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Small-angle scattering simulations for suspensions of nanocrystals

M. Schmiele[1], S. Gehrer[1], T. Unruh[1]

[1]*Friedrich-Alexander University Erlangen-Nuremberg, Chair for Crystallography and Structural Physics, Department of Physics, Erlangen, Germany*

Suspensions of nanocrystals which possess large lattice spacings d(hkl) and only a small number of unit cells along the direction of the reciprocal lattice vector G(hkl) can feature broadened Bragg peaks in small-angle scattering (SAS) patterns. The scattering from molecules located at the interface between the nanocrystals and the dispersion medium which stabilize and functionalize the nanocrystals can interfere with the scattering of the nanocrystals and affect the shape and position of their Bragg peaks. This allows to study how these molecules arrange on the surface of the nanocyrstals. As an example we study suspensions of lecithin stabilized β-tripalmitin nanocrystals which adopt a platelet-like shape. Their SAS patterns exhibit a broadened 001 Bragg peak (cf. SAXS curves in the graphical abstract). With the x-ray and neutron powder pattern simulation analysis (XNPPSA) we have demonstrated that the SAXS and SANS patterns of dilute tripalmitin (3 wt%) suspensions can be simultaneously reproduced on an absolute scale [1,2]. Thereby, powder averaged SAS diffractograms are computed for an ensemble of nanocrystals which are embedded in a dispersion medium. The crystallographic structure of the nanocrystals (CIF-file) and their geometry are taken into account and the amphiphilic lecithin molecules which cover the nanocrystals are modelled with two shells (cf. model in the right inset). From the analysis of the fitted shell thicknesses and scattering length densities it turns out that the lecithin molecules arrange rather flatly and densely packed on the surface of the nanocyrstals. Moreover, the XNPPSA method allows a reliable determination of the thickness distribution of the nanocrystals with molecular resolution [1,2]. With rising tripalmitin concentration the platelets form self-assembled stack-like structures [1,3] and finally nematic liquid-crystalline domains. The XNPPSA allows to investigate the structure and amount of such stacks in the suspensions.

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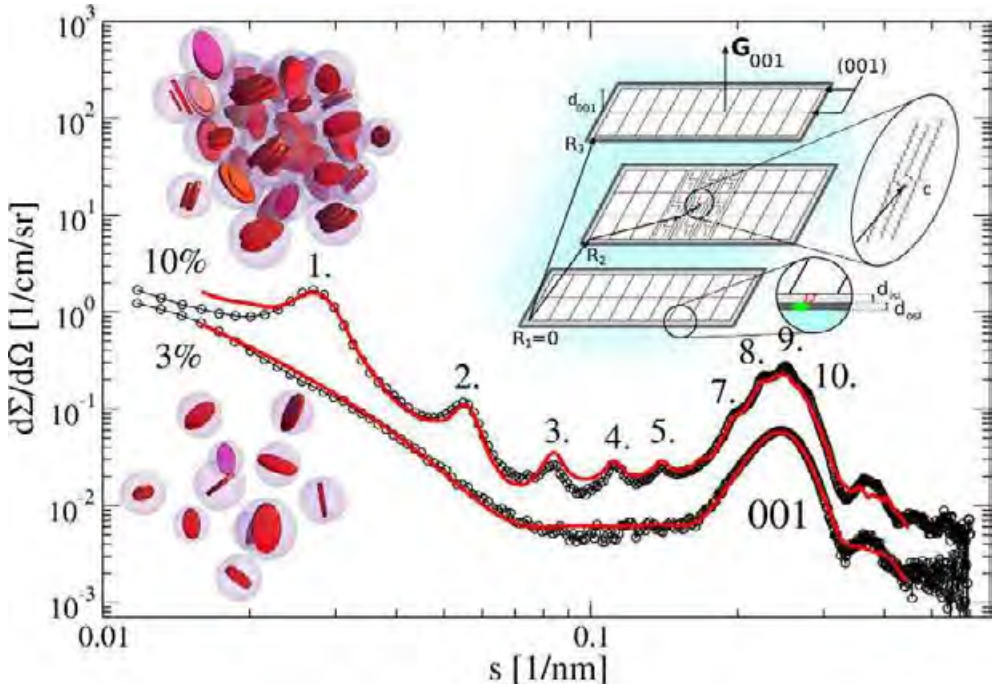

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