Structural properties of two-phase deterministic multifractals

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Abstract. In this work an analysis of the multifractal spectra, pair distance distribution function (pddf) and small-angle scattering (SAS) intensities from deterministic two-scale multifractals is performed in order to determine their structural properties. It is shown that the coefficients of the pddf are characterized by the presence of groups of distance pairs whose positions are related to the scaling factors of the fractal. It is found that the box counting dimension $D_0$ in the multifractal spectra coincides with the mass fractal dimension determined through the evaluation of scattering exponent in the fractal region of SAS curve. The length of the mass fractal region in reciprocal space is related to the relative values of the scaling factors. We illustrate these findings on a 2D Vicsek-like multifractals.

1. Introduction

In many research fields, in particular the ones concerning natural sciences, the concept of fractal geometry introduced by Mandelbrot [1] has been found to be very useful due to its simplicity in dealing with very complex structures and phenomena. Since fractal structures are statistically self-similar (i.e. random fractals), the main property of interest is the fractal fractal dimension [2], which represents a measure of the complexity of the system under examination [3]. The higher the numerical value of this parameter, the higher the irregularity of the system and its morphological complexity. Recently new experimental techniques have been developed to manufacture exactly self-similar systems (i.e. deterministic fractals) at nano and micro scales, opening new opportunities in understanding their properties and functionalities [4–9]. Thus, one of the fundamental challenge is to understand the correlations between the fractal structure and physical properties. Of particular importance is how the electromagnetic, dynamic and statistical, mechanical, thermal or optical properties of a fractal object are related to its deterministic micro-structures [10–12]. A powerful approach used to describe material’s micro-structures at nano and micro scales consists in using small-angle scattering techniques [13–15]. When analyzing random fractal structures, its main advantage relies on the possibility to extract the fractal dimension from the power law decay of the scattering intensity [16] as well as the edges of the fractal region, which appear as knees in the scattering curve on a logarithmic-scale [13–15]:

$$I(q) \sim q^{-\alpha},$$  \hspace{1cm} (1)

where $\alpha$ is the scattering exponent, $I(q)$ is the scattering intensity and $q$ is the scattering vector. In particular the exponent $\alpha$ contains informations regarding the fractal dimension of the curve. In contrast to the behavior of the power law given by Eq. (1), the scattering from single scale deterministic fractals shows a sequence of maxima and minima, which follows a power law decay, due to spatial order properties of these structures [17–26]. Therefore, additional structural parameters can be obtained such...
as the scaling factor or the iteration number. However, many fractal structures are characterized by the presence of multiple scaling factors and their combined effect on the SAS scattering curve, is not yet completely understood. In this contribution we attempt to compare different structural methods in order to obtain the fractal dimension of a multifractal with two-scaling factors. As a model, we use a 2D fractal similar to the Generalized Self-Similar Vicsek Fractal system (GSSVF) discussed in [10], and composed of disks with two different scaling factors. To this aim, first we calculate the fractal form factor and extract the fractal dimension in reciprocal space, and then, we calculate the corresponding pair distance distribution function (pdff), through a Fourier transform. We show that, at the chosen values of the scaling factors, the pdff is characterized by groups of distances from which the value of the smallest scaling factors can be roughly estimated. Finally, the box counting dimension is revealed from the dimension spectra.

2. Theoretical background
In this section we review some important concepts concerning the technique of Small Angle Scattering (SAS), providing some numerical techniques to calculate the scattering intensity from simple geometric shapes, in particular the scattering amplitude from a sphere and from a disk. A general definition of fractals and multifractals is given, focusing in detail on the determination of the multifractal spectra through the box-counting method. In addition, to obtain informations over the objects positions within a fractal polydisperse system, some general notions concerning the pair distance distribution function are underlined.

