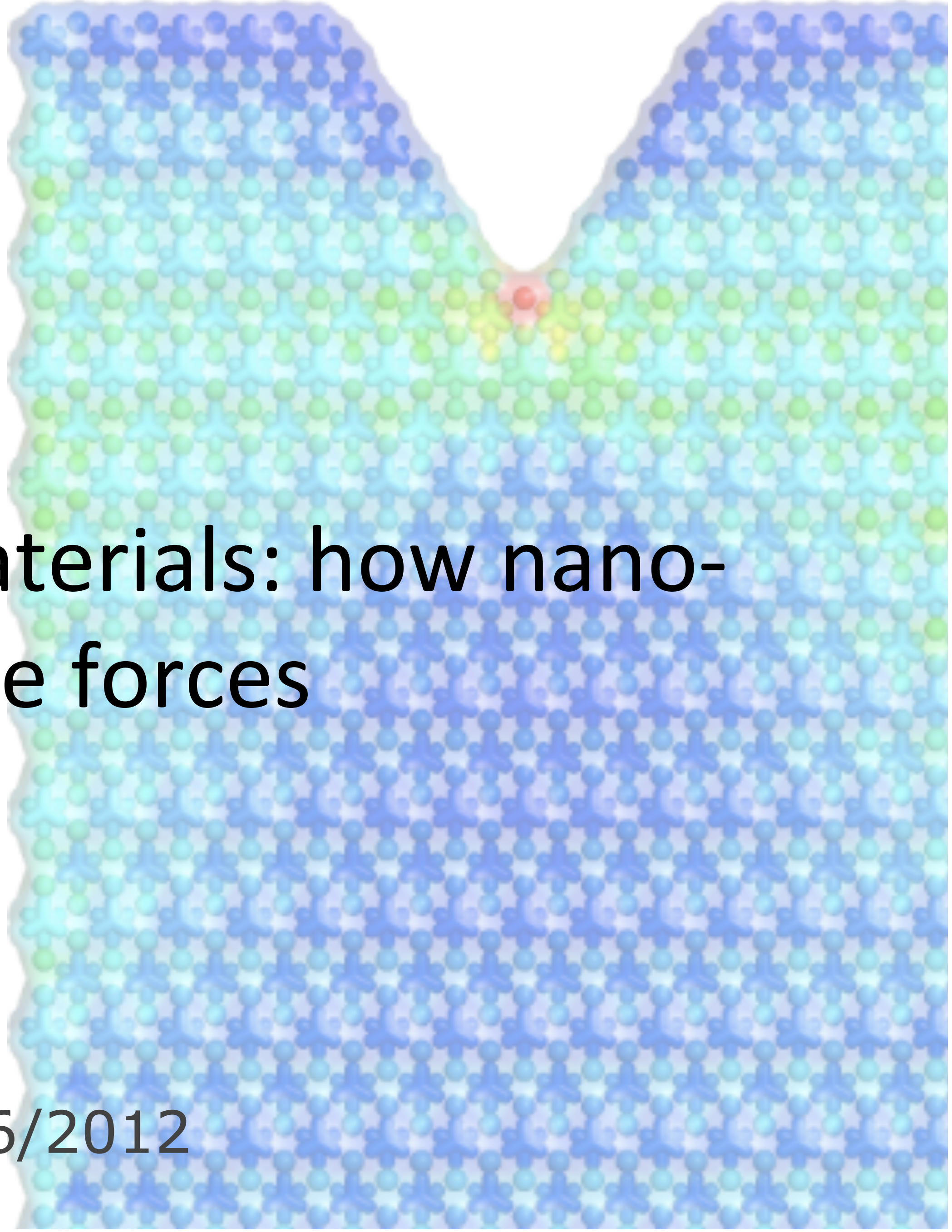
Heidelberg Institute for
Theoretical Studies

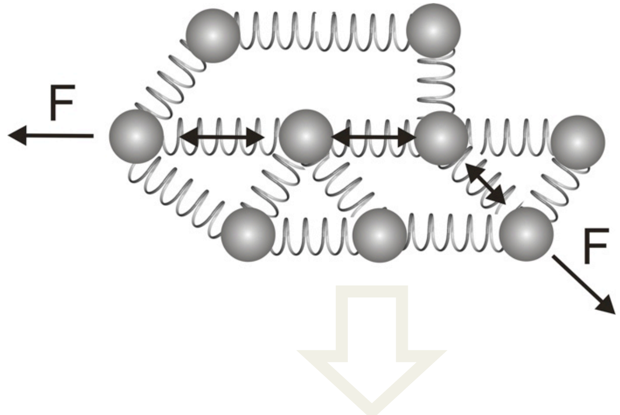
HITS

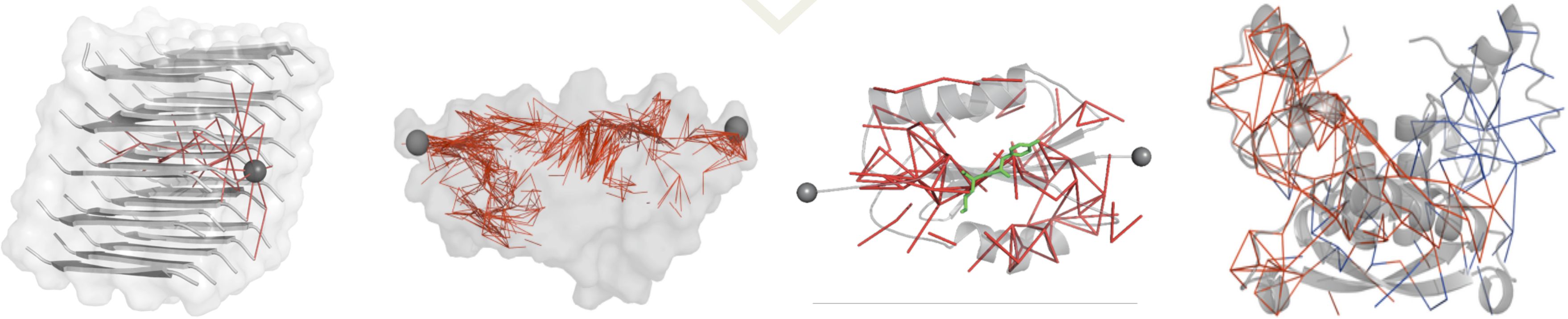
Mechanics of biomaterials: how nano-structures propagate forces



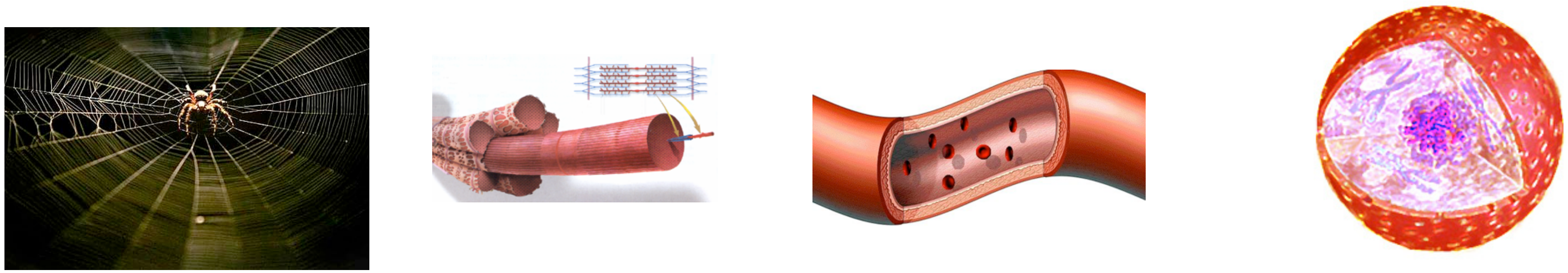
Frauke Gräter, Dresden, 06/2012

Molecular force distribution





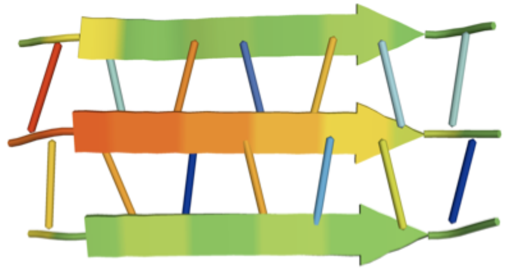
spider web | muscle | blood | gene expression



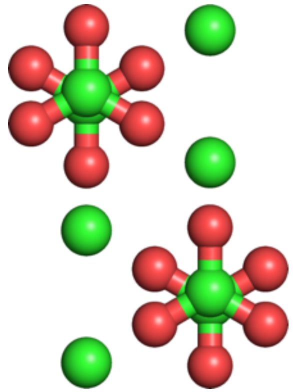
HITS

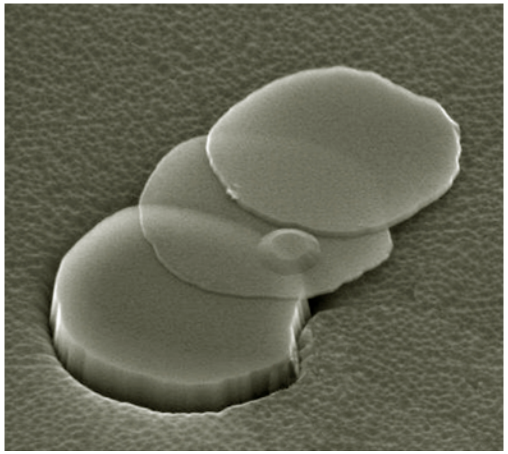
MOLECULAR (bio)mechanics – why?

