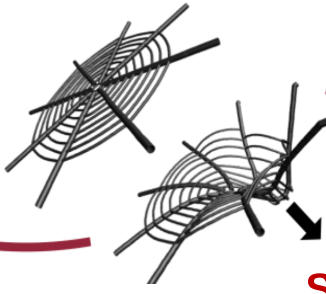
beta-sheet nanocrystal

Macroscale system (web)



Web failure (simulation, model and *in situ* experiment)





System-level mechanical tests

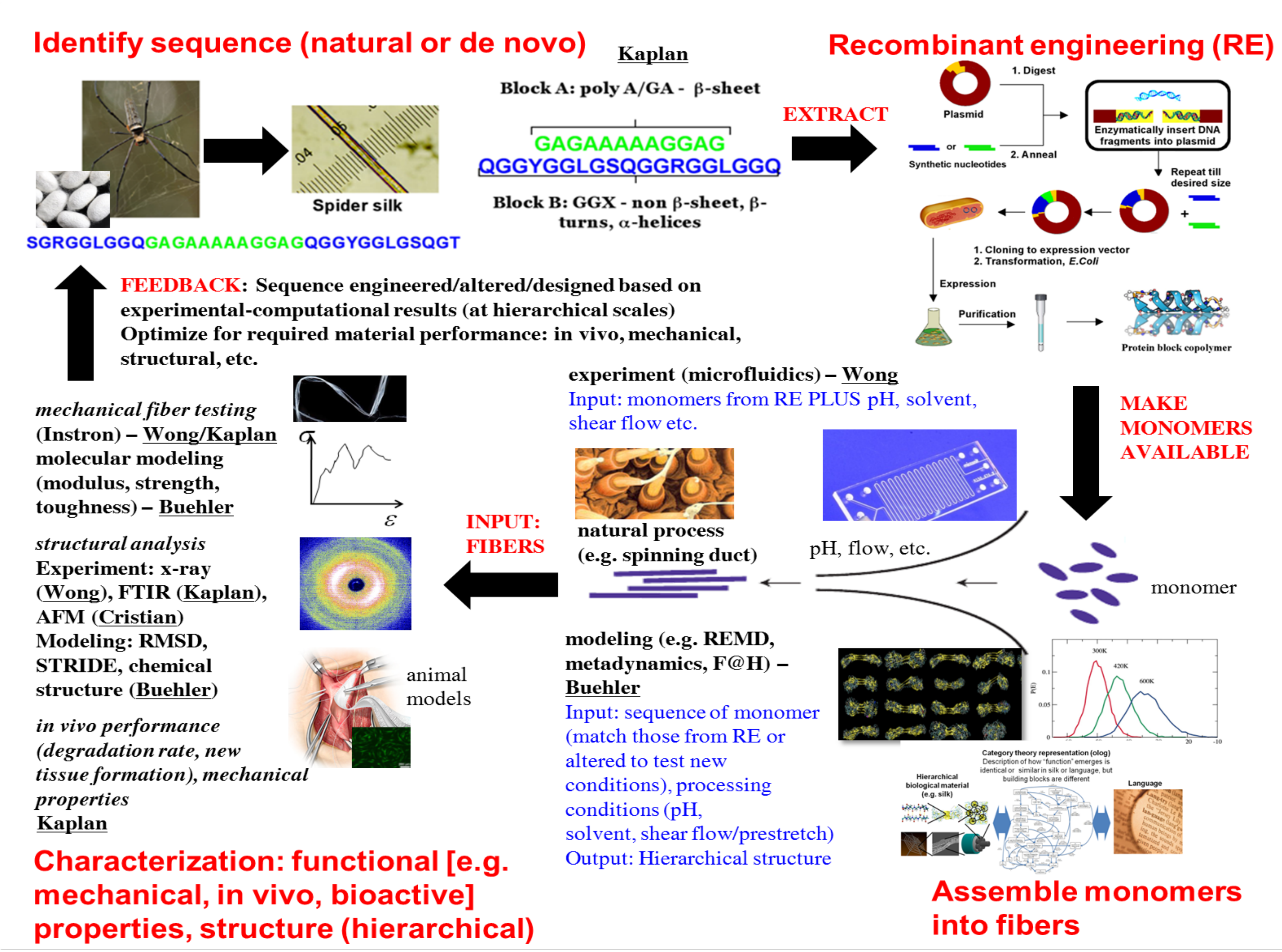
Stiffening → highly localized failure