2.1. Small angle scattering
Small angle scattering is a technique based on spatial density measurement, used to analyze structures with nano-scale sizes [13, 14, 30]. In order to characterize structures down to the nanometric region, the beam must have wavelengths comparable with the atomic distances within the sample [13, 14, 31]. Defining the wave vector of the incident beam as \( \vec{k}_i \) and the wave vector of the scattered beam as \( \vec{k}_s \), which makes an angle equal to \( 2\theta \) with the direction of the transmitted beam, the quantity measured in a SAS experiment is the differential cross section as a function of the scattering vector \( \vec{q} = \vec{k}_s - \vec{k}_i \) [13, 30]. The scattering vector \( \vec{q} \) is completely characterized by the scattering geometry and its range in a SAS experiment extends usually from \( 0 \) to \( 0.45 \) \( \text{Å}^{-1} \) [10, 13, 14, 31]. Considering a sample of \( N \) identical scatters with scattering length \( b_j \), it is possible to express the scattering length density as [10, 13, 14]:

\[
\rho(\vec{r}) = \sum_j b_j \delta(\vec{r} - \vec{r}_j),
\]

(2)

where \( r_j \) are the positions of the scatters within the sample and \( \delta \) is the Dirac’s delta function. Then, the amplitude of the scattered beam can be written as [10, 13, 14]:

\[
A(\vec{q}) = A_0 \sum_{j=1}^{N} \rho(\vec{r}) e^{-i\vec{q} \cdot \vec{r}_j},
\]

(3)

where the summation is usually replaced with an integral when the system consists of a very large number of scatters, dispersed continuously within the sample. Thus, the total scattering amplitude results to be proportional to the Fourier transform of \( \rho(\vec{r}) \) [13, 14, 30]:

\[
A(\vec{q}) = A_0 \int_V \rho(\vec{r}) e^{-i\vec{q} \cdot \vec{r}} d\vec{r},
\]

(4)

where \( V \) denotes that the integration as to take place over the scattering volume. During the time period of scattering measurements, the positions \( \vec{r}_j \) of atoms and the scattering length density distribution \( \rho(\vec{r}) \)
may change due to thermal motion of the atoms. Therefore, the resulting intensity is measured as the average over the time \([13, 14]\). Thus, we rewrite Eq. 4 as \([10, 13, 14, 30, 31]\):

\[
    I(q) = \langle |A(q)|^2 \rangle = \left\langle | \int_V \rho(\vec{r})e^{-i\vec{q} \cdot \vec{r}} d\vec{r} |^2 \right\rangle = V^2 \langle |F(\vec{q})|^2 \rangle ,
\]
where the \(\langle \ldots \rangle\) denotes the ensemble average and \(F(\vec{q})\) is the normalized scattering amplitude, given by \([10, 13, 14, 30, 31]\):

\[
    F(\vec{q}) = \frac{1}{V} \int_V \rho(\vec{r})e^{-i\vec{q} \cdot \vec{r}} d\vec{r}.
\]

For mass fractals with a single scale, the pair distance distribution function (pddf), which gives the probability density of finding the distance \(r\) between the centers of two arbitrarily taken disks inside the fractal, is given by \([32]\):

\[
    p(r) = \frac{2}{k^m (k^m - 1)} \sum_{j \neq k} C_p \delta(r - r_{jk}),
\]

where \(k\) is the number of disks, \(\delta\) is the Dirac’s delta function, \(r_{jk} \equiv |r_j - r_k|\) is the relative distance between the centers of disk \(j\) and \(k\), and \(C_p\) are the number of distances separated by \(r_p\).