silk

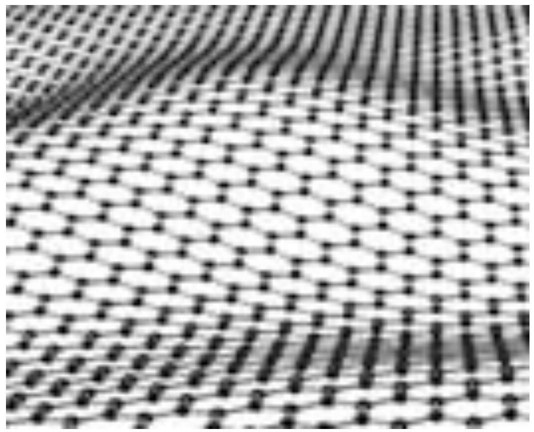


nacre





graphene

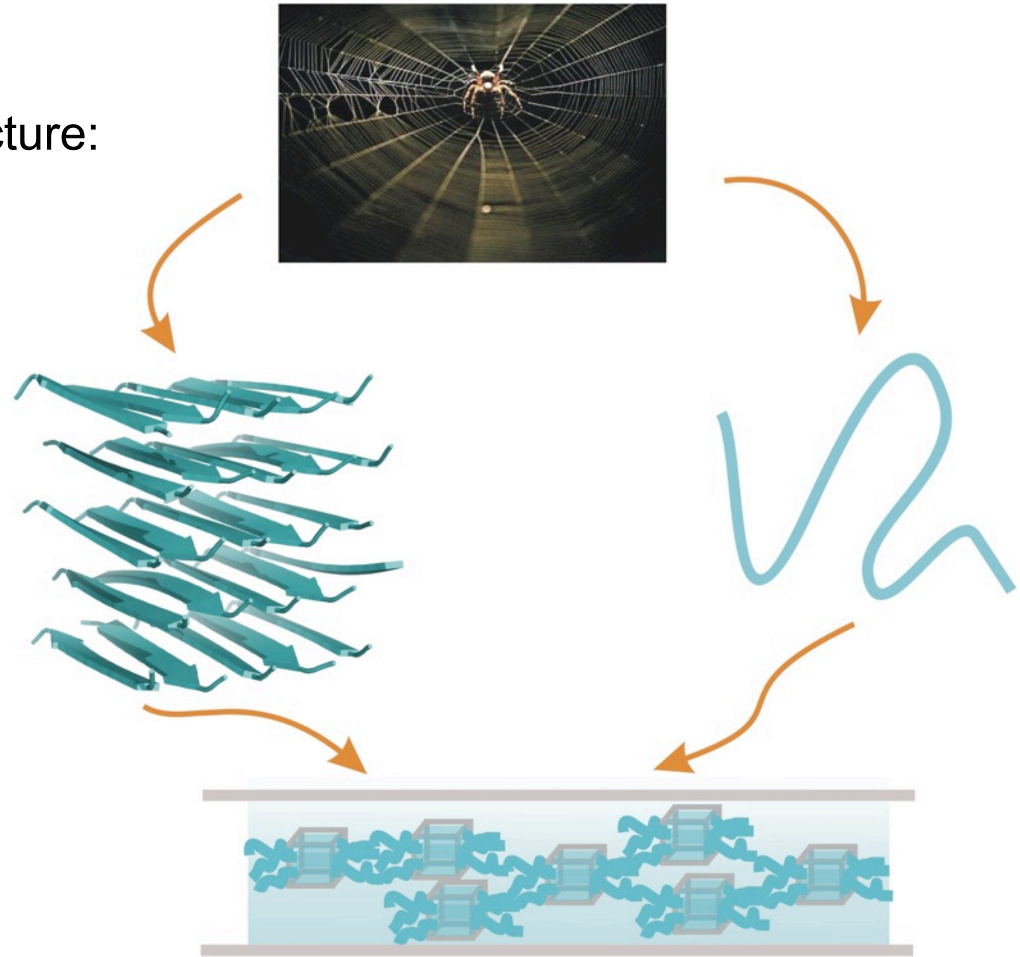


Mechanics of silk fibers

丝

silk molecular structure:

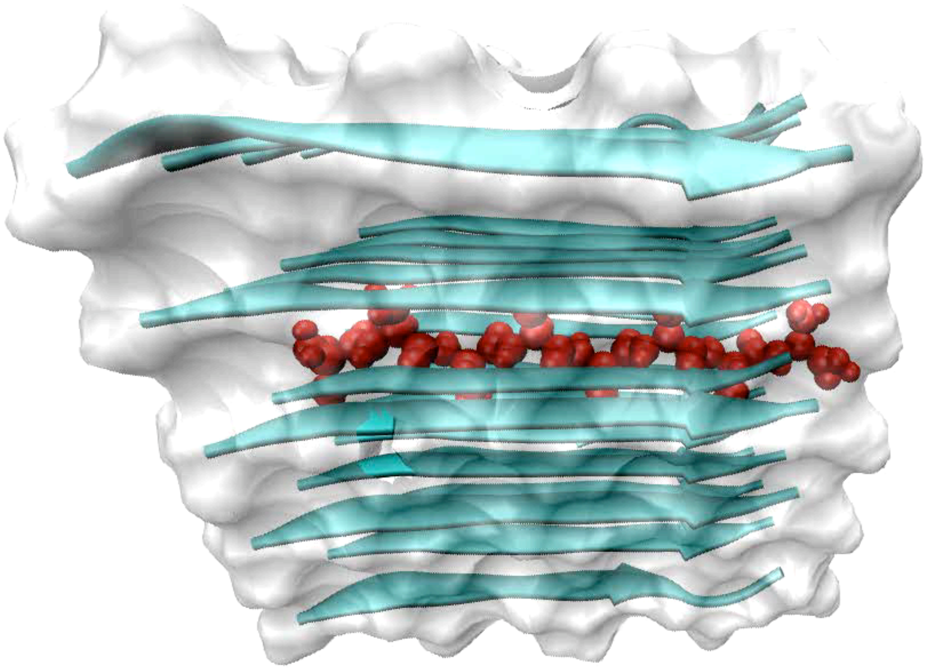
poly(alanine)



disordered
sequence
~24 aminoacids
glycine rich

How has nature designed silk to be tougher than steel?

What is the optimal design for a semi-crystalline polymer?



Strain and fracture: force distribution

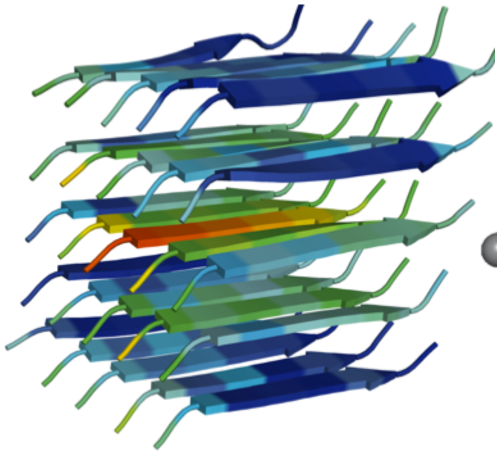
conventional design tools:
force distribution

in constructions, cars ...

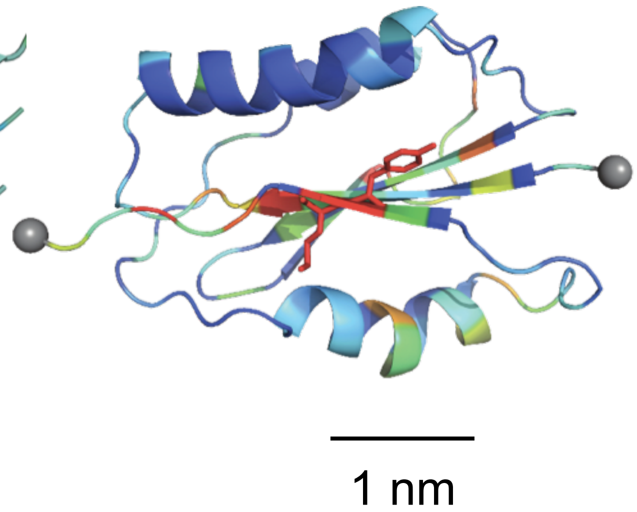
macroscopic structures:
meters

new:
force distribution in biomolecules

e.g. in silk fibers



in blood clotting factors

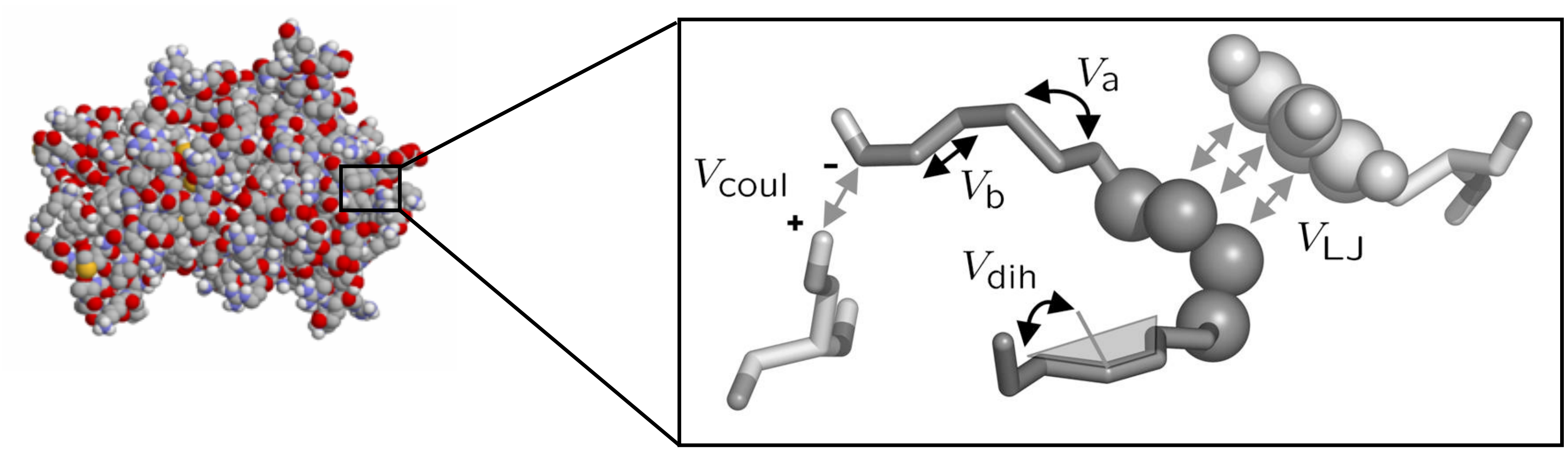


microscopic structures:
~ 10^{-9} meters

W. Stacklies, C. Vega, M. Wilmanns, F. Graeter, PLoS Comp Biol, 2009
W. Stacklies, F. Xia, F. Graeter, PLoS Comp Biol, 2009

