Structure analysis by small-angle scattering of polymer nanocomposites: from model to industrial systems

A. Banc, G. Baeza, A.C. Genix, C. Dupas, J.Oberdisse

Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Université de Montpellier, F-34095 Montpellier, France

The structure of polymer nanocomposites has important consequences on final properties, like for instance mechanical reinforcement. While the structure of the hard filler nanoparticles (NPs) is usually characterized by electron microscopy and small-angle X-ray scattering (SAXS), the chain conformation can only be measured by small-angle neutron scattering (SANS). Two main difficulties may arise with such a structural analysis. First of all, extracting reliable structural information on filler dispersion may be hindered by lack of a priori knowledge of the system. In this talk, we will discuss two examples. In the first one, additional knowledge is due to the model character of well-characterized NPs, and it can be used to analyze scattering data using Monte Carlo simulations [1]. In the second one, industrial filler NPs of high structural complexity have been used, and structural characterization of this system was only possible by quantitatively combining MC simulations, transmission electron microscopy, and SAXS [2]. Concerning the determination of polymer conformation by SANS, a second and mostly unforeseen difficulty shows up: in spite of great care in contrast-matching (undesired) NP contributions to the SANS signal, such additional intensities are systematically found in the literature. Two model cases are discussed in this talk: the first one emphasizes large-scale polymer heterogeneities reminiscent of the solution structure before nanocomposite formation. This structure is described quantitatively by a 'hairy bead' model [3]. The second one, finally, is the result of a general study of incomplete filler NP matching, evidencing for the first time that smallest NPs may induce statistical fluctuations in H-D-density in a surrounding shell, making in principle matched filler visible. Incidentally, the typical size of such mismatched polymer shells is deduced from the data [4].
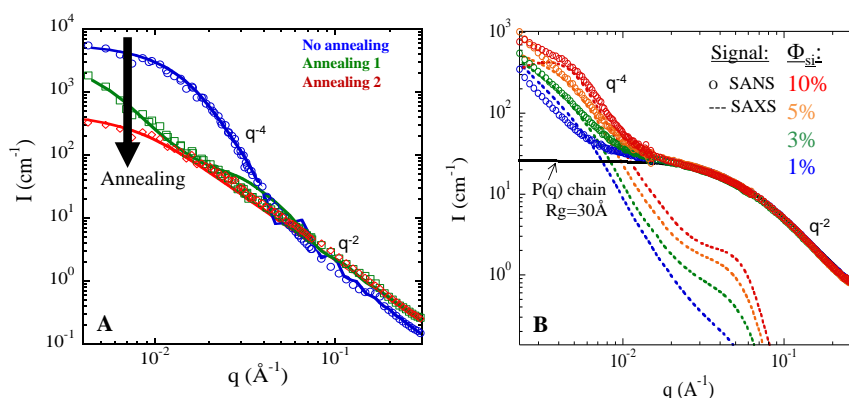

Figure: **(a)** SANS of latex matrix as function of annealing fitted with the hairy-bead model. **(b)** SAXS and SANS of nanocomposites filled with small silica NPs.

[1] A. Banc et al, Macromolecules **47 (9)**, 3219–3230 (2014); J. Oberdisse et al Soft Matter, **3**, 476-485 (2007)
[2] G. Baeza et al, Soft Matter **10**, 6686-6695 (2014)
[3] A.C. Genix et al, Macromolecules **45(3)**, 1663-1675 (2012)
[4] A. Banc et al, submitted