CPP 6 SYMPOSIUM: Polymer networks and beyond: From molecular structure to materials and biological functions

Zeit: Samstag 08:30–10:10 Raum: TU C243

CPP 6.1 Sa 08:30 TU C243

Welcome and Introduction — •Jens-Uwe Sommer —

Hauptvortrag

CPP 6.2 Sa 08:40 TU C243

Random network media and their universal properties: Landau theory and beyond — •Paul Goldbart — Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, U.S.A.

Random network solids, as formed e.g. by the vulcanization of polymeric liquids, will be examined via an order-parameter based Landau approach. Despite its simplicity, this approach yields a rich, universal picture of random solids, even at the classical level, including their heterogeneity and rigidity. By going beyond the classical level, via the incorporation of fluctuation effects, connections with percolation and random resistor networks emerge, and the scaling of the shear modulus near the random solidification transition can be determined. In addition, the influence of Goldstone-type excitations can be ascertained, and seen to be especially strong in low-dimensions. Extensions to more elaborate settings, such as vulcanized polymer blends and nematic elastomers, can be made. A simple cavity-based scheme sheds light on the origins of results first obtained via replica-based approaches.

The contributions of many collaborators, most notably Annette Zippelius, are gratefully acknowledged.

Hauptvortrag

CPP 6.3 Sa 09:10 TU C243

The inside view: computer simulations and molecular theories of entangled polymer melts, solutions and networks — •Ralf Everaers — Max-Planck-Institut für Physik komplexer Systeme,Nöthnitzerstr. 38, 01187 Dresden, Germany

Computer simulations provide unprecedented access to the microscopic structure and dynamics of polymeric systems. In particular, they are an ideal tool to study and analyze topological constraints on the dynamics of entangled polymer chains which can slide past but not through each other. We (i) show how the microscopic foundation of the tube model can be established by analyzing the topological state of polymeric liquids in terms of primitive paths, (ii) provide a unified view on loosely and tightly entangled systems, (iii) present an extension of the tube model to polymer networks which is (iv) shown to describe the microscopic and macroscopic response to strain of randomly end-linked and randomly cross-linked networks and (v) discuss the interpretation of scattering experiments addressing these issues.

CPP 6.4 Sa 09:40 TU C243

Computer simulation of polymer networks: Swelling by mixtures of explicit solvents and finite size effects — •Enno Oyen and Reinhard Hentschke — Fachbereich Mathematik und Naturwissenschaften, Bergische Universität, Wuppertal

The swelling of regular, tightly meshed model networks is investigated by a molecular dynamics-Monte Carlo hybrid technique. Chemical equilibrium between two simulation boxes, representing the gel phase and a solvent bath, respectively, is obtained by subjecting a binary Lennard-Jones fluid, serving as explicit solvents, to the particle transfer step of Gibbs Ensemble-Monte Carlo. The swelling behaviour, especially preferential absorption of a single component from a binary mixture, is studied depending on temperature, pressure, and fluid composition. In addition we investigate finite size effects comparing our simulations with an analytic theory. The latter yields finite size scaling behaviour in good accord with simulation results for both "dry"networks and gels in contact with solvent baths.

CPP 6.5 Sa 09:55 TU C243

Computer simulations on swelling and deformation experiments of polymer networks — •Michael Lang, Dietmar Göritz, and Stefan Kreitmeier — Fakultät für Physik, AG Polymerphysik, Universität Regensburg, 93040 Regensburg

Within the simulation of polymer networks using e.g. the bond fluctuation method the detailed information on the structure of the systems can be used to understand the microscopic processes during a swelling or deformation experiment. To this end we measure the mobility of each single molecule during the simulation of a swelling experiment and the subsequent simulation of a deformation experiment on the swollen network. At the same time we determine the average forces at each monomer. A comparison of this data with the information on the well known structure of the systems, the swelling ratio or the measuered force allows for a direct analysis of the dependence of macroscopic properties on the microscopic structure. Furthermore, we can test directly the assumptions of some theories on polymer networks concerning the constrained fluctuations of different parts of the network structure, which are the basis for the calculation of macroscopic properties of the systems. However, this comparison shows, that none of the existing theories models all aspects of the constrained microscopic motion or the spatial distribution of forces with sufficient detail.