HITS

Forces from MD

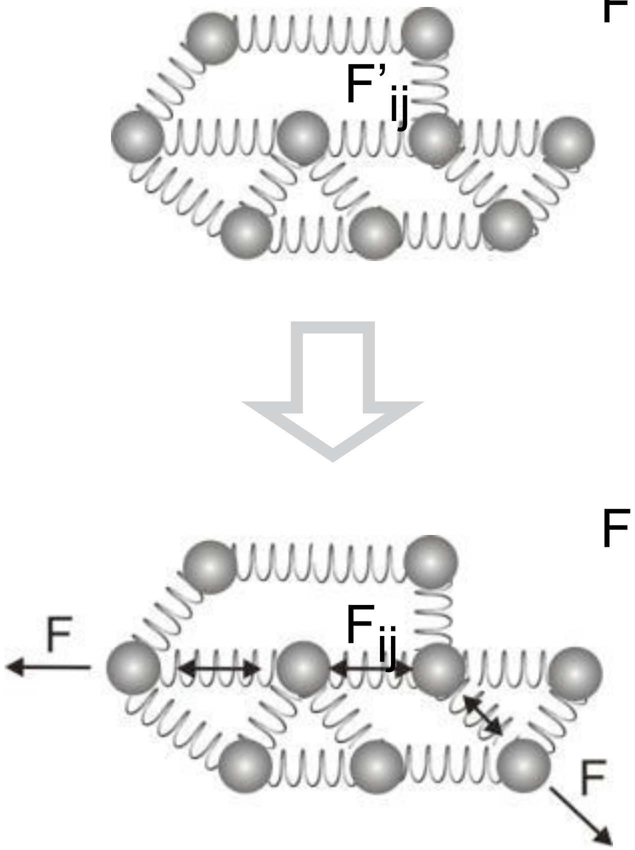


$$
\begin{aligned}
E = & \sum_{bonds} \frac{k_i}{2}(l_i - l_{i,0})^2 \\
& + \sum_{angles} \frac{k_i}{2}(\Theta_i - \Theta_{i,0})^2 \\
& + \sum_{torsions} \frac{V_n}{2}(1 + cos(n\omega - \gamma)) \\
& + \sum_{i=1}^{N} \sum_{j=i+1}^{N} (4\epsilon_{ij}((\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}) + (\frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}))
\end{aligned}
$$

↔ bonded interactions

↔ non-bonded interactions

Forces from MD



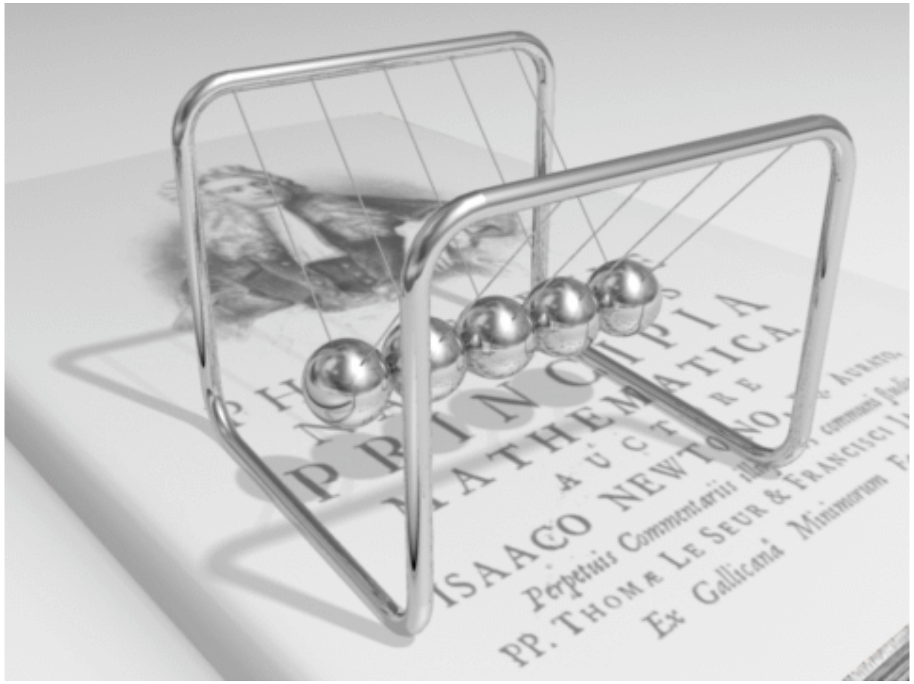
F'_{ij} force between atom i and j in relaxed state

F_{ij} force between atom i and j in stretched state

change in pairwise forces

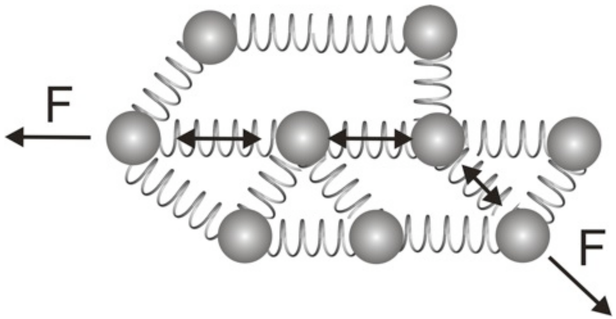
$$\Delta F_{ij} = F_{ij} - F'_{ij}$$

HITS



compare: Newton's cradle
(from wikipedia)

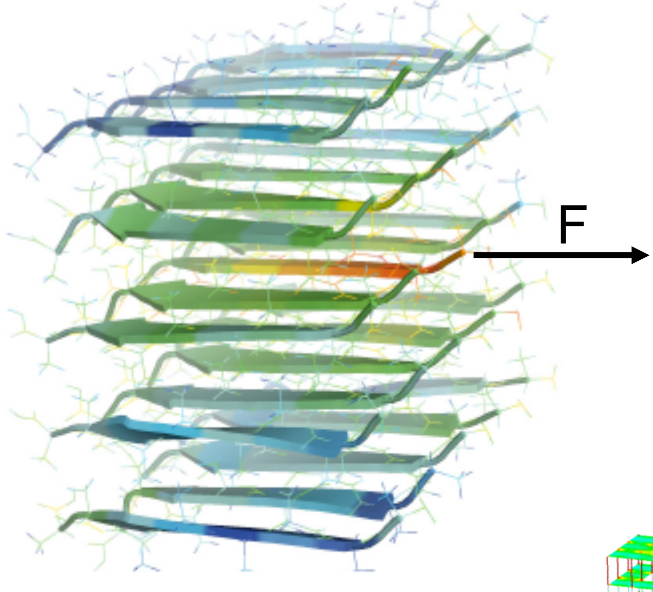
Forces from MD



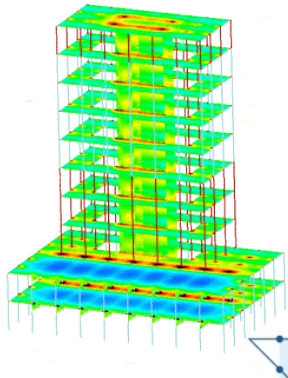
change in pairwise forces

$$\Delta F_{ij} = F_{ij} - F'_{ij}$$

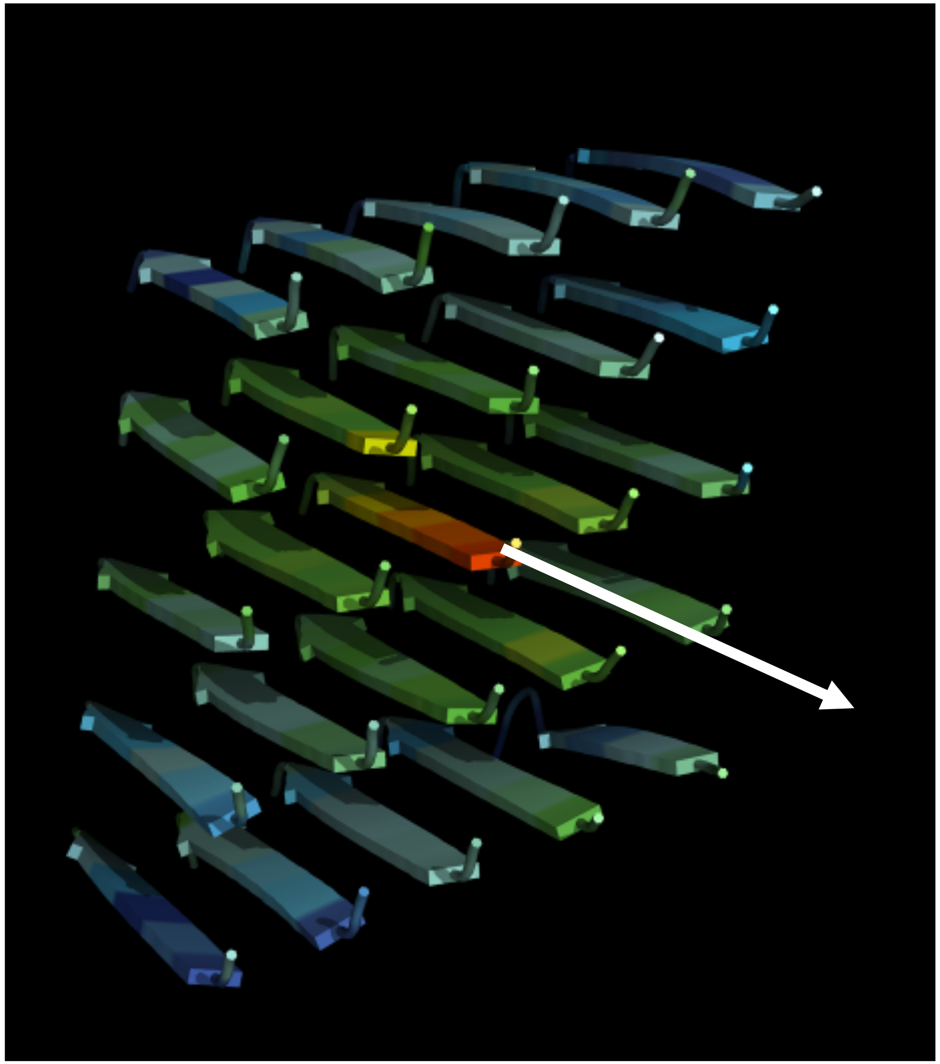
Application to proteins,
here: internal strain in a structural component of silk fibers



