CPP 29: Gels, Polymer Networks and Elastomers II

Time: Wednesday 15:00–16:15   Location: H 0106

CPP 29.1 Wed 15:00 H 0106

Structural characterization of model gels at preparation conditions and at swelling equilibrium — •Michael Lang and Reinhard Scholz — Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany

We use large scale computer simulations of star polymer model gels to separate the static and the dynamic contributions of the scattering intensity $I(q)$, allowing to determine the correlation length ξ of the corresponding polymer solution and the static correlation length Ξ combining several properties of the denser cross-link blobs. The correlation length ξ can incorporate parts of the form factor of the stars for polymer volume fractions around the overlap condition of the stars, affecting a determination of ξ from the scattering data. At swelling equilibrium, the cross-link motion is confined within a volume comparable to the size of the somewhat denser cross-link blob. Since the cross-link blob size scales $\propto \xi$, we measure $\Xi \propto \xi$ for our near ideal model networks. The confined motion of the cross-links implies a Gaussian shape for the static contribution. At swelling equilibrium, the dynamic part of the scattering intensity $I_{\mathrm{dyn}}(0)$ related to the solution-like correlation lengths is almost identical to the scattering intensity $I_{\mathrm{stat}}(0)$ of the static part. At preparation conditions, $I_{\mathrm{stat}}(0)/I_{\mathrm{dyn}}(0)$ decays with a power law following the polymer fraction of the cross-link blobs. Here, the larger volume available volume for cross-link motion stands out for increasing polymer volume fraction, reducing the concentration dependence of Ξ.

CPP 29.2 Wed 15:15 H 0106

Nonlocal elasticity explains equilibrium patterns in gels induced by phase separation — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Recent experiments found regular patterns in elastic gels, which emerged during cooling-induced phase separation. The patterns form without hysteresis, suggesting a continuous phase transition. To understand these observations, we propose an equilibrium field-based model based on phase separation between an elastic component and the solvent, augmented by nonlocal elasticity, which captures the microstructure of the gel. The model reveals a continuous phase transition from a homogenous state to patterns in stiff gels. Analytical approximations demonstrate that the pattern period is proportional to the geometric mean between the elasto-capillary length and a microscopic length scale of the gel, in good agreement with experimental observations. Our theory highlights the importance of nonlocal elasticity in soft matter systems, reveals the mechanism of equilibrium mesoscopic patterns due to elasticity, and will improve the engineering of such materials with controlled mesoscopic structure.

CPP 29.3 Wed 15:30 H 0106

Probing the microstructure properties of soft magnetic polymer hybrid materials using simulations — •Chinmay Pabshettiwar, Patrick Kreissl, Christian Holm, and Rudolf Weeber — Institute for Computational Physics, University of Stuttgart(US)

Embedding magnetic nanoparticles within a polymer hydrogel results in materials combining magnetic and viscoelastic properties, making them promising candidates for engineering and biomedical applications[1, 2]. Due to wide range of applications, it is essential to understand the coupling between magnetic nanoparticles and polymers and its effect on mechano-elastic properties. Experimentally, this is studied by analyzing the frequency-dependent magnetic susceptibility. In our study, we model this approach using computer simulations combining coarse-grained molecular dynamics and Lattice-Boltzmann hydrodynamics. Using such simulations, it is possible to switch on specific interactions, such as magnetic, steric, van der Waals, or hydrodynamic, individually. Hence, their influence on nanoparticle-polymer coupling can be studied. Using this technique, in our contribution, we study the effect of the hydrogel's mesh size on the magnetic relaxation behaviour of the nanoparticles. We compare different interaction potentials between the nanoparticle and the polymer chains. Furthermore, we obtain the AC susceptibility spectrum from the Green-Kubo approach[3] by analyzing the thermal fluctuation spectrum of magnetization in the absence of an external field.

References : [1] Filipcsei et al., 2010 [2] Weeber et al., 2018 [3] Kreissl et al., 2021

CPP 29.4 Wed 15:45 H 0106

Structure-Property Relationships of Biobased High-Performance Vitrimers — •Paulina Szymoniak[1], De-Yi Wang[2], and Andreas Schönhals[1] — [1]Federal Institute for Materials Research and Testing (BAM) Unter den Eichen 87, 12205 Berlin, Germany — [2]IMDEA Materials Institute, Eric Kandel 2, 28906 Getafe, Madrid, Spain

Epoxy vitrimers are a novel class of materials, showing great potential as sustainable replacement to classical epoxy thermosets within the frames of circular economy. Vitrimers are based on covalent adaptive networks (CANs), where dynamic bonds can break/reform and reshuffle upon a suitable stimulus, endowing polymers with unprecedented properties, such as shape-memory, self-healing, and recyclability. Here, the relationships between the microscopic structure and molecular mobility with thermomechanical performance of a novel vitrimer are studied. The material is based on glycerol triglycidyl ether (GTE) and vanillin-derivative hardener (VA), which represents an ideal biobased substitute for fossil-derived epoxy resins. The applied methodology comprises X-ray scattering, dielectric and mechanical spectroscopy, as well as calorimetry. Dielectric investigations of the materials revealed two dielectrically active processes, i.e., one related to segmental mobility, and a second broad process related to topology reshuffle. Further, GTE-VA is considered in the 'as-prepared' and 'healed' state, where the thermomechanical properties are studied as a function of recycling cycles, showing weak dependency on the healing procedure.

CPP 29.5 Wed 16:00 H 0106

Structural characterization of amphiphilic star polymer co-networks — •Reinhard Scholz[1], Michael Lang[1], Lucas Löser[2], and Kay Saalwächter[2] — [1]Leibniz Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany — [2]Institut für Physik - NMR, Betty-Heimann-Str. 7, Martin-Luther Univeristät Halle-Wittenberg, 06120 Halle, Germany

We analyze the structure of amphiphilic polymer co-networks consisting of hetero-complementary bound four functional star polymers A_4 and B_4 by computer simulations and by SAXS measurements. The computer-generated networks were characterized in an a-thermal co-solvent and in an increasingly poor solvent for the B component. In the poor solvent regime, the calculated pair distribution reveals a long-range radial oscillation, corresponding to the formation of dense B clusters and a pronounced peak in the scattering intensity. All simulated scattering data are decomposed into scattering from the time average density and from thermal fluctuations around this background, revealing an increased correlation length around the phase transition. Polymer networks consisting of complementary four functional stars of poly ethylene glycol (PEG) and poly caprolactone (PCL) were synthesized via covalent coupling of complementary end groups. Their SAXS data in different solvents were analyzed with a combination of model functions deduced from the computer simulations, revealing excellent agreement between observed and simulated length scales of the nanophase separation.