Towards a dynamical understanding of biological materials

HALOS symposium, 28/01/2022 Felix Roosen-Runge, Malmö University





Hierarchical Biological Structures and Dynamics

Single protein



- active sites
- localized dynamics
- → essential for biological function

Crowded solution



- protein interaction
- diffusion-reaction
- → essential for cellular processes

Cross-linked fibers



- mechanical rigidity
- viscoelasticity
- → functionality of biomaterials

→ multi-scale problem for experiments and modeling



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Scattering as a multi-scale method



M Grimaldo, FRR et al. Q.Rev.Biophys. 52 (2019) e7

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Scattering as a multi-scale method



kinetics of structural evolution

(time-resolved and pump-probe studies)

- **DIFF** Laue diffraction (crystals)
- W/SAXS wide/small-angle X-ray scattering
 - SLS static light scattering

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(coherent scatt.)

- NBS neutron backscattering
- TOF neutron time of flight



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collective dynamics

- NSE neutron spin echo
- X-PCS X-ray photon correlation spectroscopy
 - DLS dynamic light scattering

self-dynamics

- NBS neutron backscattering
- TOF neutron time of flight
- THz THz and dielectric spectroscopy
- NMR NMR spectroscopy
- PFG pulse-field gradient NMR
- FCS fluorescence correlation spectroscopy
- FRET Förster resonance energy transfer
- FRAP fluorescence recovery after photobleach.

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Sample system: Elastin & Elastin-like Peptides

Elastin

- key protein in extracellular matrix
- provides elasticity to tissues
- hierarchical structure of fibers
- hydrophobic units + crosslinks

Elastin-like peptides (ELPs)

- mimicking elastin's hydrophobic repeat unit: (VPGXG)_n
- model system with tunable properties

Mechanism of Elasticity: chain collapse



Mechanistic microscopic picture including structure and dynamics???



HALOS Project: structural relaxation in elastin films













Biofilms-Research Center for Biointerfaces (Malmö University)

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Condensation of ELP chains (VPGVG)₃





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Chain dynamics of ELPs

Chain dynamics (TOF-QENS)

- 10–100 picosecond time scales
- subnanometer length scales



- → despite dense condensates: local chain dynamics preserved
- $\rightarrow\,$ no rigid stacking, but flexible assemblies

 \rightarrow systematic, but mild changes

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work in progress

- detailed integrative analysis
- complementary computer simulations
- → consistent picture of microscopic mechanism



Structural relaxation in elastin hydrogels

central question for mechanistic understanding

which structural feature stores and releases mechanical energy?





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Dynamics for radiation-sensitive materials

X-ray photon correlation spectroscopy



Challenges

- radiation-caused processes / damage
- → low-dose protocol: X-ray speckle visibility spectroscopy
- potentially complex relaxation (model-free analysis needed)

Theoretical work in progress

• optimize pulse lengths/sequences



• matrix formalism for arbitrary relaxation function

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Summary

- Dynamics in biological material is relevant
- Scattering as suitable multi-scale methods



unlinked ELP chains



- condensation
- high chain flexibility preserved

Elastin hydrogels



• work in progress: multi-scale relaxation in radiation-sensitive matter

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