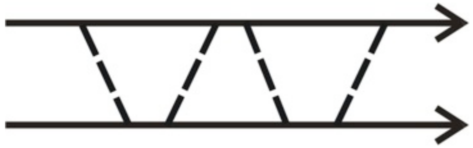
Compare:
force distribution
in large structures

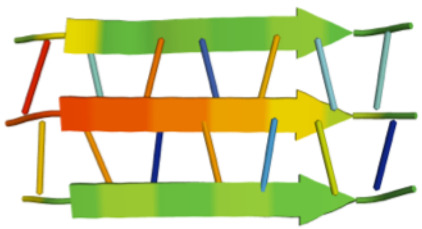


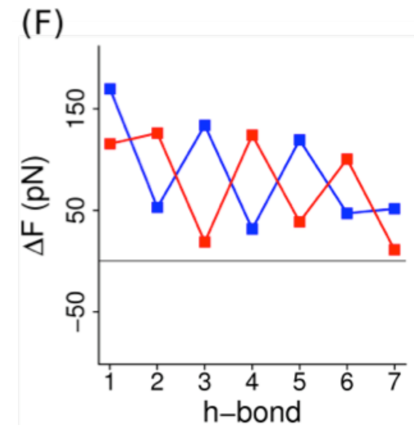
Mechanics of silk fibers



zigzag pattern of
hydrogen bonds
crucial for stabilization





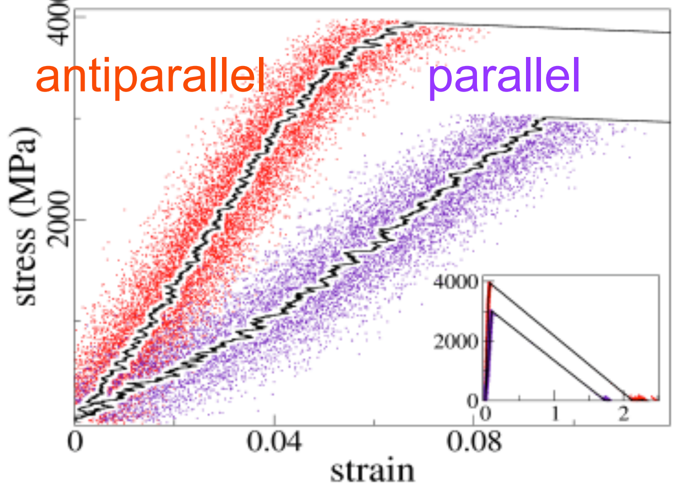


HITS

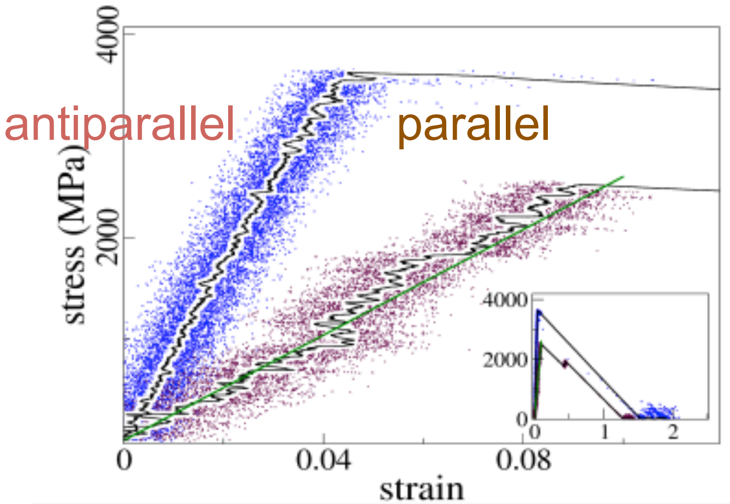
Mechanics of silk fibers

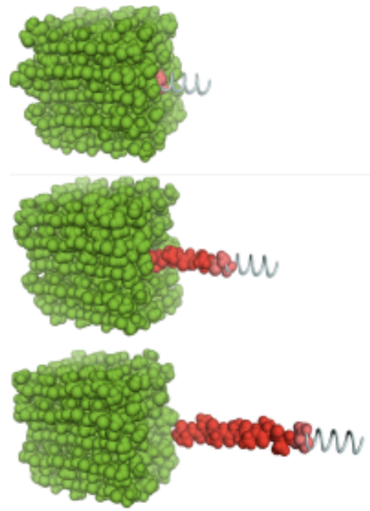
stress-strain curve
from Molecular Dynamics

