

CPP 58: Polymer Networks and Elastomers

Time: Friday 9:30–11:30

Location: ZEU 255

Invited Talk

CPP 58.1 Fri 9:30 ZEU 255

Studies of polymer thermosets using scattering techniques — ●MATS JOHANSSON — Department of Fibre & Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Thermoset polymers are complex macromolecular structures where the macroscopic properties depend on several different structural features such as crosslink density, rigidity on a molecular level, and internal secondary bond interactions. The final thermoset structure not only depend on the in-going monomers structure but also how these form the network i.e. the polymerization process. The presentation will describe how a combination of scattering techniques and traditional physical and chemical characterization techniques can reveal new insights on the structure / property relationship for thermoset polymers. It is moreover demonstrated that this approach also can be used to monitor the network formation in-situ i.e. how the structures evolves on a nanoscale during polymerization.

CPP 58.2 Fri 10:00 ZEU 255

Effect of π - π stacking interactions on mechanical properties of lignin-based thermosetting resins — ●JULIANA RIBCA¹, BENEDIKT SOCHOR², MARIE BETKER^{1,2}, STEPHAN V. ROTH^{1,2}, MARTIN LAWOKO¹, MICHAEL A. R. MEIER^{3,4}, and MATS JOHANSSON¹ — ¹Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden — ²Deutsches-Elektronen Synchrotron (DESY), Hamburg, Germany — ³Institute of Organic Chemistry (IOC), Materialwissenschaftliches Zentrum MZE, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — ⁴Institute of Biological and Chemical Systems-Functional Molecular Systems (IBCS-FMS), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

The transition towards a more sustainable global carbon economy can be achieved by replacing petroleum-based materials with bio-based alternatives. Lignin is the most abundant aromatic resource in nature and a largely unused by-product of the pulp and paper industry. It is considered a good replacement for fossil-based aromatics. One promising strategy for lignin valorization is to produce thermosetting resins. Further applications of these resins require the understanding of their physicochemical properties. An important role on these properties are playing π - π stacking interactions. Different configurations of π - π stacking interactions are favored between the lignin chains, due to the presence of aromatic rings. In this study, it was investigated the effect of π - π stacking interactions on mechanical properties of lignin-based thermosets by small and wide-angle X-ray scattering methods.

CPP 58.3 Fri 10:15 ZEU 255

Strain hardening of hydrogenated acrylonitrile butadiene rubber — ●CHRISTOPH GÖGELEIN¹ and MARJAN HEMSTEDT - VAN URK² — ¹Arlanxeo Deutschland GmbH, Kaiser-Wilhelm-Allee 40, 51369 Leverkusen — ²Arlanxeo Netherlands B.V., Urmonderbaan 24, 6167 RD Geleen, The Netherlands

Therban hydrogenated acrylonitrile butadiene rubber (HNBR) is a specialty elastomer used in the automotive and oil and gas markets. It is well known that HNBR with acrylonitrile (ACN) contents above 39 wt% shows strain-induced crystallization (SIC), caused by the crystallization of alternating ethylene-ACN units (Obrecht, 1986). For HNBR polymers with ACN contents lower than 36 wt%, crystallization occurs in longer ethylene units derived from hydrogenated butadiene sequences (Uschold & Finlay, 1974). Besides these well-established findings, there is an ongoing debate up to which temperature SIC occurs for HNBR (Narynbek Ulu, et al., 2017) (Shaw, 2019). Therefore, crystallization of the polymers was studied, using regular and isothermal differential scanning calorimetry at varying storage times. Furthermore, we investigated strain hardening behavior of HNBR networks with varying ACN contents from room temperature (RT) up to 100 °C, as well as at varying crosslink densities and filler loadings. Our results show that there is a significant strain hardening behavior for HNBR vulcanizates with high ACN content, i.e. for > 39 wt% ACN content. The effect is still observed at 60 °C, but not at 80 °C. Surprisingly, strain hardening doesn't enhance the fatigue lifetime for the samples under investigation.

