Spatial statistical analysis of micro-structures of nano silica particle gels

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The characterization of the micro-structure of a material is crucial for controlling its properties and function. For instance, understanding diffusion and flow through micro-structures is of great importance in various fields ranging from drug development over food processing to chromatography. However, the characterization of such micro-structures is difficult. Especially, the link between the theory describing the physics and chemistry involved in their formation and obtained observations still has to be found. Here, we are approaching this challenge using tools from spatial statistics summarizing the spatial properties of clusters. Hence, the central question arises which combination of spatial summary statistics characterizes and, hence, discriminates simulated or observed micro-structures best.

In particular, we are studying the characterization of micro-structures of nano silica particle gels pursuing the goal of identifying an appropriate model describing the particle aggregation process. For this purpose, experimental scanning transmission electron microscopy (STEM) micrographs as presented in Figure 1 are investigated. Since we are interested in a three-dimensional reconstruction, a method allowing comparisons between two- and three-dimensional data is required.

As a model, reaction-limited cluster aggregation (RLCA) is used to describe the formation of nano silica particle gels. This process is controlled by a collision probability P which mimics the repulsive interaction between the particles. Several micro-structures with varying values for P are regarded giving rise to different configurations. The resulting point patterns of centers of particles are analyzed as realizations of spatial point processes. In order to compare different configurations in a least-squares type approach, these point patterns were characterized using spatial functional summaries including, among others, the empty space function, the pair-correlation function and a so called cluster function. The focus of this talk will be on this spatial statistical analysis.

Keywords: Spatial cluster analysis, micro-structures, 3D reaction-limited cluster aggregation.

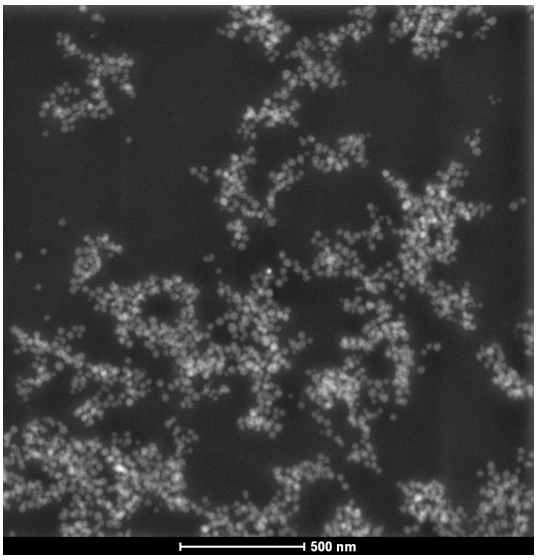

Figure 1: Micrograph of a 90 nm slice of 5 wt% aggregated nano silica obtained with STEM.

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