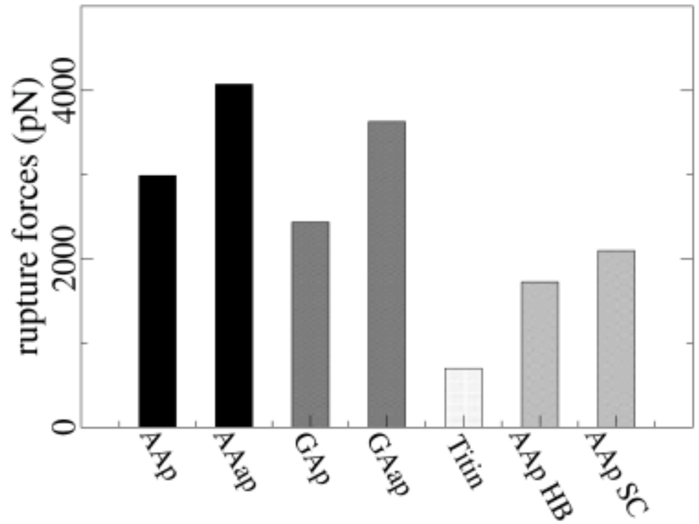
GA



AA





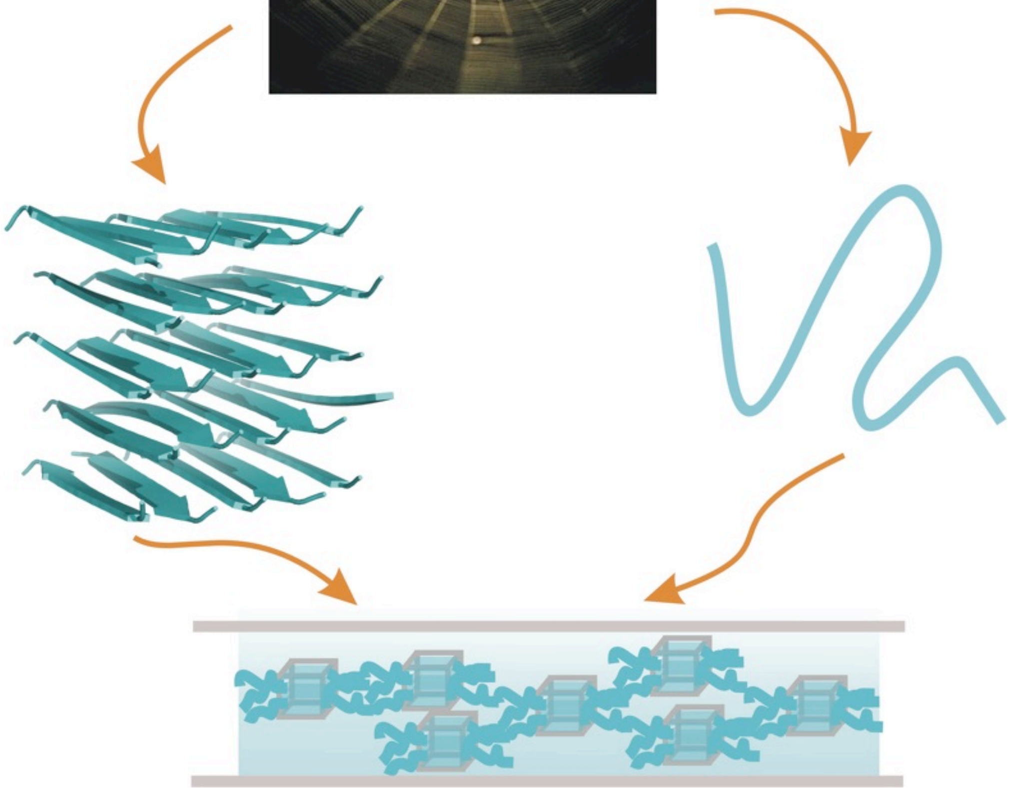


HITS

Mechanics of silk fibers

丝

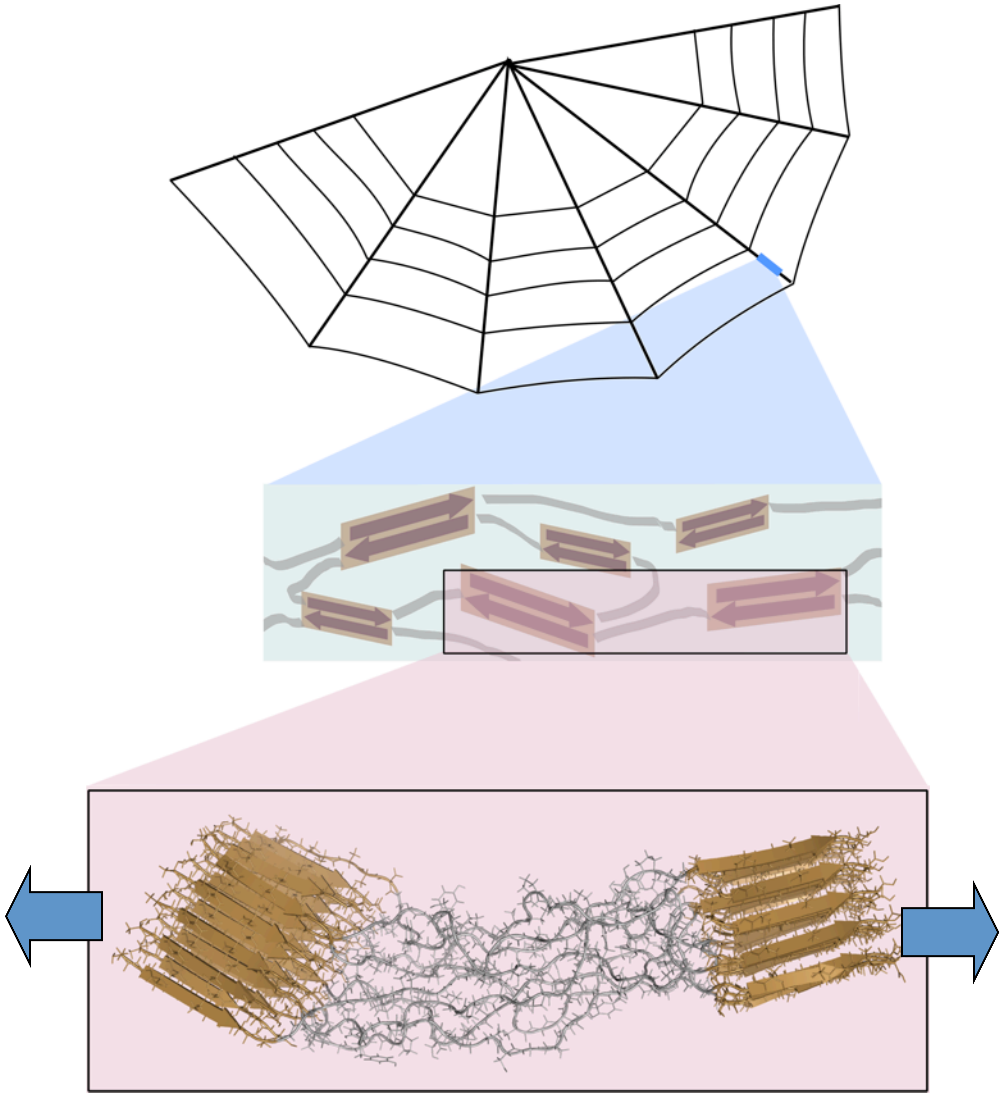
silk molecular structure:



Design of a semi-crystalline polymer:
interplay of amorphous and crystalline phase!

HITS

Mechanics of silk fibers

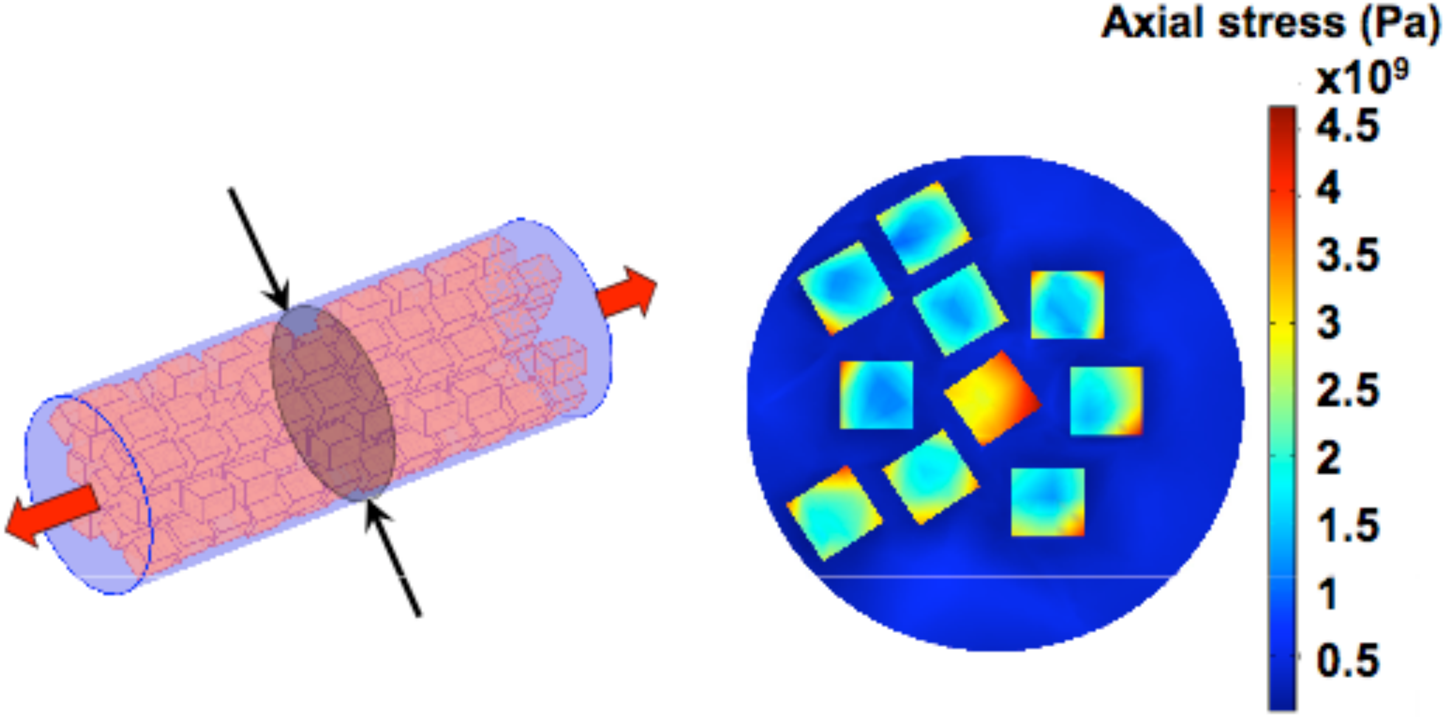


coarse_graining:

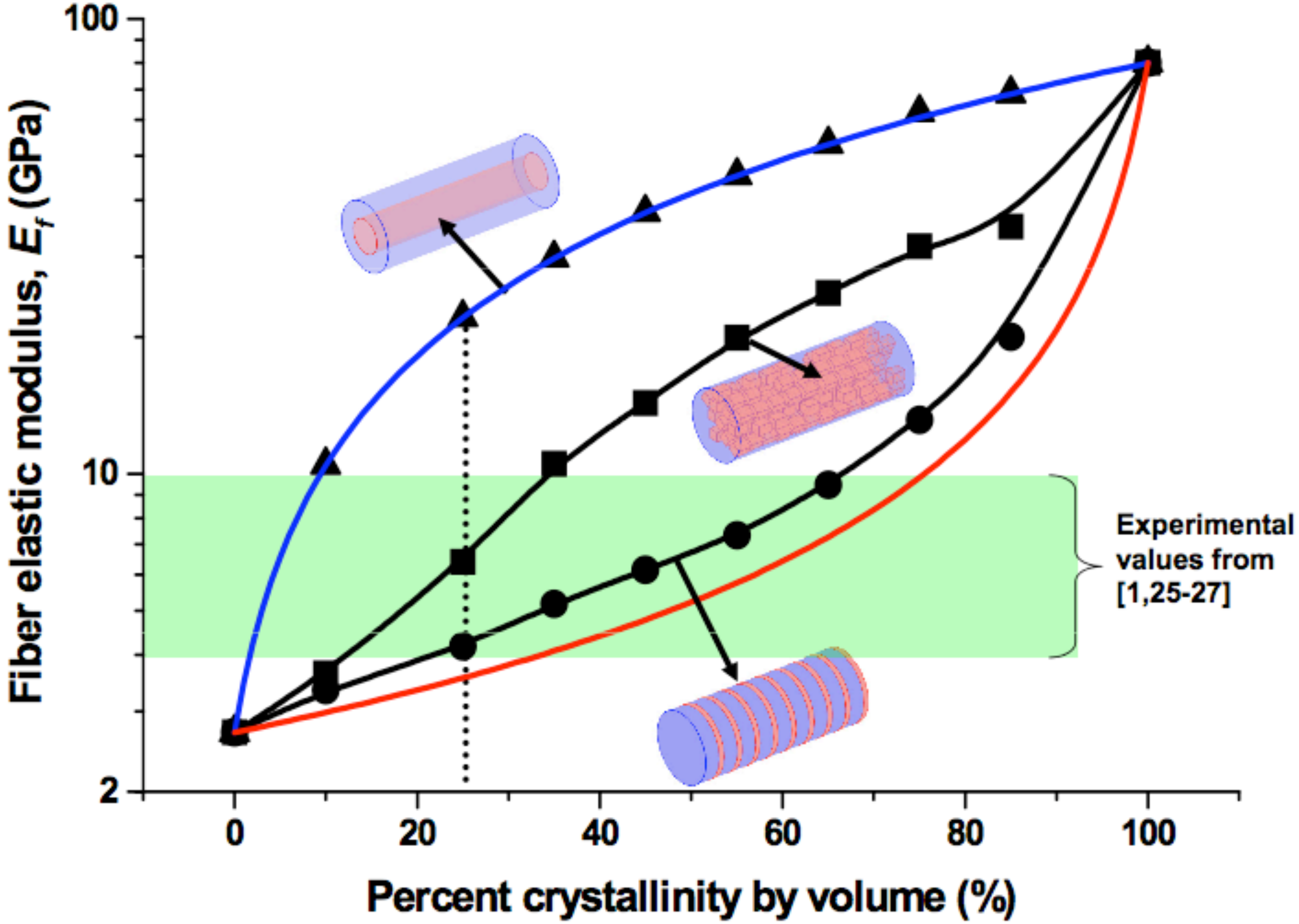
obtain elastic parameters from these all-atom simulations