CPP 58.4 Fri 10:30 ZEU 255

From Cellulose Model Surfaces to Elastic Papers — ●CASSIA LUX, SABRINA KERZ, and REGINE VON KLITZING — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Paper is a hierarchical material based on cellulose which allows functionalization on different length scales. The resulting multilateral use is especially crucial with regard to reducing plastic use and waste and replacing it with renewable and biodegradable resources. A novelty in terms of mechanical robustness and controllable fluid mechanics are elastic papers, prepared through the functionalization of the paper fibers with elastomeric particles that concentrate at the fiber-fiber-crossing points. In order to study the particle adsorption, planar cellulose model surfaces are prepared to mimic the surface of a cellulose fiber. The elastomeric core shell particles have a pH-responsive polycation shell, and their adsorption to the negative charged cellulose surface is studied in dependence of e.g. pH-value. The question we address is how the properties of the cellulose surface and the particles affect the contact area between both, and what effect the adsorption has on the elastic behavior of the particles. A special focus is to resolve the core-shell structure of the particles by Indentation AFM.

CPP 58.5 Fri 10:45 ZEU 255

Structure, phase behavior and mechanical properties of the surface of amphiphilic co-polymer networks — ●KEVIN HAGMANN¹, NORA FRIBICZER², SEBASTIAN SEIFFERT², CAROLIN BUNK³, FRANK BÖHME³, and REGINE VON KLITZING¹ — ¹Institute for Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt — ²Department of Chemistry, Johannes Gutenberg University Mainz, D-55128 Mainz — ³Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden

The underlying study focuses on the structure, phase separation and mechanics of the surface of amphiphilic co-polymer networks (ACNs). [1] The amphiphilic networks are synthesized from tetrameric star-shaped polymers, combining tetra-poly(ethylene glycol) (hydrophilic) and tetra-poly(ϵ -caprolactone) (hydrophobic) to form a 3D gel network. The topology and near surface structure of the networks are studied with atomic force microscopy (AFM). We put special emphasis on AFM phase imaging under various solvent conditions to identify nanophase separation at the interface. Additionally, we like to present the relation between surface structure and swelling and the resulting mechanical and rheological properties laterally and orthogonally to the gel surface of ACNs. In order to evaluate heterogeneities and phase separation, the mechanical and rheological behavior at the interface of the ACNs will be presented on various length scales (nm - μ m). The study shows that the environmental conditions have a strong effect on the gel structure and on nano/microrheological properties. [1] Hagmann et al.; *Polymers* 2022.

CPP 58.6 Fri 11:00 ZEU 255

A mean field model for reversible networks made of star polymers — ●MICHAEL LANG¹, KIRAN SURESH KUMAR^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Straße 6, 01069 Dresden, Germany — ²Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

We extend our recent approach [1] for linear equilibrium polymers with cyclization towards reversible networks made of star polymers. These model systems are particularly suited to test generalizations of the theory that account for the formation of cyclic network defects. Monte-Carlo simulation data and our mean field model demonstrate that the lack of pending loops in networks made by a hetero-complementary coupling of the stars leads to a pronounced shift of the position of the gel point of conventional networks towards lower concentrations. Larger cyclic structures in the networks, on the contrary, can develop a stabilizing effect on the network structure and can cause a reduction of the critical concentration for gelation for a suitable set of system parameters. Remarkably, this leads then to the opposite effect of finite loops as known for conventional irreversible gels.

[1] Lang, M.; Kumar, K. S. *Macromolecules* 54 (2021) 7021, 10.1021/acs.macromol.1c00718.

CPP 58.7 Fri 11:15 ZEU 255

Thermal Conductivity of Semicrystalline Polymer Networks: Crystallinity or Cross-Linking?

— ●MANOJ KUMAR MAURYA¹, JAMES WU², MANJESH KUMAR SINGH¹, and DEBASHISH MUKHERJI²
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Understanding the heat flow in polymers is at the onset of many developments in designing advanced functional materials. Here, however, amorphous linear polymers usually exhibit a very low thermal conductivity κ , often hindering their broad applications. In this context,

two common routes to increase κ are via semicrystallinity and cross-linking. It can therefore be inferred that the combination of these two effects may result in a further increase of κ with respect to the systems where only one of these two effects is important. Using molecular dynamics simulations, we investigate κ in semicrystalline polymer networks. Contrary to a prior understanding, we show that a combination of cross-linking and crystallinity does not always increase κ . Instead, a delicate competition between the lattice periodicity, the cross-linker types, and the bond density dictates the tunability of κ in these complex macromolecular systems. These results are also compared with the existing experiments.