A deterministic multifractal model for complex structures

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Abstract. An idealized deterministic multifractal-based model is suggested for describing the structure of complex hierarchical materials. The corresponding pair distance distribution function and the small-angle scattering form factor is calculated from a system containing a macroscopic number of randomly oriented multifractals with uncorrelated positions. We show how to extract various structural information of the fractal both from real and reciprocal space data, such as: the scaling factors, the overall and fractal dimensions, and the size of the basic objects composing the fractal. The obtained results give additional insights into the structure of multifractal systems at nano- and micro-scales.

1. Introduction

Recent advances in materials science and nanotechnology have led to the development of new techniques and methods for creating complex nanoscale and micro metric materials. Many of these materials are characterized by a sort of self-similarity, either statistical, where only the statistical properties remain invariant at various magnifications, or exact, where an intrinsic pattern repeats itself exactly under scaling [1–7]. Such advanced materials are known as fractals [8] and they have enhanced physical properties (mechanical, thermal, optical etc.) as compared with traditional materials [9]. This makes them very good candidates for satisfying the ever increasing needs of the contemporary society in various technical, industrial and bio-medical applications.

Their improved physical properties are most often correlated with their the geometric structure, and therefore at nano and micro scales small-angle scattering (SAS) technique [10] is most often used to investigate their structural properties. To this aim, several theoretical models based on fractal geometry have been suggested so far to describe the corresponding SAS intensity, including mass, surface and fat fractals [12–25]. These models allows to extract various structural parameters from experimental SAS data, such as: fractal dimension, scaling factors, number of particles in a given iteration, the overall size of the fractal or the size of the particle forming the fractal.

The existing models can describe structures where at a given scale the material is characterized by a single scaling factor. However, in a more general case, some materials can exhibit several scaling factors interwoven at a given scale. They are known as multifractal materials, and their geometry is much more complex than that corresponding to regular fractals.

In order to characterize such structures, we develop a new model, and calculate the corresponding form factor from a macroscopic number of randomly oriented and non-interacting 3D deterministic multifractals with two different scaling factors. The results show that in the fractal region the SAS curve is characterized by the presence of Guinier, fractal and Porod regions. In the fractal region, the
SAS curve is characterized by a complex superposition of maxima and minima on a power law decay, with the scattering exponent equal to the fractal dimension $D_0$ in the multifractal spectra.

2. Theoretical model and small-angle scattering intensity

The deterministic multifractal model is built following a top-down approach, where we consider as initiator ($m = 0$) a ball of radius $r_0 = l_0/2$ centered inside a cube of edge $l_0$. The ball is then replaced by smaller balls according to the iteration rule described below. First, we choose a Cartesian system of coordinates whose center coincide with the ball center. At first iteration ($m = 1$) we replace the initial ball with 8 smaller balls of radii $\beta_{s_1}r_0$ (Fig 1 left side, black balls) and with 1 ball of radius $\beta_{s_2}r_0$ (Fig. 1 left side, blue ball). The coefficients $0 < \beta_{s_1} \leq 0.5$ and $0 < \beta_{s_2} \leq 0.5$ are called the scaling factors. For exemplification, we fix here their values to $\beta_{s_1} = 0.25$ and $\beta_{s_2} = 0.5$. The second iteration ($m = 2$) is obtained by following the same procedure for each of the 9 balls. The resulting structure is shown in Fig. 1 right side, and it is called a multifractal since it is generated by using multiple scaling factors at a given iteration.

We consider that the obtained fractal structures are composed of balls with scattering length density (SLD) $\rho_b$ immersed in a solid matrix with SLD $\rho_m$. Thus, the scattering contrast is defined by $\Delta\rho = \rho_b - \rho_m$ and the total scattering intensity can be written as [10]

$$I(q) \equiv n|\Delta\rho|^2V^2\langle|F(q)|^2\rangle,$$

where $n$ is the concentration of multifractals inside the matrix, $V$ is the volume of each multifractal, the symbol $\langle\cdots\rangle$ represents the averaging over all orientations, the quantity $F(q) \equiv (1/V)\int_V \exp(-iq \cdot r)dr$ is the normalized form factor, and $q$ is the scattering wavevector.

3. Results and discussions

We start by introducing the probability density of finding the distance $r$ between the centers of two arbitrarily balls inside the fractal [19], such as:

$$p(r) = \frac{2}{N(N-1)} \sum_{r_p} C_p \delta(r - r_p),$$

Figure 1. (Color online) The first two iterations for the multifractal model with the scaling factors $\beta_{s_1} = 0.25$ and $\beta_{s_2} = 0.5$. 
where \( N = 9^m \), \( m = 0, 1, \cdots \), is the number of balls at \( m \)-th iteration, \( C_p \) are the number of distances separated by \( r_p \), and \( \delta \) is the Dirac delta function. The quantity given by Eq. (2) is called the pair distance distribution function and is related to the fractal structure factor through a Fourier transform.