HITS

Fiber scale: continuum mechanics

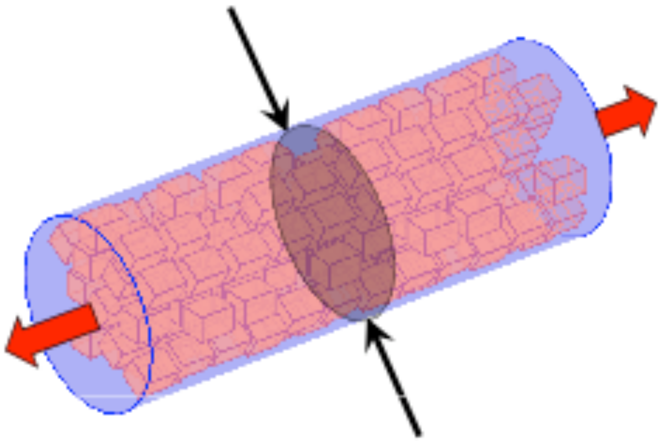


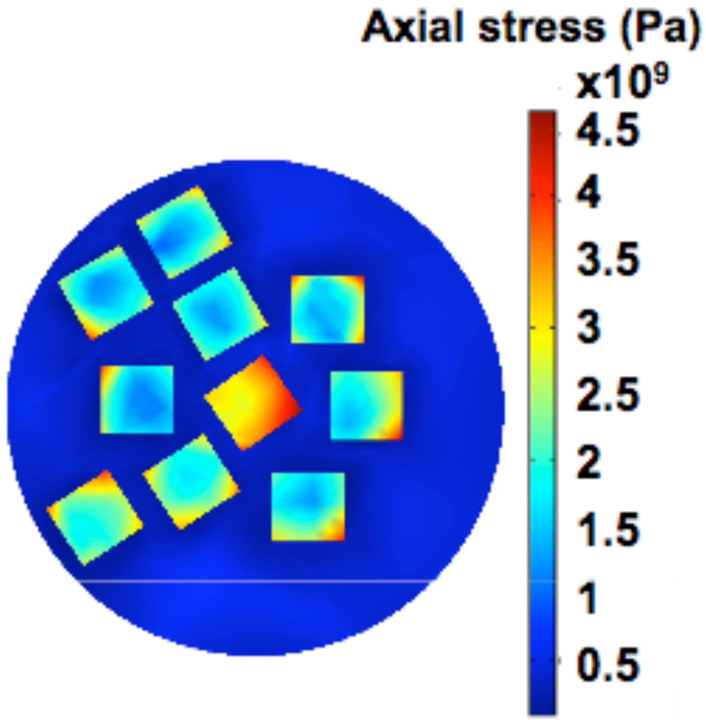
Fiber scale: continuum mechanics



Fiber scale: continuum mechanics

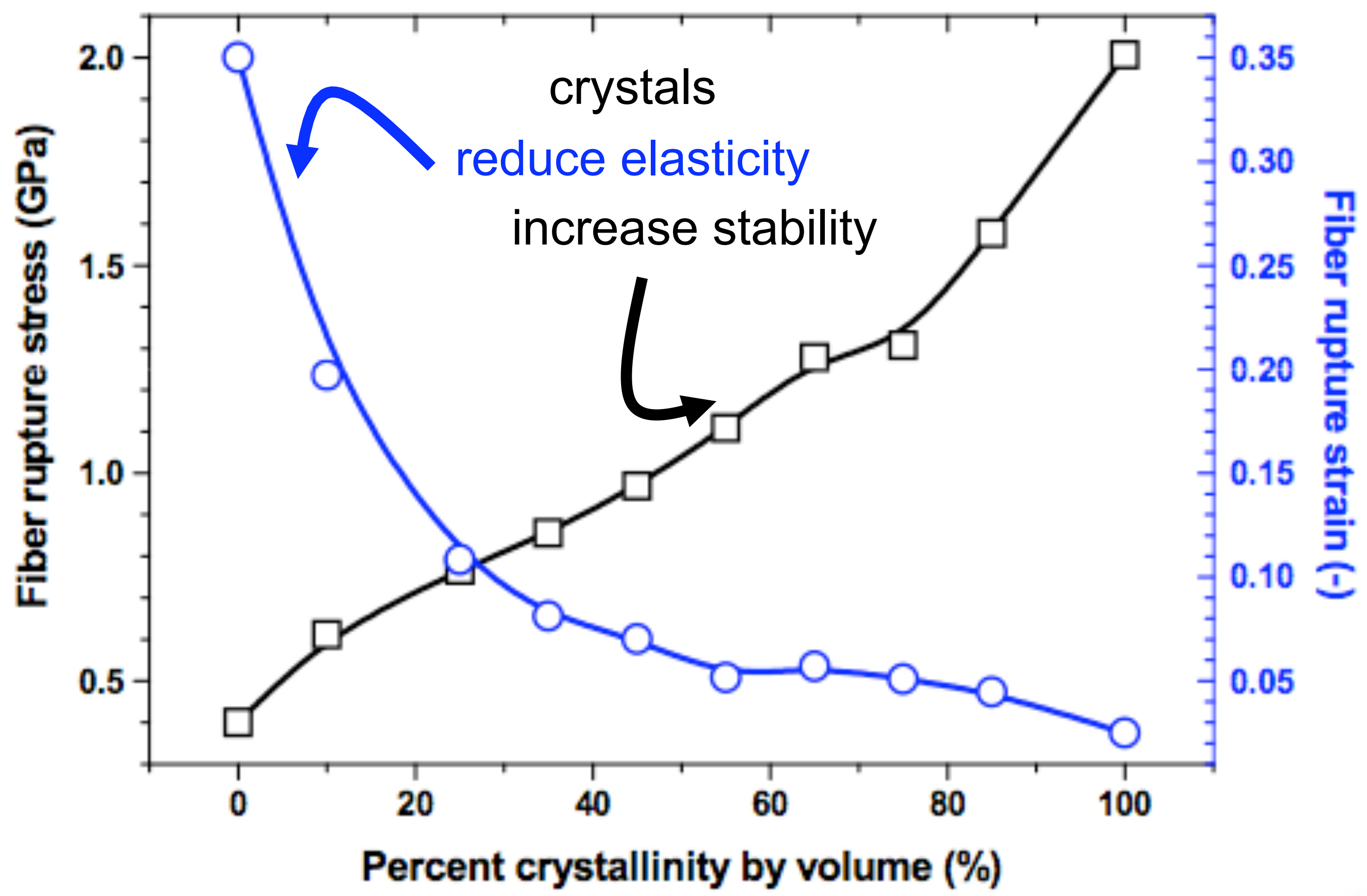
rupture stress at crystals
from molecular scale:
2 GPa





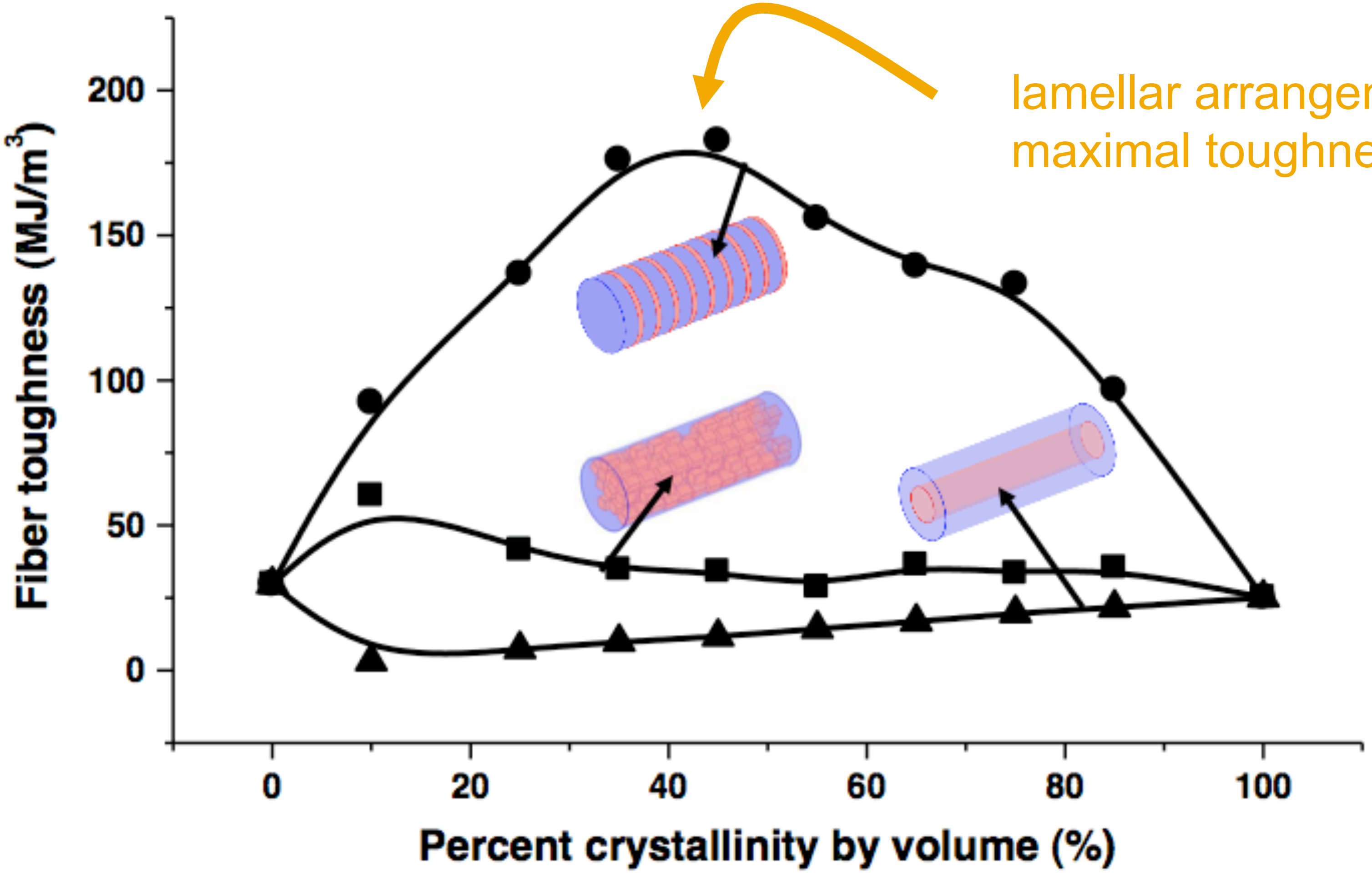
HITS

Fiber scale: continuum mechanics



HITS

Fiber scale: continuum mechanics



lamellar arrangement gives maximal toughness!