Link macroscale web failure back to molecular mechanisms

Based on: *Nature Materials*, 2010; *Nature*, 2011, in submission

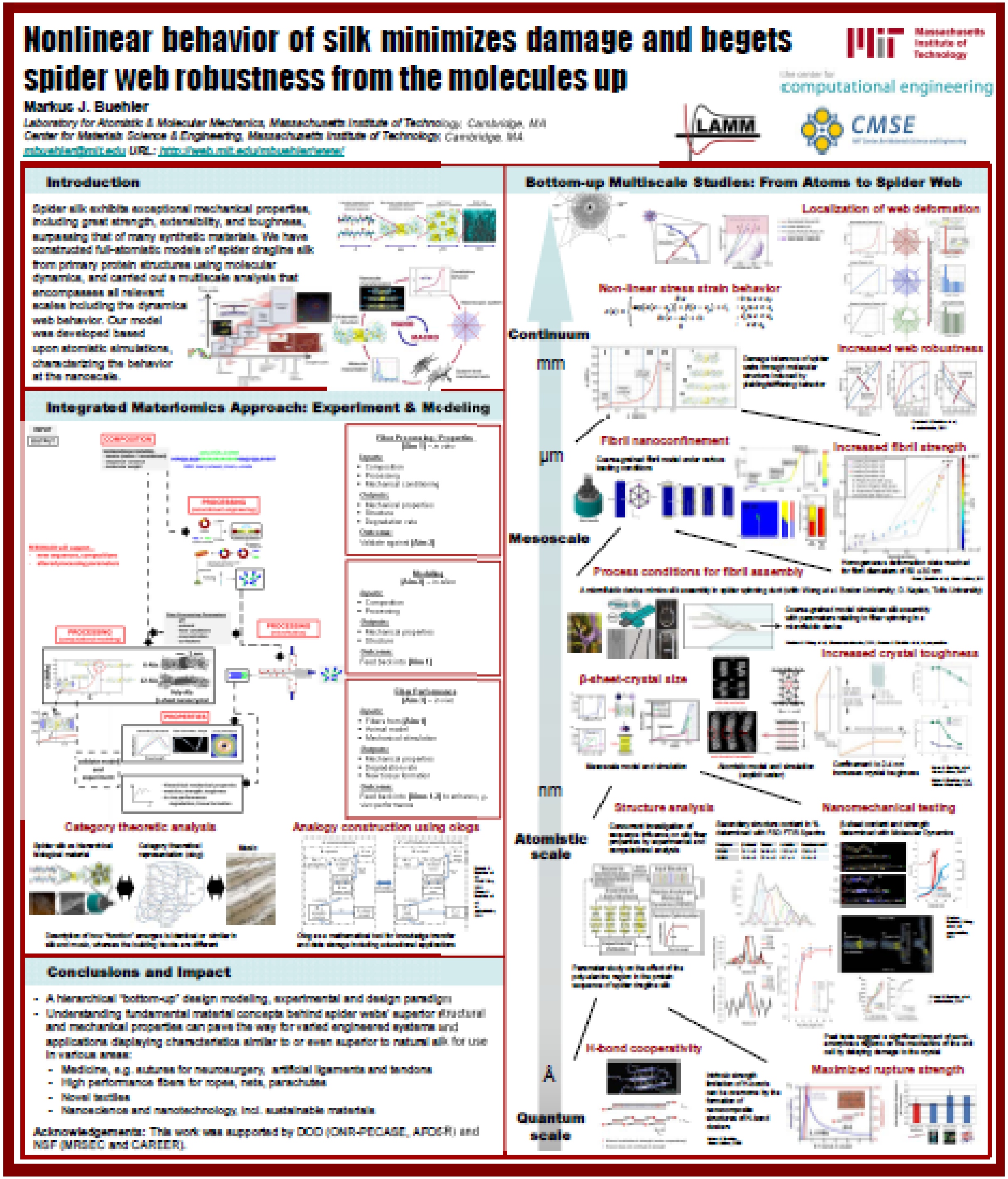
Problem solved: Source of great strength of silk (comparable to steel) despite material being constructed from weak H-bonds (e.g. water)

