X-ray characterization of three possible edible oleogelators: Experiment and Theory

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April 10, 2023

Abstract

Three oleogeletors molecules (Triacontane (TC), Stearic acid (SA), and Behenyl Lignocerate (BL)) were studied individually, in pairs, or all together to make an oleogel using triolein as the oil. WAXS, SAXS and USAXS were used to elucidate the solid structures from angstroms to a few micrometers. A two-dimensional mapping of atomic positions for each molecule was carried out to understand the crystalline multilayer structures formed. We assumed that the molecules were rigidly extended and that they underwent no significant (hindered) rotations so that the free energy is determined by the Lennard-Jones interactions of closely-packed multilayers. TC molecules were predicted to form a tilt angle of ϑ_t [?] 33°, yielding a SAXS line at q[?] 0.194 A^{-1}, in acceptable agreement with the measured q=0.181 $^{-1}$.For SA crystals ϑ_t [?] 33° (predicted) yielding a SAXS line at q=0.150 $^{-1}$ compared to q=0.159 $^{-1}$ (observed). No mixed crystals were observed for any pair of molecules or when all three were used. USAXS data showed that SA forms large nanocrystals compared to TC and BL. All three combinations of molecular pairs showed basic scatterers smaller or similar to those of individual molecules. The theory presented here, together with the experimental results, showed why no mixed crystals are formed from two or all three molecules. Data from the USAXS region suggested that, when using all three molecules, a more compact fractal structure was obtained, compared with those if one or two of the molecules were used.

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