in agreement with: Hagn et al, Nature, May 2010

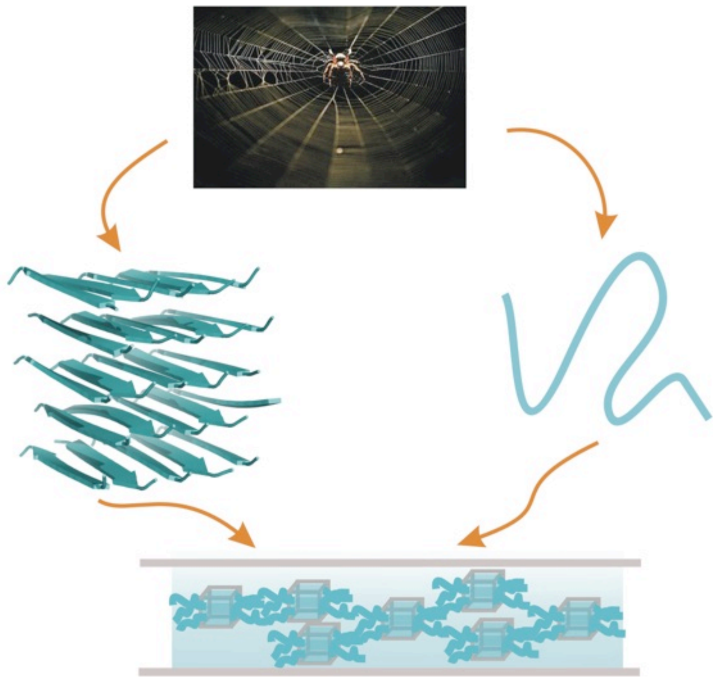
Conclusions

丝

silk self-assembles on steel into vertical beta sheets

force distribution helps to reveal crucial force-carrying motifs in proteins

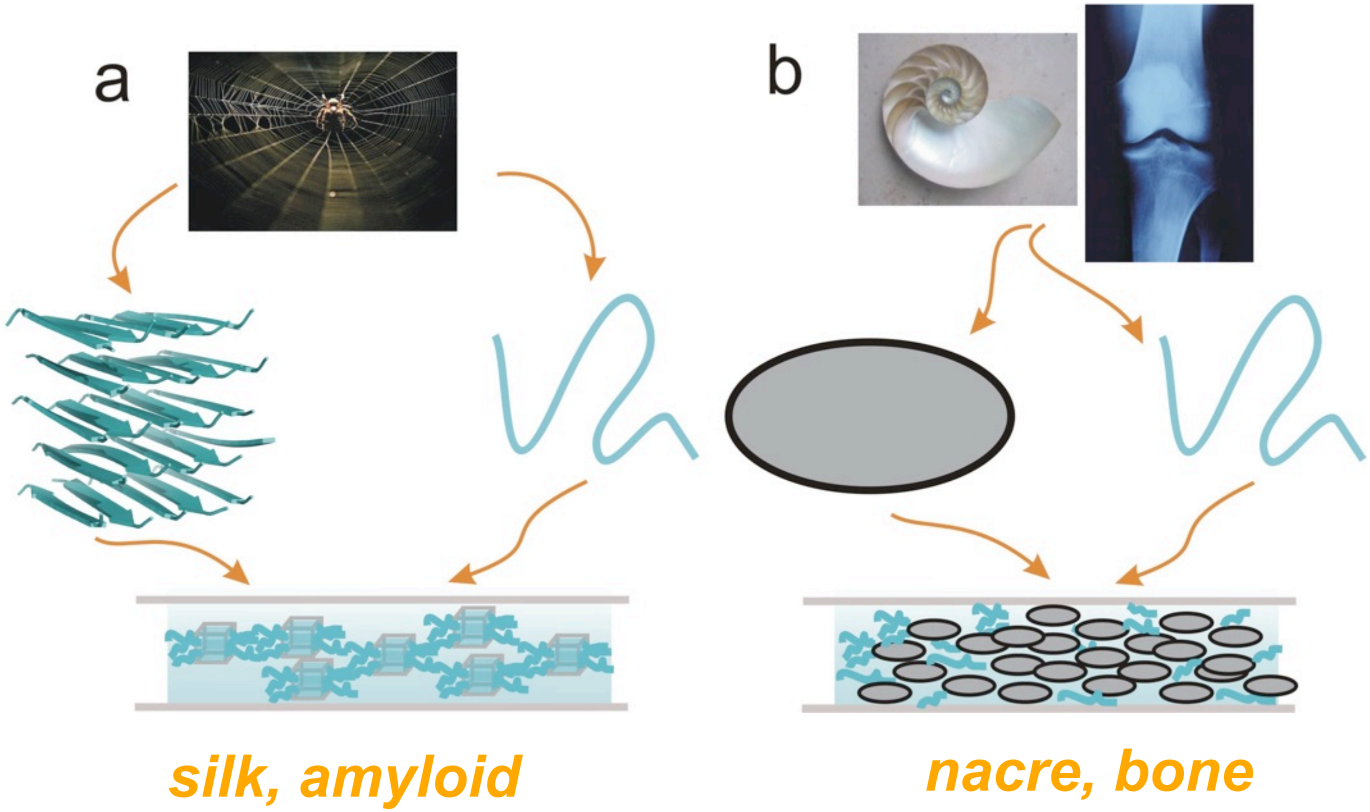
lamellar arrangement in fibers is optimal for mechanical toughness!



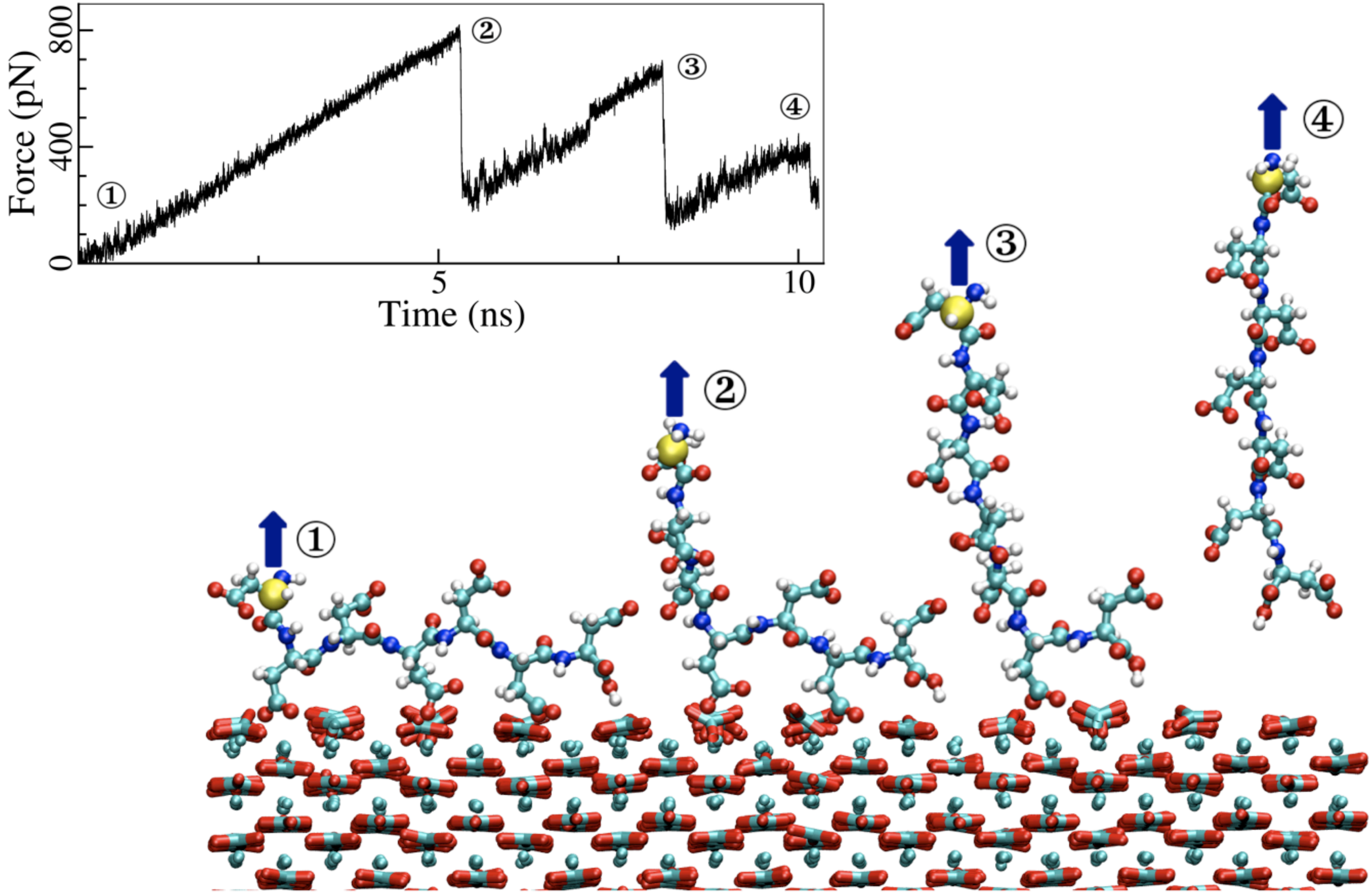
our approach:
- simple
- transferable
- can be automated
- can guide design of semi-crystalline materials poly-amides etc

