Prospects for investigating deterministic fractals: Extracting additional information from small angle scattering data

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Abstract. We examine a general problem of small angle scattering from deterministic fractals: whether one can extract some additional information from the small angle scattering data apart from the fractal dimension and the edges of the fractal region. It is shown that for single-scale mass fractals one can additionally obtain the fractal iteration number, the scaling factor, and the number of structural units composing the fractal, provided the quality of fractal samples is high enough.

Fractals, one of the most beautiful and interesting group of objects, appeared in the scientific literature quite recently [1]. Right after that, the fractals attracted much attention of a broad community of investigators in various fields. Nearly at the same time, the connections were revealed between fractal structures and the intensities of small-angle neutron or X-ray scattering (see, e.g., reviews [2,3] and references therein). In particular, it was shown that within the fractal region of a mass fractal, the SAS intensity decays in the momentum space according to the power law $I(q) \sim 1/q^D$, where $D$ is the fractal dimension. The majority of SAS studies focus on determining the fractal dimension and the edges of the fractal region, within which the object behaves as a fractal. For random (stochastic) fractals, it is rather difficult to extract more information from the SAS data, because the fine structure of spatial correlations of particles, forming the fractal, is usually smeared due to the randomness. Presently, various deterministic fractals can be artificially created due to a rapid progress in nanotechnologies. As was recently shown [4], deterministic fractals, being exact self-similar objects, allow us to obtain more information from the scattering data.

In the papers [5,6], we constructed the generalized 3D Cantor and Vicsek sets (Fig. 1), whose dimensions are controlled by the scaling factor of fractal. The SAS intensities from these deterministic fractals were calculated analytically, and the obtained results exhibit a number of general features, common for deterministic mass fractals with a single scale [4]. If the fractals, composing a sample, are randomly oriented and placed, then the SAS intensities represent minima and maxima superimposed on the power-law decay $I(q) \sim 1/q^D$ (the generalized power-law decay). In the reciprocal fractal region, the curve $I(q)q^D$ is approximately log-periodic with the period equal to the logarithm of the fractal scaling factor (Fig. 2), and this log-periodicity of the scattering curves is a consequence of the self-similarity of the fractal. As was shown [4-6], the minima and maxima amplitudes are...
damped with increasing fractal polydispersity, i.e., variance in fractal sizes in the sample. Physical reasons for such a behaviour are quite clear: the fractal dimension dictates the power law $I(q) \sim 1/q^D$ for the intensity only on the average. Polydispersity smears the spatial correlations between the units composing the fractal and, hence, the intensity becomes smoother.

For a mass fractal with a single scale, one can extract a number of parameters from the scattering intensity even in the presence of polydispersity (Fig. 2): (i) The fractal dimension from the generalized power-law decay. (ii) The fractal scaling parameter from the period on the logarithmic scale. (iii) The number of fractal iteration, which is equal to the number of periods of function $I(q)q^D$. (iv) The lower and upper fractal edges from this diagram as the beginning and end of the "periodicity region". The edges allow us to estimate the fractal size and the smallest distance between fractal units in real space. (v) The total number of structural units, of which the fractal is composed, by the relation $N_m=(1/\beta s)^m D$, where $m$ is the iteration number.

The analysis of SAS data for deterministic fractals represents an important step in the structural investigations of complex systems. One can expect that the required samples of deterministic fractals of higher quality will be obtained with the help of modern nanotechnologies and investigated by SAS in near future.

![Figure 1. The initiator and first three iterations for the generalized self-similar Vicsek fractal, a deterministic fractal immersed in 3D, at the scaling factor $\beta s = 1/6$.](image1)

![Figure 2. The log-periodicity of the scaled SAS intensity $I(q)q^D$ in the fractal region of the generalized Vicsek sets. The period in the log-scale is equal to log$_{10}(1/\beta s)$. Here $l_0$ and $D_r$ are the average fractal size and its relative variance, respectively, and $m$ is the iteration number.](image2)

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