

Structure of filler aggregates in polymer nanocomposites: a reverse Monte Carlo approach to the analysis of complex spectra

D. Musino, C. Schmitt-Pauly, A.C. Genix, A. Banc, J. Oberdisse

Laboratoire Charles Coulomb (L2C), CNRS, Université de Montpellier, 34090 Montpellier
France

julian.oberdisse@umontpellier.fr

Polymer nanocomposites are mixtures of nanoparticles and polymer chains, where the filler particles are usually added to enhance mechanical properties, e.g. of car tire materials. Performance depends to a great extent on the structure of the filler, i.e. its dispersion state in the polymer matrix, which itself depends on mixing protocols, but also on the thermodynamics of the system. The latter can be tuned by performing either chemical surface modifications of the nanoparticles, or by playing with the mass and/or grafting properties of the polymer chains.

In this talk, some straightforward ways to obtain information from small-angle scattering on the structure of nanocomposites will be presented [1], before presenting two (very) recently developed methods, the correlation-hole analysis [2], and a reverse Monte Carlo path to aggregate statistics [3]. As application, we will present recent results on nanocomposites close to industrial applications, with particular emphasis on the impact of grafting of small molecules on such structures [4, 5]. If there is time, chain structure will also be discussed, with a quick outlook on why contrast-matching with SANS in nanocomposites often fails [6].

REFERENCES

- [1] A.-C. Genix and J. Oberdisse, Structure and dynamics of polymer nanocomposites studied by X-ray and neutron scattering techniques. *Current Opinion in Colloid & Interface Science* 2015, 20, 293-303 (2015).
- [2] A.-C. Genix and J. Oberdisse, Determination of the local density of nanoparticle assemblies, under review.
- [3] D. Musino et al, to be submitted.
- [4] D. Musino, A.-C. Genix, C. Fayolle, A. Papon, L. Guy, N. Meissner, P. Weda, T. Bizien, T. Chaussée, J. Oberdisse, Synergistic effect of small molecules on large-scale structure of simplified industrial nanocomposites, submitted.
- [5] C. Schmitt-Pauly, A.-C. Genix, J. G. Alauzun, J. Jestin, M. Sztucki, P. H. Mutin, J. Oberdisse, Structure of alumina-silica nanoparticles grafted with alkylphosphonic acids in poly(ethylacrylate) nanocomposites, *Polymer* 2016, 97, 138-146
- [6] A. Banc, A.-C. Genix, C. Dupas, M. Sztucki, R. Schweins, M.-S. Appavou, J. Oberdisse, Origin of small-angle scattering from contrast-matched nanoparticles: A study of chain and filler structure in polymer nanocomposites, *Macromolecules*, 48, 6596–6605 (2015).