# APS March Meeting 2019

## Monday–Friday, March 4–8, 2019; Boston, Massachusetts

## Session P49: Tribology of Polymers and Soft Materials II: Friction and Slip

2:30 PM–5:30 PM, Wednesday, March 6, 2019
BCEC Room: 252A

Sponsoring Units: DPOLY GSOFT DFD GSNP
Chair: Catheryn Jackson

## Abstract: P49.00013 : Mechanical and thermodynamic properties of $A\beta_{42}$ , $A\beta_{40}$ and α-synuclein fibrils from molecular-scale simulation*

5:18 PM–5:30 PM

← *Abstract*

**Presenter:**
Adolfo Poma
(Biosystems and Soft Matter, Polish Academy of Sciences)

**Authors:**
Adolfo Poma
(Biosystems and Soft Matter, Polish Academy of Sciences)

Horacio Vargas
(Polymer Theory, Max Planck Institute for Polymer Research)

Mai Suan Li
(Theoretical Physics, Polish Academy of Sciences)

Panagiotis Theodorakis
(Theoretical Physics, Polish Academy of Sciences)

Atomic force microscopy (AFM) is a versatile tool to characterise the mechanical properties of biological systems. However, AFM deformations are tiny, which makes impossible the analysis of the mechanical response by experiment. Here, we have employed a simulation protocol to determine the elastic properties of several biopolymers (i.e. biological fibrils) . For these systems, the simulation approach is sufficient to provide reliable values for three different types of elastic deformation, i.e. tensile ($Y_L$), shear (S), and indentation ($Y_T$). Our results enable the comparison of the mechanical properties of these fibrils. In particular, we find a significant elastic anisotropy between axial and transverse directions for all systems. In addition, our methodology is sensitive to molecular packing of the fibrils . Interestingly, our results suggest a significant correlation between mechanical stability and aggregation propensity (rate) in amyloid systems, that is, the higher the mechanical stability the faster the fibril formation takes place.

*This research has been supported by the National Science Centre, Poland, under grant No. 2017/26/D/NZ1/00466 and the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 665778.

**4:54PM P49.00011: Contact and slip mechanics between crosslinked hydrogel surfaces using in situ microscopy*** ALISON DUNN (Presenter), CHRISTOPHER L JOHNSON, JIHO KIM, SHABNAM Z BONYADI, University of Illinois at Urbana-Champaign — The contact mechanics of soft-soft interfaces provide a backdrop for the slip mechanics due to the conformal contact at the interface, in which any surface asperities are fully compressed, and the apparent area of contact is the real area of contact. However, assumptions regarding the nature of the soft material as a thermal, semi-dilute mesh network, poroelastic solid, or other, will control the contact mechanics, especially over time. In this work we show detailed measurements of contact areas with polyacrylamide hydrogels during microindentation and slip which are revealed through particle inclusion and/or exclusion microscopy. The particles are green fluorescent polystyrene spheres of 0.5 or 1 μm in diameter. We identify time-dependent contact mechanics in migrating, stationary, and self-mated "Gemini" contact. Our data suggest that for long times, Gemini contact approaches a constant-pressure contact model, which depends upon the equilibrium osmotic pressure of the sample. Finally, we present for the first time asymmetric contact areas as visualized by in situ particle exclusion which manifests as a flow field around the probe. The results of this work begin to connect hydrogel material properties with surface mechanics.

*This work was support by NSF Award Number 1751945.

**5:06PM P49.00012: Wall slip of complex fluids: Interfacial friction versus slip length*** BENJAMIN CROSS, CHLOÉ BARRAUD, LiPhy, Université Grenoble Alpes, CYRIL PICARD, LILIANE LÉGER, FREDERIC RESTAGNO (Presenter), Université Paris-Sud, ELISABETH CHARLAIX, LiPhy, Université Grenoble Alpes — If the slip length is an useful notion notion to describe the friction of simple fluids, we will show that the slip length is not appropriate for viscoelastic liquids. Rather, the appropriate description lies in the original Navier's partial slip boundary condition, formulated in terms of an interfacial friction coefficient. We establish an exact analytical expression to extract the interfacial friction coefficient from oscillatory drainage forces between a sphere and a plane, suitable for dynamic SFA or atomic force microscopy noncontact measurements. We use this model to investigate the boundary friction of viscoelastic polymer solutions over 5 decades of film thicknesses and 1 decade in frequency. The proper use of the original Navier's condition describes accurately the complex hydrodynamic force up to scales of tens of micrometers, with a simple Newtonian-like friction coefficient that is not frequency dependent and does reflect closely the dynamics of an interfacial depletion layer at the solution-solid interface.

REF: Cross, B., Barraud, C., Picard, C., Léger, L., Restagno, F., & Charlaix, É. (2018). Wall slip of complex fluids: Interfacial friction versus slip length. *Physical Review Fluids*, *3*(6), 062001.

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**5:18PM P49.00013: Mechanical and thermodynamic properties of $A\beta_{42}$ , $A\beta_{40}$ and α-synuclein fibrils from molecular-scale simulation*** ADOLFO POMA (Presenter), Biosystems and Soft Matter, Polish Academy of Sciences, HORACIO VARGAS, Polymer Theory, Max Planck Institute for Polymer Research, MAI SUAN LI, PANAGIOTIS THEODORAKIS, Theoretical Physics, Polish Academy of Sciences — Atomic force microscopy (AFM) is a versatile tool to characterise the mechanical properties of biological systems. However, AFM deformations are tiny, which makes impossible the analysis of the mechanical response by experiment. Here, we have employed a simulation protocol to determine the elastic properties of several biopolymers (i.e. biological fibrils) . For these systems, the simulation approach is sufficient to provide reliable values for three different types of elastic deformation, i.e. tensile ($Y_L$), shear (S), and indentation ($Y_T$). Our results enable the comparison of the mechanical properties of these fibrils. In particular, we find a significant elastic anisotropy between axial and transverse directions for all systems. In addition, our methodology is sensitive to molecular packing of the fibrils . Interestingly, our results suggest a significant correlation between mechanical stability and aggregation propensity (rate) in amyloid systems, that is, the higher the mechanical stability the faster the fibril formation takes place.

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# Wednesday, March 6, 2019 2:30 PM - 5:18 PM

## Session P50 DPOLY DMP: Organic Electronics II: Structure and Morphology BCEC 252B - Dean DeLongchamp, National Institute of Standards and Technology - Tag(s): Focus