

Stabilization of Amorphous Form of Organic Compounds in Porous Media: Influence of the Pore Structure on the Adsorption and Crystallisation Processes in the Pores

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The physicochemical properties of a number of solid materials are fundamentally determined by their crystallinity. In pharmaceutical technology the transition from amorphous to crystalline state plays a special role, since the bioavailability of the drug is influenced by its state, i.e., amorphous form of drugs have much higher bioavailability compared to the corresponding crystalline form of the same drug. However, the main problem of amorphous substances is their tendency to recrystallisation or reaction with the environment. To overcome this problem, nanoconfinement of the drug in porous carrier is used. It was shown, that not only the pore size, but mainly the interaction of the drug with the pore walls determine the crystallinity of the resulted particles. Within the same pore size, stronger interactions between the drug and the carrier lead to amorphous particles inside the pores, whereas in case of weak interactions rather crystals are formed. However, only qualitative studies on this matter were made. Thus, the aim of this work is to establish functionality between the pore structure, solute-wall interactions and amorph-crystalline phase transitions of large organic molecules confined in porous carriers. Here we focus on the influence of the adsorptive properties of the carrier on the crystallization of organic materials from supercritical CO₂ (“adsorptive crystallization”). Nanoporous materials, aerogels, are used as carrier materials since they are highly transparent so that the particle characterization by optical methods is enabled. Aerogels with different pore size, surface area and surface functional groups are produced. Adsorption and crystallization of several organic compounds in these aerogels are studied using a magnetic suspension balance and supercritical fluid chromatography. Thermodynamic properties (enthalpy and entropy of adsorption) are derived respectively to characterize the interaction between the solute and the aerogel. The results are supported by modeling with cellular automata.