S. Xiao, BJ 2009, Soft Matter 2010; M. Cetinkaya, BJ 2011, PCCP 2011

Nano-structured biomaterials

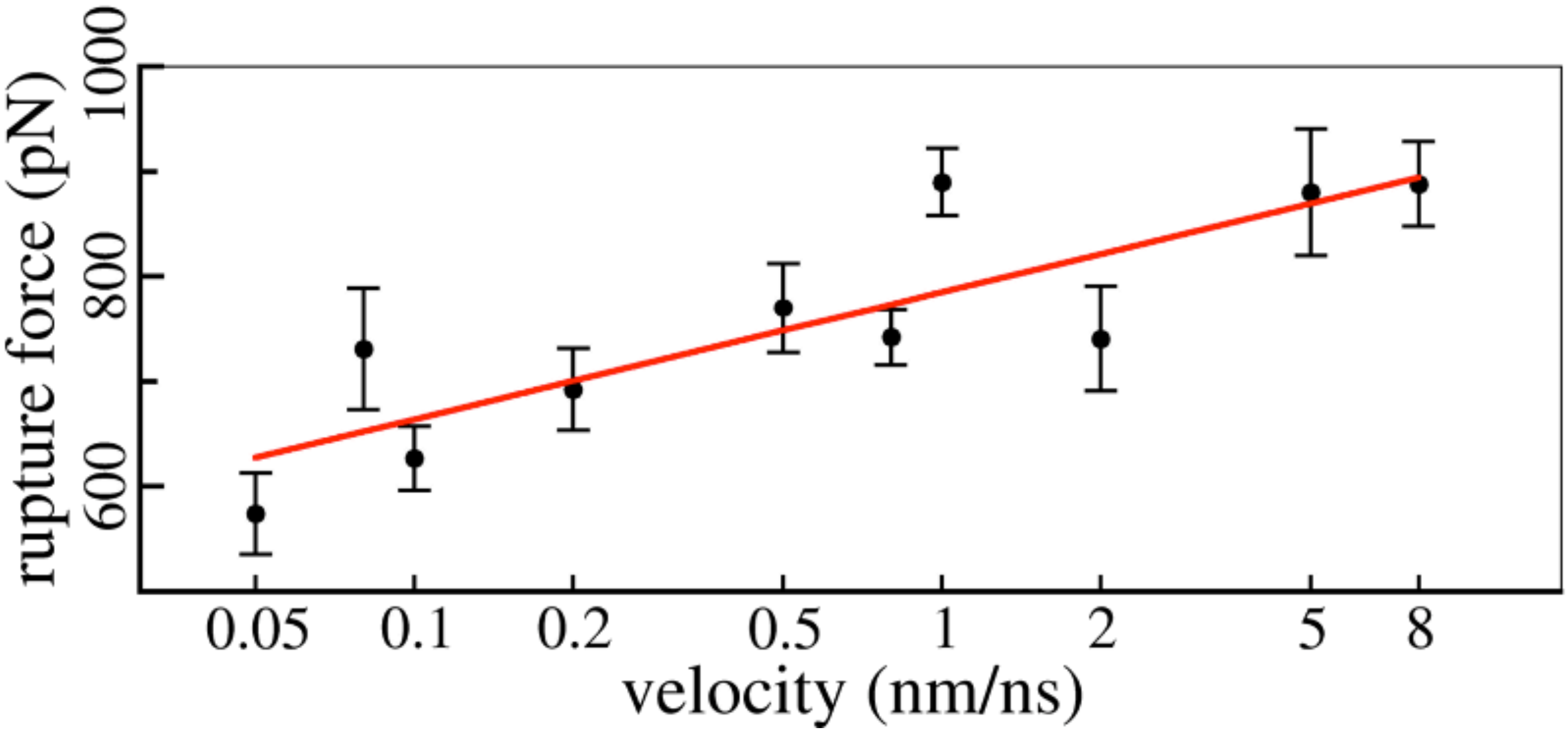


Nacre: aragonite + protein



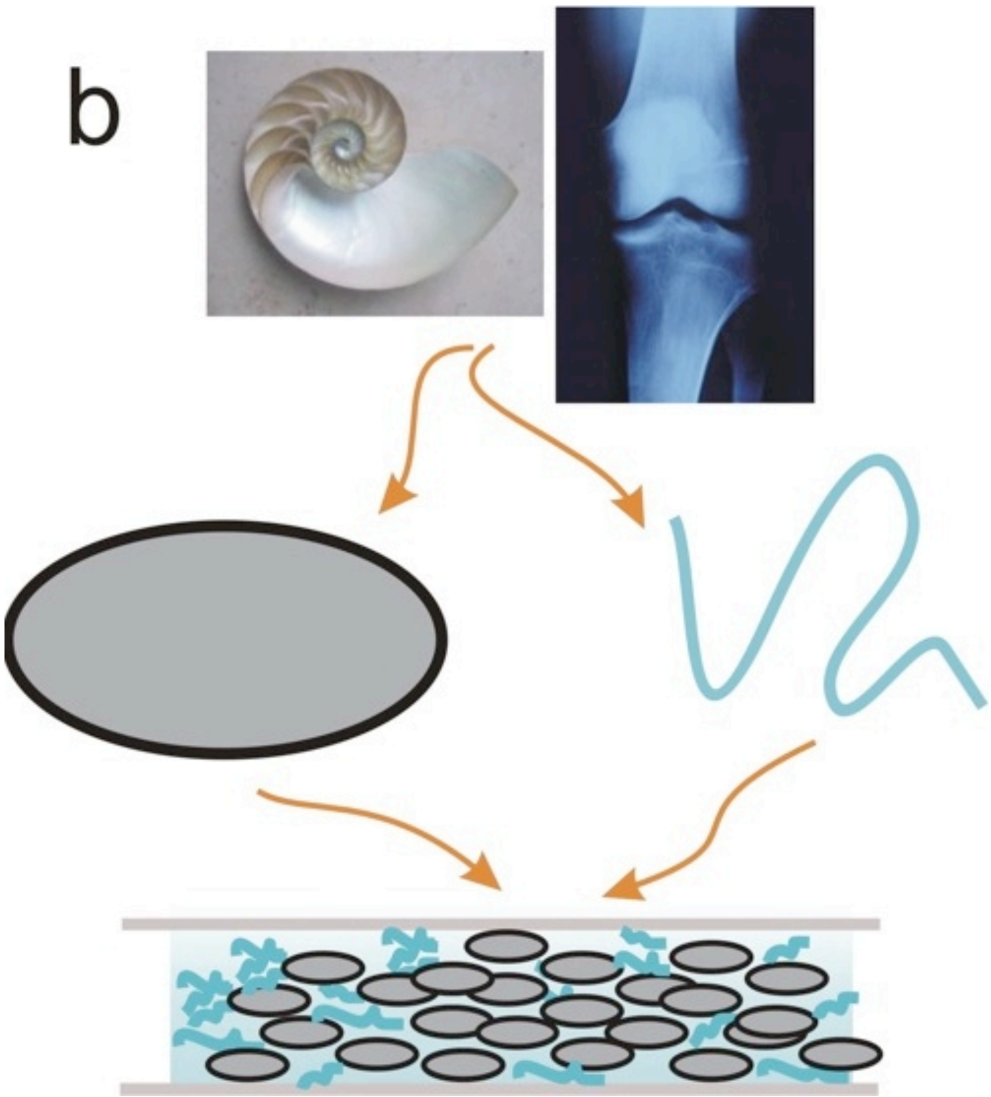
Shijun Xiao et al, J. Phys. Chem C, 2011

Nacre: aragonite + protein



extrapolation: 60pN-/+30pN

Nacre: aragonite + flaws



aragonite tablets -
a few tens of nanometers
in height:

flaws at the nanoscale?

in and with

PICB Shanghai

Heidelberg Institute for Theoretical Studies

experiments

Matthias Mayer, Bernd Bukau, ZMBH Heidelberg
Joerg Langowski, DKFZ, Heidelberg
Tobias Dick, DKFZ, Heidelberg
Suat Ozbek, COS, Heidelberg
Edward Lemke, EMBL, Heidelberg
Jasna Brujic, New York Univ.
Julio Fernandez, Columbia Univ.
Matthias Wilmanns, EMBL, Hamburg
Mathias Rief, TU Munich,
Joachim Spatz, MPI Stuttgart
Hermann Gaub, LMU Munich
Reinhard Schneppenheim, Uni-Klinik, Hamburg
Jianping Ding, SIBS, Shanghai

simulations/theory

Yi Xiao
Huazhong Univ, Wuhan
Bernd Markert, Univ Stuttgart
G. Caetano-Anolles
UIUC, Illinois
Gerrit Groenhof,
MPI Goettingen
Dave Thirumalai,
Univ Maryland

HITS

Thanks!

Senbo Xiao, Carsten Baldauf, Fei Xia, Ilona Baldus, Li Wenjin, Wolfram Stacklies, Christian Seifert, Scott Edwards, Jian Chen, Murat Cetinkaya, Cedric Debes, Agnieszka Bronowska, Bogdan Costescu

$$:
in Germany:
Klaus Tschira foundation
DFG, DAAD, BMBF, AvH, MPG
Toyota
in China:
NSFC