Nanocomposites and nanomaterials

Phase transitions of 1-octadecene in silica gel based nanocomposites

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Nowadays rapid development of different fields of nanotechnology caused growing interest to physical properties of nanostructured materials such as thin films, small particles, etc. The nanocomposites based on the substances inside the porous matrixes attract special attention. Confining of molecular species inside the pores may cause the formation of new crystalline phases, different from ones of the bulk media; also it may influence the molecular mobility, temperature and character of phase transitions, such as melting and crystallization.

The aim of our work is characterization of the influence of pore size and surface coverage of silica matrix onto the phase transitions of 1-octadecene.

A set of silica gels with different pore size and surface area were chosen for the experiment. Particularly the silica gels KCK-2.5, KCC-4, KCM-6c with the pore diameters 10.3, 4.7 and 2.3 nm correspondingly as well as Silica gel for column chromatography (United Chemical Technologies (UCT), 100-200 Mesh fraction, 6 nm pore diameter), and the samples of corresponding silicas after chemical functionalization with octadecyltrichlorosilane (C_{18}) or trimethylchlorosilane (-SiMe₃) were used.

The melting temperature (m.t.) of 1-octadecene confined in the silica pores decreases with the reduction of the pore size (fig. 1). The functionalization of silica with $-SiMe_3$ groups resulted in further decrease of confined 1-octadecene m.t.: temperature decrease to 1.5, 2 and 3 K was observed for correspondingly for trimethylsilylated KCK-2.5, UCT and KCC 4 in compare with unmodified ones. At the same time the modification of silicas with $-C_{18}$ groups resulted in growth of 1octadecene m.t. in compare with unmodified silicas.

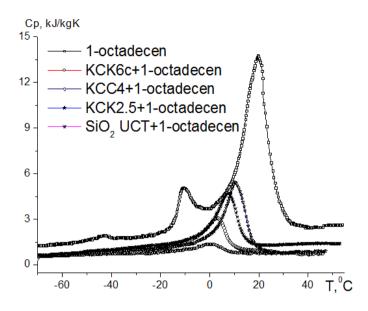


Fig. 1. Temperature dependencies of specific heat capacity of neat 1-octadecene and 1-octadecene confined inside the pores of silica gels.

The values of 1-octadecent m.t. for both unmodified (hydroxylated) and trimethylsilylated silicas demands on the pore size in accordance with Gibbs-Tolmen equation for melting in confined media. At the same time the octadecene inside the pores of SiO_2 - C_{18} silicas formed two crystalline structures: surface co-crystallite of 1-octadecene and grafted - $C_{18}H_{37}$ groups as well as neat 1-octadecene crystallites in the pore voids.