### 2.1.1. Scattering from a disk

We consider here a disk of radius \(R\) and area \(S = 4\pi R^2\), and denote \(\vec{q} = \{q_x, q_y\}\) and \(\vec{r} = \{x, y\}\) the components of the scattering vector in reciprocal space and respectively of the position vector in real space. Passing to a spherical coordinates system, \(F(\vec{q})\) can be expressed as \([33]\):

\[
    F(q) = \frac{2J_1(q)}{q}.
\]

The total scattering intensity is therefore \([13, 14, 33]\):

\[
    I(q) = |F(q)|^2.
\]

Fig. 1 shows SAS scattering intensity of a disk of radius about 2 nm (orange), given by Eq. 8 represented in a double logarithmic scale. For comparison the scattering intensity of a sphere with radius about 20 nm is also shown (green). The results clearly show that it is possible to distinguish two main regions: the Guinier region and the Porod one. For very small values of \(q\) (i.e. when \(q < \pi/R\)) the curve is a plateau (Guinier region), with \(I(q) \propto q^0\), which provides informations about the overall structure of the sample \([13, 14, 18, 30, 31]\). As \(q\) increases the curve falls off, following a power-law decay, denoted as Porod law (Eq. 1) where the exponent \(\alpha\) is equal to 4, when the system consists of spheres (three dimensional), and is equal to 2 for disks (two dimensional) \([18, 30, 31]\).

### 2.2. Fractals and multifractals

A fractal is an object which exhibits dilatation symmetry, that is a self-similarity property under scale transformations \([1,3]\). A real object can be a fractal only within a range of values imposed by its effective physical dimension and by the size of the basic building blocks of its structure \([11,13]\). In the case of fractals the most important characteristic is the fractal dimension \(d\). The meaning of this quantity can be explained considering a sphere of radius \(r\) around a point inside the object, taken into account. If the object is a line (1D) the mass \(M(r)\) within the sphere will be proportional to \(r\); if the object is a sheet then \(M(r) \propto r^2\) while if the object is a fractal then \([1,3,18,29,31]\):

\[
    M(r) \propto r^d,
\]

where \(1 < d < 3\) is the fractal dimension \([13]\). For those fractal structures constructed by using an iterative process consisting of an initiator and a generator (iterative operation), the fractal dimension can
be determined analytically. For a fractal with \( n \) scaling factors \( \beta_{si}, i = 1, \ldots, n \), each one having \( k_i \) scattering units, the fractal dimension can be obtained from \([1, 3]\):

\[
k_1 \left( \frac{1}{\beta_{s1}} \right)^d + k_2 \left( \frac{1}{\beta_{s2}} \right)^d + \ldots + k_n \left( \frac{1}{\beta_{sn}} \right)^d = 1.
\] (11)

Since a fractal object consists of an ensemble of fractal supports, whose fractal dimension generally differs from that of the whole, knowing the fractal dimension of a set is generally not enough to characterize its geometry or a particular physical phenomenon occurring on it \([1, 3, 10, 27, 28]\). Thus, in order to understand physical systems with multiple scaling factors (known as multifractals), it is necessary to characterize the distribution of measures inside the system \([27]\). A convenient way to reflect this distribution is by determining not a single fractal dimension, but a whole spectra of fractal dimensions, known as the \textit{dimension spectrum}. For this purpose, let us consider a grid of boxes of various sizes \( l \) covering a domain \( D \) and a phenomenon occurring \( k \) times in \( D \) and define the probability that an instance of the phenomenon occurs in the \( i \)-th box as \([1, 3, 27]\): \( p_i = \frac{k_i}{k} \), where \( \mu \) is the corresponding probability measure. Then, we can introduce the quantity:

\[
Z(s) = \sum_i p_i^s,
\] (12)

which is similarly to the partition function used in thermodynamics. Thus, the generalized dimension spectrum \( D_s \) can be written in terms of the partition function as:

\[
D_s = \frac{1}{1 - s} \lim_{l \to 0} \frac{\ln Z_s(l)}{-\ln l},
\] (13)

where we take into account that \( Z_s \) has a power-law behaviour in the limit \( l \to 0 \) and the number of boxes \( N \to \infty \), so that \( Z_s \propto l^{D_s(s-1)} \). As a consequence:

\[
D_s = \lim_{l \to 0} \frac{1}{1 - q} \frac{\ln \sum_{i=1}^N p_i^s(l)}{-\ln l},
\] (14)

with \( p_i = N_i(l)/N \) being the relative weight of the \( i \)-th box.
The plot of $D_s$ over $s$ is generally a monotonically decreasing one. The higher the difference between fractal dimensions at smallest and respectively at the largest values of $s$, the more heterogeneous the multifractal. In the case of simple fractals, the curve is a straight line whose intercept with $D$-axis, gives the fractal dimension. In the following we shall use this property of dimension spectrum to distinguish between mono and multifractals.

