

MONTPELLIER, FRANCE

JUNE 16<sup>TH</sup> – 17<sup>TH</sup> 2011

The third European workshop on nanocomposites and polymer dynamics was held in Montpellier, in the south of France, on Campus St. Priest of University of Montpellier II. Anne-Caroline Genix and Julian Oberdisse (both from Laboratoire Charles Coulomb, CNRS/University of Montpellier) planned and organized this two-day meeting, together with Wim Pyckhout-Hintzen (Jülich, Germany), Gerald J. Schneider (Munich, Germany), and Marc Couty (Michelin, France).

The general idea of this workshop was to bring together scientists from Europe (in fact also from further away) working on the many different facets of polymer nanocomposites, both experimentally and theoretically. The broad range of phenomena which may appear when one incorporates nanofillers in polymer matrices, which act and possibly intermingle on different time and length scales, manifests itself sometimes through striking macroscopic (e.g. rheological or mechanical) properties, and sometimes in subtle shifts in dynamics at the scale of a monomer, which in turn may considerably influence the macroscopic response. This interplay is usually system dependent, which motivates research on many different model systems. The latter appear to be a perfect playground for theory and simulation, as it is necessary to extract the fundamentally relevant ingredients from a large body of experimental evidence, using sophisticated modelling. A second reason for the broad coverage of systems lies in the close connection with applications: indeed, a car tyre containing poly(styrene-butadiene) rubber is not optimized for the same performance as a bio-sourced and -degradable polymer used in thin film packaging.

The talks presented in Montpellier reflect this interest in the same problem but from many different points of view, and gave a nice overview of the activities in the field. As with the previous two editions (in 2006 and 2008), it was chosen to split the program into two parts. The first part was a series of two invited lectures covering almost the entire morning sessions by internationally recognized experts in the field. The central idea of these lectures is not only to provide an introduction to the field for PhD-students and post-docs, but also to define common elements of language and identify common problems occurring in the broad field of nanocomposites. Thursday morning, François Boué from Labora-

toire Léon Brillouin (Saclay, France) gave a valuable and pedagogical introductory lecture entitled "Structure and mechanical reinforcement in nanocomposites". He covered the basics of polymer physics, common experimental set-ups and guidelines for interpretation to study the structure and rheology of polymer melts and rubbers. He then introduced model filler and matrix systems, and finished with recent advances in nanocomposite chain and filler structure, at rest and under deformation. The second morning session, entitled "Numerical simulations of polymer dynamics" was devoted to polymer dynamics, with particular emphasis on the different simulation methods. Jean-Louis Barrat from University Joseph Fourier (Grenoble, France) gave an enlightening lecture on the different levels of modeling currently applied to polymer properties. Starting with a quick overview on quantum simulations and 'exact' force fields, he presented the basic mesoscopic models of polymers on different length scales, up to self-consistent field theory. J.L. Barrat took care to relate the models to experimental data, and also discussed some simple rules on how to choose an appropriate model. In addition, he also presented the mechanisms of Monte Carlo and molecular dynamics simulations used to explore phase space. The lecture ended with an example on the mechanical properties of glassy polymers.

The participant talks were opened with a presentation by O. Pravaz (Fribourg, Switzerland) on in-situ polymerization as a route towards properties tuned polymer-colloid nanocomposites. It became clear from the presentation that the preparation of nanocomposites of controlled dispersion advances steadily. A complete session on the rather hot topic of chain labelling in nanocomposites followed, including talks by M. Meyer (Jülich, Germany) on polymer grafted silica nanoparticles, M. Tatou (Orsay, France) on reinforcement and polymer mobility in silica-latex nanocomposites, A.S. Robbes (Saclay, France) on magnetic nanocomposites with tuneable filler anisotropy, and F. Schneider (Jülich, Germany) on microgel-polymer blends. A second session was devoted to the characterization of nanocomposites using physical methods on micro- and macroscales. H. Zhang's (Paris, France) nice presentation on cavitation in carbon black filled styrene-butadiene rubber probed by real time small angle X-ray scattering fueled a lively dis-

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cussion on the problem of cavitation. A. Bogner (Lyon, France) presented three electron tomography methods applied to polymer nanocomposites, which gave a complementary view on structural characterization as compared to scattering techniques. F. Grillard (Bordeaux, France) reported on surprising temperature memory effects in the electrical and mechanical properties of nanotube composites. The session ended with a communication by A. Chevillard (Montpellier, France) on biobased nanocomposites for controlled release applications, giving insights in the complex world of biopolymers used for nanocomposites.

The last session of the workshop, following the morning lectures on polymer dynamics by J.L. Barrat, was dedicated to polymer dynamics. V. Boucher (San Sebastian, Spain) gave a talk on a microscopic view of polymer dynamics in polymer nanocomposites, by relating segmental dynamics, glass transition temperature, and physical aging. C. Mark (Jülich, Germany) investigated a model system where he could separate interface- from melt-dynamics. T. Narita (Paris, France) presented a talk on the dynamics of silica particles in hybrid hydrogels studied by dynamic light scattering, and correlated the influence of the gel structure and the surface chemistry with the silica motion, a problem central to all nanocomposite studies. Two theoretical talks

concluded the session. K. Hagita (National Defence Academy, Japan) presented coarse-grain simulation studies on filled polymer nanocomposites, and showed that his group was able to reconstruct the filler structure under strain using scattering and computer simulations. The workshop ended with A. Lyulin's (Eindhoven, The Netherlands) brilliant talk on molecular-dynamics simulations of polymers in nanoconfinements.

In the eyes of the participants, the particular focus of the workshop on nanocomposites and polymer dynamics, the combination of pedagogical lectures with communications on recent advances on many different systems and techniques, and the many occasions to discuss science informally on-site, in front of posters or during the workshop dinner on a nice summer evening, accompanied by a Jazz group, made this a successful meeting. The workshop was organized as an open topical meeting of the European network of excellence Softcomp, but would not have been possible without financial support from Softcomp, CNRS Montpellier, University of Montpellier, and the Languedoc-Roussillon region.

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