Explicit analysis of small-angle scattering patterns in terms of scale-dependent heterogeneity

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Small-angle x-ray scattering (SAXS) is intuitively related to the concept of heterogeneity: a sample that is homogeneous at the nanometer scale does not scatter. From a mathematical point of view, however, the notion of heterogeneity is somewhat hidden behind the concept of correlation function. In the present communication we present an explicit analysis of SAXS in terms of scale-dependent heterogeneity.

The main idea is the following (Figure 1). Imagine a biphasic material comprising two phases: A (volume fraction ϕ_A and electron density ρ_A), and B (ϕ_B=1-ϕ_A, ρ_B). To quantitatively characterize the heterogeneity of the material at a given length scale R, take a sphere of radius R and throw it randomly in the material. The average electron density ρ_R within the sphere is a random variable that depends on where the sphere has fallen. The average value is $\phi_A \rho_A + \phi_B \rho_B$, independently of the size of the sphere. However, the variance of ρ_R, $\sigma^2_\rho(R)$ is size-dependent. If the sphere is very small the variance is $(\rho_A-\rho_B)^2\phi_A(1-\phi_A)$, and it becomes vanishingly small for large sizes of the sphere. The curve $\sigma^2_\rho(R)$ *versus* R characterizes explicitly the scale-dependent heterogeneity of the material. We show how that curve can be calculated from SAXS patterns and we also discuss how structural information (surface areas, pores sizes) can be extracted from it.

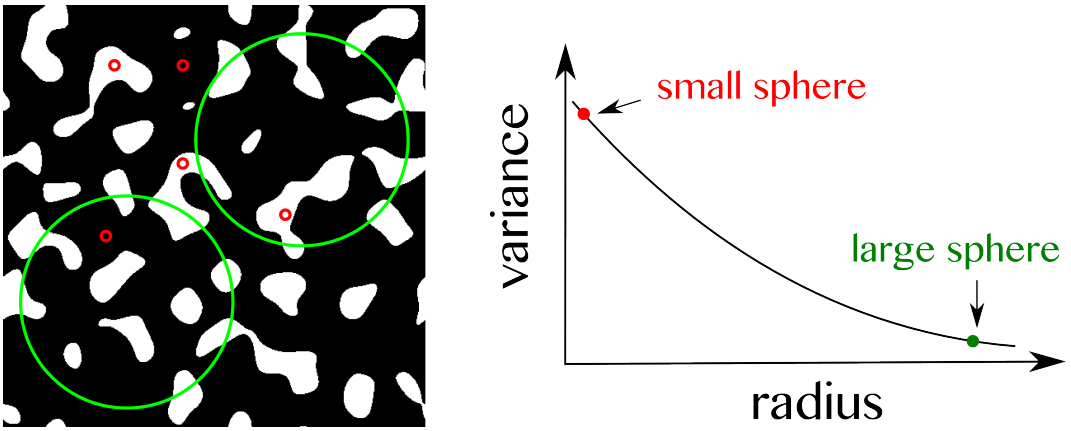

Figure 1. The scale-dependent heterogeneity of a material (left) can be characterized by throwing randomly spheres of radius R in it and counting the number of electrons they contain. This number is a random variable, the variance of which is a measure of the heterogeneity of the material at scale *R*.