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"Investigations on the collapse- and aggregation behaviour of dissolved polyacrylates in the presence of divalent cations"

Polyacrylic acid sodium salts are water soluble polymers and belong to the class of the so-called polyelectrolytes. In technical applications they are used as scale inhibitors, as absorbers and as precipitation agents in waste water treatment. In fundamental research they serve as model polyelectrolytes. In the present work, diluted aqueous solutions of polyacrylic acid sodium salts are investigated by means of scattering methods to gain information about the collapse and aggregation process. Upon addition of small amounts of calcium, copper and lead ions the collapse and aggregation process is initialised. The divalent cations bind specifically to the carboxylic groups. As a result, the polyelectrolyte chains become more hydrophobic and collapse. The extent of the collapse increases with increasing amount of added divalent cations. In the presence of calcium ions, the extent of chain collapse increases with increasing temperature. The overall dimensions of the collapsing chains are determined by means of combined static and dynamic light scattering (SLS and DLS). Phase diagrams are calculated from the data of combined SLS and DLS experiments of polyacrylic acid in the presence of calcium and copper ions. Selected samples of polyacrylic acid in the presence of calcium ions are subdued to temperature dependent small angle neutron scattering (SANS) experiments to gain insight into the internal structure of collapsing chains. With non linear least squares (NLS) methods, theoretical scattering functions are fitted to the experimental data. Solutions of polyacrylic acid in the presence of lead ions are subdued to small angle x-ray scattering (SAXS) experiments. To interpret the data from the SAXS experiments, a new theoretical scattering function is presented in the current thesis. Scattering functions known from literature and the scattering function presented in the current thesis are fitted to the SAXS data by means of NLS methods. The differences between the theoretical scattering functions and the results of the NLS calculations are discussed in detail. Anomalous SAXS (ASAXS) experiments reveal the spatial distribution of the lead ions that are bound to the polyacrylic acid chains and enable the calculation of their amount. The aggregation behaviour of polyacrylic acid in the presence of calcium and copper ions upon crossing the phase boundary is investigated by means of time resolved SLS (TR-SLS). The scattering curves of the aggregating polyelectrolyte chains are compared with theoretical models. The mechanism of aggregation is interpreted by means of scaling laws.