CPP 2: Polymer Physics I

Time: Monday 10:00-12:30

CPP 2.1 Mon 10:00 H40

Multiscale modeling of block-copolymer-nanomaterials — •STEPHAN ALEXANDER BAEURLE¹, TAKAO USAMI², and ANDREI GUSEV³ — ¹Department of Chemistry and Pharmacy, Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93053 Regensburg, Germany — ²Polymer Design Laboratory, Mitsubishi Chemical Group Science and Technological Research Center, Yokkaichi, Mie 510-0885, Japan — ³Department of Materials, Institute of Polymers, ETH, CH-8093, Zurich, Switzerland

A detailed knowledge about the physics and chemistry of multiphase materials on different length and time scales is essential to tailor their macroscopic physical and mechanical properties. A better understanding of these issues is also highly relevant to optimize their processing and, thus, their elucidation can be determinant for their final industrial application. In this presentation we introduce an analytical and numerical multiscale modeling approach, to explain and predict the peculiar stress relaxation behavior of block-copolymer-based thermoplastic elastomers at long times, which are subjected to a nonlinear extensional strain. We compare our theoretical results to the stress relaxation measurements performed on poly(styrene-isoprene-styrene) triblock copolymers and show that they correctly describe the crossover from power-law to stretched-exponential relaxation behavior, observed below the glass transition temperature of the polystyrene crosslinks. Our study confirm the importance of the chain-pullout mechanism in the stress relaxation process and demonstrates the involvement of multiple time- and structural-length-scales.

CPP 2.2 Mon 10:15 H40 Bicontinuous AB-diblock-copolymer mesophases: geometric arguments in favour of an "alternating" Im3m phase based on the I-WP surface — \bullet G.E. SCHROEDER-TURK¹, S.T. HYDE², and A. FOGDEN² — ¹Inst. für Theor. Physik I, Univ. Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen — 2 Applied Maths, Res. School of Phys. Sciences, Australian National University, 0200 ACT, Australia Bicontinuous phases in AB-diblock-copolymers are well known. In the "coreshell" Gyroid phase, immiscibility of A and B blocks leads to two intertwined identical networks of block A separated by a matrix of block B. The Gyroid triply-periodic minimal surface (TPMS) lines the middle of the B domain. For AB diblock copolymers, an "alternating" phase (as found in linear ABC terpolymers) with one network consisting of A and the other of B blocks does not exist. Chain stretching frustration is crucial to the phase stability analysis of these systems. Variations of the domain thickness, i.e. of the length between the TPMS and the center of the network channels, is unavoidable and incurs an entropic penalty for stretching of the polymer chains. We present an analysis of these variations for various TPMS of cubic symmetry. We demonstrate that the Gyroid is the bicontinuous geometry with the smallest frustration. The I-WP geometry is another TPMS where the two networks are not identical. The domain thickness variations are small for one network and large for the other. We argue that the I-WP may be suitable for an AB-diblock alternating phase in an asymmetrically polydisperse polymer system where one moiety has a wide and one a narrow molecular weight distribution.

CPP 2.3 Mon 10:30 H40

Core-shell filler in a block copolymer matrix: morphology and properties — •LESZEK JAKUCZEK^{1,2}, JOCHEN GUTMANN^{2,3}, and DANUTA ZUCHOWSKA¹ — ¹Wroclaw University of Technology,Wroclaw,Poland — ²Max Planck Institute for Polymer Research,Mainz,Germany — ³J.Gutenberg University,Mainz,Germany

Physical modification of block copolymer matrices has drawn much attention due to the remarkable possibility of property tailoring. Numerous structures can be prepared by changing the properties of the matrix (e.g. block length) or those of the nanofiller (dimensions, type of modification). Simultaneously interesting research problems- e.g. possible spatial arrangements of constitutive elements- can be addressed.