3. Results and discussions

3.1. Theoretical model

We focus here in the construction a fractal system similar to a Generalized Self-Similar Vicsek Fractals (GSSVF), discussed in Ref. [10]. Our fractal initiator consists of a disk of radius $r_0$ placed inside a square of edge $l_0$, such that their center coincide and $r_0 = l_0/2$. In order to obtain the first iteration we choose a Cartesian system whose origin coincide with the center of the square and disk. The first iteration $m = 1$ consists in replacing the initial disk with five other disks. The central disk has the scaling factor $\beta_{s2} = r_2/r_0$ where, $r_2$ stands for its radius, while, the other four disks have the scaling factor $\beta_{s1} = r_1/r_0$ where $r_1$ stands for their radius. The central disk is located in the center of the square, while the other four disks are shifted from the origin by the vectors:

$$a_j \equiv l_0 \beta_j = l_0(\beta_{s1}, \beta_{s2}) = l_0\left(\frac{\beta_{s1} + \beta_{s2}}{2}, \frac{\beta_{s1} + \beta_{s2}}{2}\right).$$

(15)

The next iteration ($m = 2$) is obtained by carrying out the same procedure to each disks of the first iteration. By repeating the same procedure in the limit of high number of iterations we obtained a multifractal with two scaling factors, similar to GSSVF. Fig. 2 shows the first three iterations when $\beta_{s1} = 0.45$ and $\beta_{s2} = 0.1$.

3.2. Fractal form factor

Taking into account the previous mathematical procedure to generate a fractal system, it is possible to calculate analytically the form factor of the $m$th generation throughout the so called Generative Function $G_m(q)$, defined by the disks centers positions. From the generative function for a GSSVF system at the $m$th, defined in [10], we derive the generative function for our system taking into account the presence of two scaling factors. Assuming $G_0(q) = 1$, we write:

$$F_m(q) = F_0(r_mq) \prod_{i=0}^{m} G_i(q),$$

(16)

hence, SAS intensity becomes [10]:

$$\frac{I_m(q)}{I_m(0)} = \langle |F_m(q)|^2 \rangle.$$

(17)

Figure 2. Three first iteration of two scale multifractals model for $\beta_{s1} = 0.45$ and $\beta_{s2} = 0.1$. Starting from the left we have: first iteration ($m = 1$), second iteration ($m = 2$) and third ($m = 3$).
Figure 3. Figure (a) shows scattering intensity of the 3th order iteration of GSSVF fractal system. Figure (b) displays the coefficients $C_p$ in Eq. (7) for the pddf at $m = 4$, with $\beta_{s1} = 0.45$, $\beta_{s2} = 0.1$. 

In Fig. 3(a) we show the scattering intensity obtained for the third fractal iteration. The results show that it is possible to distinguish three regions: the Guinier, the fractal and the Porod regions. The Guinier region is presented as a plateau and provides information about the overall structural properties of the fractal, as discussed in [13, 18]. The fractal region is determined by the maximal and minimal distances between the disks centers and is characterized by a succession of maxima and minima on a power-law decay with scattering exponent $\alpha = 1.76$ (see Eq. (1)). By using numerical values $\beta_{s1} = 0.45$, $k_1 = 4$, $\beta_{s2} = 0.1$ and $k_2 = 0.1$ in Eq. (11) we obtain also $d \simeq 1.76$. Note that the length of the fractal regime increases with increasing the iteration number, since the distances between the scattering units of the fractals decrease [10, 18, 31]. However, in a SAS experiment only 3 or maxim 4 iterations are visible. For the chosen numerical values in Fig. 3(a), the fractal regime is clearly seen within the range $6 \lesssim q \lesssim 100$. Beyond the fractal regime, one obtain as expected, the Porod region where the exponent of the power-law decay is $\alpha = 2$, i.e the scattering intensity is equal to the one of the initiator.