Fig. 2a) shows the coefficients \( C_p \) of the pair distance distribution function from Eq. (2) for the multifractal model shown in Fig. 1, at \( m = 4 \). The coefficients have been calculated numerically by a simple combinatoric analysis. The graph shows a succession of sharp maxima, which indicates the most common distances inside the fractal, for a given \( r \). For the suggested model, the most common distances are about \( 2 \times 10^4 \) and they correspond at \( r/l_0 \simeq 0.77 \). However, the self-similarity of the fractal manifests in the log periodicity of the group of distances on the log-linear scale. The minima correspond to the least common distances, and it can be clearly seen in Fig. 2a) that they appear at \( r/l_0 \simeq 0.03, 0.11 \) and \( 0.42 \). They relate to the scaling factor through \( \log_{10}(1/\beta_s) \), and thus from the minima position we recover the scaling factor 0.25, which corresponds to \( \beta_s \) in the model of Fig. 1. Furthermore, inside each group there are additional less-pronounced minima, such as at \( r/l_0 \simeq 1.19 \) and 0.62 in the last group, and which reveal the existence of a second scaling factor, with the value 0.5. Indeed for the suggested model this is the case and this numerical value corresponds to \( \beta_{s_2} \).

At \( m = 0 \) the system consists from a single ball of radius \( r_0 = \beta_{s_1}l_0/2 \) and form factor \( F_0(q) = 3 \left( \sin(qr_0) - 3qr_0 \cos(qr_0) \right) / (qr_0)^2 \). At first iteration, the multifractal can be constructed as a sum of the eight balls from the corner, with radius \( r_1 = \beta_{s_1}l_0/2 \), together with the single ball of radius \( r_0 = \beta_{s_2}l_0/2 \) situated in the center. Therefore at \( m = 1 \) we can write:

\[
F_1(q) = \frac{1}{V_a + V_b} \left( V_a G(q) F_0(\beta_{s_1}l_0q/2) + V_b F_0(\beta_{s_2}l_0q/2) \right),
\]

where \( V_a \) is the total volume of balls with radii \( \beta_{s_1}l_0/2 \), \( V_b \) is the volume of the single ball from the center, \( G(q) = \cos(qz_2l_0(1 - \beta_{s_1}/2)) \cos(qy_0l_0(1 - \beta_{s_1}/2)) \cos(qx_2l_0(1 - \beta_{s_1}/2)) \) is the generative function which gives the position of the eight balls, and \( q_x, q_y \) and \( q_z \) are the components of the scattering wavevector \( q \).

For \( m = 2 \) we follow a similar procedure and obtain

\[
F_2(q) = \frac{V_c G(q) G(\beta_{s_1}q) F_0(\beta_{s_2}l_0q/2) + V_d G(q) + G(\beta_{s_2}q) F_0(\beta_{s_2}l_0q/2) + V_e F_0(\beta_{s_2}l_0q/2)}{V_c + V_d + V_e},
\]

where, \( V_c \) is the volume of the balls with radii \( \beta_{s_2}l_0/2 \), \( V_d \) is the volume of the balls with radii \( \beta_{s_2}\beta_{s_1}l_0/2 \), and \( V_e \) is the volume of the ball with radius \( \beta_{s_2}^2l_0/2 \) (see Fig. 1 right part).

The scattering intensities for the first two iterations are obtained by introducing Eqs. (3) and (4) into Eq. (1) (see Fig. 2b). The results show that starting with the first iteration, the scattering curve

**Figure 2.** (a) The coefficients \( C_p \) in the expression (47) for the pair distance distribution function of the multifractal model at \( m = 4 \). (b) The normalized scattering intensity form the multifractal at first three iterations.
is characterized by the presence of three main regions: Guinier at small $q_0$ (the plateau on a double logarithmic scale), intermediate/fractal and respectively a Porod region at high $q_0$. The end of the Guinier region provides information about the overall size of the fractal \cite{19}. In the fractal region the scattering exponent equals the fractal dimension $D_f = 1.64$ while in the Porod region the exponent is $-4$ as expected. The length of the fractal region increases with the iteration number since the distances between balls become smaller. Thus, the border between fractal and Porod region can be used to estimate the size of the smallest balls, which are of the same order as the distances between them.

4. Conclusion
A deterministic multifractal model with two scaling factors is introduced and a combined real and reciprocal space analysis is performed. We show that the corresponding pair distance distribution function may reveal both scaling factors in real space. In the fractal region, the exponent of the scattering intensity equals the fractal dimension, and thus together with the Guinier and Porod regions, various structural properties can be determined. This analysis can be useful for for modeling small-angle scattering intensities from complex structures at nano and micro scales.

In practice, by using a Fourier transform of the scattering data, a real space analysis can be used to complement a reciprocal space analysis, and thus to have a better image on some structural parameters of the fractal.

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