S. Cranford, A. Tarakanova *et al.*, *Nature*, *in revision*



Identify sequence (natural or de novo)
Kaplan
Block A: poly A/GA - β-sheet
GAGAAAAAGGAG
QGGYGGLGSQGGRGGLGGQ
Block B: GGX - non β-sheet, β-turns, α-helices
Spider silk
.04
SGRGGLGGQGAGAAAAAGGAGQGGYGGLGSQGT
EXTRACT
Recombinant engineering (RE)
1. Digest
Plasmid
or
Synthetic nucleotides
2. Anneal
Enzymatically insert DNA fragments into plasmid
Repeat till desired size
+
1. Cloning to expression vector
2. Transformation, E.Coli
Expression
Purification
Protein block copolymer
FEEDBACK: Sequence engineered/altered/designed based on experimental-computational results (at hierarchical scales)
Optimize for required material performance: in vivo, mechanical, structural, etc.
experiment (microfluidics) – Wong
Input: monomers from RE PLUS pH, solvent, shear flow etc.
MAKE MONOMERS AVAILABLE
mechanical fiber testing
(Instron) – Wong/Kaplan
molecular modeling
(modulus, strength, toughness) – Buehler
σ
ε
INPUT: FIBERS
natural process
(e.g. spinning duct)
pH, flow, etc.
monomer
structural analysis
Experiment: x-ray (Wong), FTIR (Kaplan), AFM (Cristian)
Modeling: RMSD, STRIDE, chemical structure (Buehler)
animal models
in vivo performance
(degradation rate, new tissue formation), mechanical properties
Kaplan
modeling (e.g. REMD, metadynamics, F@H) – Buehler
Input: sequence of monomer (match those from RE or altered to test new conditions), processing conditions (pH, solvent, shear flow/prestretch)
Output: Hierarchical structure
300K
420K
600K
0.1
0.05
0
P(E)
Category theory representation (olog)
Description of how "function" emerges is identical or similar in silk or language, but building blocks are different
Hierarchical biological material (e.g. silk)
Language
Characterization: functional [e.g. mechanical, in vivo, bioactive] properties, structure (hierarchical)
Assemble monomers into fibers

Poster #8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Introduction
Spider silk exhibits exceptional mechanical properties, including great strength, extensibility, and toughness, surpassing that of many synthetic materials. We have constructed full-atomistic models of spider dragline silk from primary protein structures using molecular dynamics, and carried out a multiscale analysis that encompasses all relevant scales including the dynamics web behavior. Our model was developed based upon atomistic simulations, characterizing the behavior at the nanoscale.
Integrated Materiomics Approach: Experiment & Modeling
Category theoretic analysis
Analogy construction using ologs
Conclusions and Impact
- A hierarchical "bottom-up" design modeling, experimental and design paradigm
- Understanding fundamental material concepts behind spider webs' superior structural and mechanical properties can pave the way for varied engineered systems and applications displaying characteristics similar to or even superior to natural silk for use in various areas:
- Medicine, e.g. sutures for neurosurgery, artificial ligaments and tendons
- High performance fibers for ropes, nets, parachutes
- Novel textiles
- Nanoscience and nanotechnology, incl. sustainable materials
Acknowledgements: This work was supported by DOD (ONR-PECASE, AFOSR) and NSF (MRSEC and CAREER).
Bottom-up Multiscale Studies: From Atoms to Spider Web
Localization of web deformation
Non-linear stress strain behavior
Increased web robustness
Continuum
mm
μm
Fibril nanoconfinement
Increased fibril strength
Mesoscale
Process conditions for fibril assembly
Increased crystal toughness
β-sheet-crystal size
nm
Structure analysis
Nanomechanical testing
Atomistic scale
H-bond cooperativity
Maximized rupture strength
Å
Quantum scale