3.3. Pair distance distribution function

By calculating the pddf of the fractal, according to Eq. (7), we can reveal the real-space characteristics of the model shown in Fig. 3(b). At $m = 4$ we can see in Fig. 3(b), that the coefficients of the pddf are characterized by the presence of groups of distance pairs whose positions are related to the scaling factors of the fractal. In particular the ratio between each pairs of minima, with good approximation, coincides with the smallest scaling factor $\beta_{s2} = 0.1$ of the fractal system. In Fig. 3(b) it is possible to distinguish four main minima at about $2.5 \times 10^{-3}$, $2.5 \times 10^{-2}$, $2.5 \times 10^{-1}$ and $2.5 \times 10^0$. This clearly shows that the ratio of successive minima is about 0.1, and which coincides with the scaling factor $\beta_{s2} = 0.1$.

3.4. Multifractal spectra

The calculated dimension spectrum according to Eq. (14) is shown in (Fig. 4 - orange). The spectrum is almost a straight line, underlining the high dimensional homogeneity of the system. The results also show that $D_0 \simeq 1.76$, which coincide to the to the fractal dimension, determined both theoretically (Eq. (11)) and through the evaluation of the scattering exponent in the fractal region of the SAS form factor (Eq. (1)). This also show that at the chosen numerical values of the scaling factors, the multifractal model can be considered, with good approximation, as a mono fractal.

Conclusions

In this contribution we have presented and discussed a theoretical model which can be used to analyze SAS intensity from a deterministic two phase multifractal system. The model is a two dimensional system whose basic building units are disks. The latter ones are distributed as to form a fractal system.
Figure 4. Plot of the dimension spectrum $D_s$ (Eq. 13) for the model shown in Fig. 2

similar to the GSSVF presented in [10]. The two scaling factors of the system are $\beta_{s1} = 0.45$, for the external disks, and $\beta_{s2} = 0.1$ for the central disk. The model can be easily generalized to other values of the scaling factors as well as other number of particles. Based on this model we calculated the fractal form factor and we shown that this can be characterized by the presence of tree main regions: at low $q$ the Guinier region which gives informations about the overall sizes of the fractal, at intermediate values of $q$ we have the fractal regions, where the exponent of the scattering intensity coincides with the fractal dimension $D_0$ of the system, while at high values of $q$ the scattering intensity decays following the Porod law behavior. By computing the corresponding pddf we demonstrated that it is possible to numerically determine the smallest scaling factor $\beta_{s2}$ by analyzing the ratio between the function minima. Also, the number of minima coincide with the fractal iteration number. Analysis of the dimension spectra reveals the weak multifractality of the model, since it is close to a straight line. The value of the box-counting dimension $D_0$ is about 1.76, which is in very good agreement with both the analytic value obtained from Eq. (11), and with the scattering exponent of the intensity in the fractal region (see Fig. 3). The results point out a number of general features, common for deterministic mass fractals with two scaling factors, which can be used to understand experimental data and can be generalized for fractal systems with more than two scaling factors. Thus, generally it is possible to extract several information from a combined analysis of the scattering intensity, the pddf function and from the generalized dimension spectra: fractal dimension, scaling factor(s), number of fractal iterations and the degree of heterogeneity in the multifractal.

The results obtained can be applied for various structures, whose geometries are based on iterations of fractal systems, like magnetic cluster structures, chemical compounds artificially assembled, and so forth. We consider her mass fractals composed of the same units, but the developed approach can be used also for mass fractal systems containing units of various shapes and sizes and to surface fractals as well. By taking into account the polydispersity, one can analyze random fractals as well, such as the structure of DLA clusters with or without interactions [34].

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