PS-grafted nanoparticles (polysiloxane microgel) were used as the filler. The inorganic cores were synthesized in a sol-gel process and surface modified with ATRP initiator. Controlled polymerization allowed to obtain well-defined polymer shells (Mw- up to 30 kg/mol; Mw/Mn about 1,10).

PS-grafted nanoparticles were used to modify the PS-PI diblock and

PS-PI-PS triblock copolymers. All samples were prepared via solution casting. Upon changing the filler type and loading, the influence of such parameters as Mw of grafted chains, grafting density and particle dimensions on the properties of host matrix could be extensively evaluated. Nanocomposites were thoroughly characterized- morphology changes were identified and visualized using SAXS and TEM. Additional information was obtained from rheological and thermal analyses (by the DSC).

15 min. break

CPP 2.4 Mon 11:00 H40 Thermal and chemical glass transition of two nanocomposite systems — ROLAND SANCTUARY, •JÖRG BALLER, RAVI BACTA-VATCHALOU, JAN KRISTIAN KRÜGER, BARTOSZ ZIELINSKI, and MAR-TINE PHILIPP — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a, avenue de la Faïencerie, L-1511 Luxembourg

Epoxy resins modified with different kind of nanoparticles, so-called nanocomposites, reveal properties which are interesting from the fundamental and technical point of view. E.g. nanoparticles of Al2O3 strongly increase the viscosity of the composites which leads to a modified glass transition behaviour: Tg as well as the distribution of relaxation time is changed as a function of nanoparticle content. However surface-treated SiO2 particles almost have no effect. Addition of a suited hardener to these nanocomposites leads to reactive adhesive systems. These systems undergo a chemical glass transition during the curing process. Despite of the big difference in viscosity between the epoxy resins filled with Al2O3 and SiO2 particles, curing of these systems doesn't seem to be sensitive to the type of filler particles. Moreover the kinetics of the chemical reaction is faster compared to systems without nanoparticles. Concerning the thermal glass transition, the influence of filler particles is completely different for the epoxy resin and the cured system (e.g. opposite shift of Tg). MDSC, Brillouin spectroscopy and rheology data is presented and discussed for these systems before, during and after chemical curing.

CPP 2.5 Mon 11:15 H40 Structure Property Relationships of Polymeric Nanocomposites based on Polyhedral Oligomeric Silsesquioxanes — NING HAO, MARTIN BOEHNING, and •ANDREAS SCHÖNHALS — Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, D-12205 Berlin

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvement (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally scaled composites.Different polymer based nanocomposites are prepared where, polycarbonate and polystyrene are used as polymer matrices. As molecular nanofillers polyhedral oligomeric silsesquioxanes (POSS) with different substituents (Phenethyl-, Chlorpropyl-) are used. The property structure relationships of these nanocomposites are investigated by dielectric spectroscopy, gas transport measurements (permeation, sorption) and density measurements as well. The results are discussed with regard to the phase structure of the nanocomposites and the properties of the different POSS. This includes the construction of phase diagrams. Especial attention is paid to characterize the interfacial region between the polymeric matrix and nanoparticles. This regards also to estimate the length scale of interaction between the nanoparticle and the matrix.

CPP 2.6 Mon 11:30 H40

Shear and elongational properties of melts of reactively compatibilized PA 6/ABS blends — CHRISTIAN SAILER and •ULRICH ALEXANDER HANDGE — Institute of Polymers, Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich

Reactive compatibilization is a technologically commonly applied method in order to improve the interfacial adhesion in multiphase polymer blends. In this study, we investigated the influence of reactive compatibilization on the rheological properties and the morphology of polyamide 6/acrylonitrile-butadiene-styrene (PA 6/ABS) blends in the melt. Three different blends with different types of morphology (disperse morphology and cocontinuous structure) were prepared. Then linear viscoelastic shear, melt elongation and subsequent recovery experiments were performed. The linear viscoelastic shear properties of the blends were discussed using the fractional Zener model. In melt elongation, we investigated the deformation of the blend morphology using atomic force microscopy and quantified the stretch ratio of the extended drops and domains. The analysis of our recovery experiments after melt elongation revealed that the interfacial tension and reactive compatibilization strongly influence the elasticity of the blends (C. Sailer, U.A. Handge, submitted). We discuss our experimental results for the blends by taking into account the formation of polymer chains grafted with PA 6 via reactive compatibilization.

