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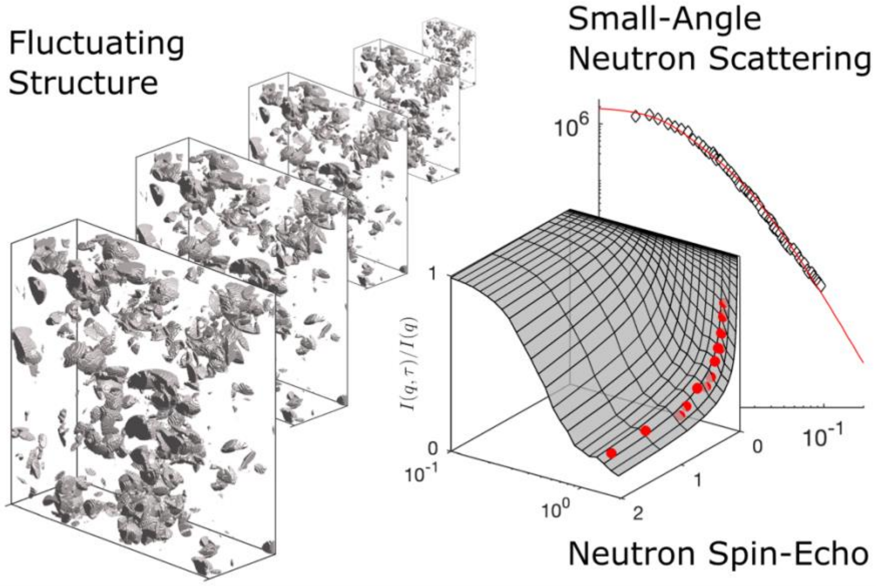
Analyzing thermal fluctuations in aerogels via inelastic neutron scattering and stochastic models

Cedric J. Gommes[a,*]

[a] Department of Chemical Engineering, University of Liège B6A, Allée du Six Août 3, B-4000 Liège, Belgium

* Cedric.Gommes@uliege.be

GRAPHICAL ABSTRACT



ABSTRACT

All soft nanomaterials, and aerogels in particular, are subject to thermal motion so that their structure randomly fluctuates with time. Combining elastic and inelastic neutron scattering - such as Small-Angle Neutron Scattering (SANS) and Neutron Spin Echo (NSE) experiments – offers the possibility of characterizing both a structure and its fluctuations with nanometer and nanosecond resolutions.

In the case of aerogels, thermal motion is limited by the way in which the building blocks of the structure are interconnected. The good connectivity of aerogels at macroscopic scale endows them with elastic properties, but the mobility of the structures at smaller scale can be

much larger with possibly many dangling branches. Characterizing the scale-dependent mobility through neutron scattering is therefore tantamount to characterizing the scale-dependent connectivity of the material.

Like most scattering methods, however, inelastic neutron scattering provides indirect information in the form of a correlation function, which in this case is a Van-Hove correlation function. The latter specifies the probability for two points at a given distance from another to both belong to the solid phase of the material, *at two different times*. Converting this type of data into time-dependent structures can only be achieved through models.

We present here a general time-dependent stochastic model of hierarchical structure, with fractals as a particular case, which enables one to jointly analyze elastic and inelastic scattering data [1]. A hierarchical structure is obtained by combining Boolean models of spheres with various sizes, each of which describes a particular level in the hierarchy. Thermal fluctuations are modelled by letting the spheres move either ballistically or diffusively. Analytical expressions are obtained for the van-Hove correlation function in both cases, which can be used for data fitting.

The use of the model is illustrated with previously published small-angle neutron scattering (SANS) and neutron spin-echo (NSE) data measured on silica aerogels synthesized in acidic conditions or via a two-step acid-base procedure [2]. In addition to structural differences, the approach provides insight into the different scale-dependent mobility of the aggregates that make up the aerogels, in relation with their different connectivities.

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