CPP 2.7 Mon 11:45 H40

Collective rearrangement under shear of a polycrystalline soft material — •TERESA BAUER^{1,2}, JULIAN OBERDISSE¹, and LAURENCE RAMOS¹ — ¹Laboratoire des Colloïdes, Verres et Nanomatériaux (UMR CNRS-UM2 5587), CC26, Université Montpellier 2, France — ²Lehrstuhl für Biophysik E22, Technische Universität München, Germany

Polycrystalline soft materials show interesting rheological behaviour in creep experiments. Initially the instantaneous shear rate decreases as a power law with time in a similar manner as a solid. This power law regime is followed by an abrupt increase of the shear rate, indicating a fluidization of the sample, and finally reaches a stationary flow with a high constant shear rate. Here we studied how this behaviour is coupled to a structural rearrangement of the sample by conducting in situ rheology and Synchrotron (ID2 ESRF) SAXS measurements on a polycrystalline surfactant hexagonal columnar phase simultaneously. We show that a collective reorientation of the crystallites occurs at the onset of flow. We discuss how the fluidization time, which scales with the shear modulus and the applied stress, is related to structural changes.

CPP 2.8 Mon 12:00 H40

Skotometrical Investigation of Volume Changes during Rapid Deformation of Elastomers — •MICHAEL KERSCHER, GERALD JO-HANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

Polymer composites consisting of a filler and an elastomer are indis-

pensable for daily life. Thus, an enormous effort is done to understand their properties. When trying to derive constitutive equations for elastomers, the constance of volume on deformation is one of the major assumptions to be made. Already several decades ago, however, experiments showed a volume expansion, albeit very small. Therefore, a constant volume has still been assumed even though these experiments were only performed at small strain rates or with slow measuring processes not considering a possible effect at short time intervalls.

In our contribution, we show the influence of deformation velocity on volume expansion at high deformation rates. For this purpose, in our experiments we use an optical dilatometer based on the principle of a scotometer (from greek " $\sigma\kappa\sigma\tau\dot{\alpha}\delta\iota$ ": darkness) which allows measurement of volume changes in the range of a few milliseconds.

Our experiments point to a by far higher volume change than expected from slow deformation which then relaxate in the range of several milliseconds. These new results have to be taken into consideration when trying to fully understand the laws behind the deformation of elastomers.

CPP 2.9 Mon 12:15 H40

How to stop ageing of biosynthetic PHB - 'melt irradition' — •ANTJE BERGMANN^{1,2} and ANTHONY OWEN¹ — ¹Fakultät für Physik, Universität Regensburg — ²Fakultät für Physik, Universität Karlsruhe (TH)

Bacterially processed polyhydroxybutyrate (PHB) is a semicrystalline polymer. Its properties are similar to those of some conventional plastics such as polyethylene (PE). Unfortunately, it undergoes an ageing process, which is characterised by an increasing embrittlement while stored at room temperature. Using various structural analysis methods and comparing the results with those obtained by mechanical measurements we investigated the mechanisms of ageing and found that both a progressive crystallisation process and physical ageing are responsible for the ageing phenomenon.

On the basis of that knowledge we tried out different treatments on the samples in order to prevent the progressive embrittlement. Whereas annealing treatments and the use of plastizisers were not suitable to stop the ageing process completely, irradiation of amorphous PHB with electrons turned out to be a successful method - we call this procedure 'melt irradiation'. An elastic network can be established within the amorphous regions, even though the samples are highly crystalline. This new PHB morphology shows the desired elastic mechanical properties, and the samples are no longer prone to ageing.