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CLASSIFICATION OF OVERLAYER PRECIPITATES BY NOVEL HIERARCHICAL SYSTEMS-SUPERFRACTALS

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ABSTRACT

The formalism introduced allows a new insight into the symmetry hidden in the mathematical formulation of fractals. We prove that application of the logarithmic scales uncovers hidden relation between fractals and crystals and prove that this symmetry can be classified according to symmetry groups of conventional crystallography. The latter result allows us to introduce the concept of superfractals, which generalizes the idea of conventional fractals. We show that idea of superfractals offers a new tool for characterization of surface precipitates.

INTRODUCTION

The concept of fractal has become a powerful tool in analysis of common aspects of many complex processes observed in physics, biology, chemistry or earth sciences. Brownian motion, turbulence, colloidal aggregation or biological pattern formation can be fully understood only when the idea of self-similarity or fractal structures is applied [1]. The hallmark of a fractality is a hierarchical organization of its elements, described by discrete scaling laws which makes the fractal, regardless on magnification or contraction scale, looks the same. This property of fractals is called self-similarity, self-affinity or self-replicability. Although there are fractal sets that show no self-similarity, for the reason that will become evident later, we will focus our attention to the self-similar ones.

The aim of the paper is to show one to one correspondence between inherent to fractals self-similar mappings and translational symmetry in $\mathbf{R}^3$. We will show that for some fractals we can find isomorphism of injective mappings on a fractal and a crystal lattice. As the natural consequence of this isomorphism there arises the concept of a more general class of hierarchical systems-superfractals. We will show that the superfractals can be assumed as some kind of modulated fractals or equivalently the conventional fractals within the (n+k)-dimensional space projected onto the nD space.

A self-similar symmetry of a fractal is a transformation that leaves the system invariant, in the sense that, taken as a whole it looks the same after transformation as it did before, although individual points of the pattern may be moved by the transformation. We say that $\mathbf{K} \subset \mathbf{R}^n$ satisfies the scaling law $\mathbf{S}$, or is a self-similar fractal if $\mathbf{S}$:$\mathbf{K}$=$\mathbf{K}$. Let us limit our considerations to fractals in which the self-similarity is can be realized only via linear maps, i.e., transformations which point $\mathbf{r}=(x_1, x_2, x_3) \in K \subset R^3$ transform into point $\mathbf{r'}=(x_1'$ $x_2', x_3')$ according to the formula

$$x_i' = S_{i1} x_1 + S_{i2} x_2 + S_{i3} x_3 \tag{1}$$

The vector form of Eq. (1) can be written as $\mathbf{r'} = \mathbf{S} : \mathbf{r}$, where $\mathbf{S}$ is the matrix of linear transformation (1). If we orient coordinate axes along the eigenvectors of matrix $\mathbf{S}$ (i.e., $\mathbf{x} =(x_1, x_2, x_3) \rightarrow (\varepsilon, \eta, \rho)$ then the mapping (1) reduces to transformation $\mathbf{S}:(\varepsilon, \eta, \rho) \rightarrow (\lambda_1\varepsilon, \lambda_2\eta, \lambda_3\rho)$. In the case of infinite-size fractals also the inverse $\mathbf{S}^{-1}$ mapping fulfills the self-similarity conditions $\mathbf{S}^{-1}:\mathbf{K} = \mathbf{K}$ and for any $\mathbf{x} \in K$, we have

$$\mathbf{S}^{-1}:\mathbf{x}=\mathbf{S}_1^{-1} \circ \mathbf{S}_2^{-1} \circ \mathbf{S}_3^{-1}:\mathbf{x}=(\lambda_1^{-1}\varepsilon, \lambda_2^{-1}\eta, \lambda_3^{-1}\rho) \tag{2}$$

For n-tuple superpositions of $\mathbf{S}^{-1}$ the above relations are valid provided that substitution $(\lambda_i)^n \rightarrow (\lambda_i)^{-n}$ is performed. We can define a more general transformation of the type $\mathbf{S}^{(m,n,l)} = (\mathbf{S}_1)^n \circ (\mathbf{S}_2)^m \circ (\mathbf{S}_3)^l$, where $(\mathbf{S}_i)^n$ denotes n-tuple superposition of transformation $\mathbf{S}_i$. By analogy to the linear algebra the set of all allowed transformations $\mathbf{S}^{(m,n,l)}$ of a given fractal $\mathbf{G}$ can be called the dual space $\mathbf{G}^*$. Action of $\mathbf{S}^{(m,n,l)}$ transforms any point $\mathbf{x} \in \mathbf{R}^3$ according to the formula

$$\mathbf{S}^{(m,n,l)} : \mathbf{x} = (\lambda_1^{\,n}\, \varepsilon, \lambda_2^{\,m}\, \eta, \lambda_3^{\,l}\, \rho) \tag{3}$$

where m, n, l are arbitrary (negative or positive) integers. In view of Eq. (3) we have that $\mathbf{S}^{(m,n,l)}:\mathbf{G} \subset \mathbf{G}$, i.e $\mathbf{S}^{(m,n,l)}$ are the injective scaling mappings. Evidently the subset of self-smilar transformations $\mathbf{G}_s^* = \{ \mathbf{S}^{(n,n,n)} \} \subset \mathbf{G}^*$. For any linear $\mathbf{S}_1$ by definition we have $\mathbf{S}_1:\mathbf{F}_1 = \mathbf{F}_1$ and for any $\mathbf{x}_o \in \mathbf{F}_1$ we have $\mathbf{S}_1: \mathbf{x}_o = \lambda_1 \mathbf{x}_o$, consequently $(\mathbf{S}_1)^m: \mathbf{x}_o = \lambda_1^m: \mathbf{x}_o$. Using the logarithmic scale we have $\log(x_m/x_o) = m \ln \lambda_1$. This is nothing but 1D crystal lattice with the lattice spacing given by $a_1= \ln \lambda_1$. Using the multi-logarithmic scale we obtain that the family of mappings $\mathbf{S}^{(m,n,l)}$ is isomorphic with a 3D crystal lattice. This means that the isomorphism $\mathbf{S}^{(m,n,l)} \rightarrow (ma_1, na_2, la_3)$ holds. Thus, in view of the arguments given above the symmetry of this crystal lattice can be classified according to conventional symmetry elements like rotations, inversion or mirror planes (32 point groups) and space groups.

REAL FRACTAL SYSTEMS

In real systems the position of species that form the fractal structure often deviate from ideal mathematical fractal. In conventional physical systems, in which the allowed positions of its elements are uniformly distributed within $\mathbf{R}^3$-space the position fluctuations are usually follow the Gaussian (normal) distribution. In the self-similar fractal its elements are nonuniformly distributed, however in the logarithmic scale the uniform distribution of allowed positions are restored. If all conditions necessary for the normal (Gaussian) probability distribution P(x) (in the log scale) are fulfilled the position variation are described by the well-known log-normal distribution

$$P(x) = \frac{1}{\sqrt{2\Pi}\sigma x} \exp\left(\frac{(\ln x - \mu)^2}{2\sigma^2}\right) \tag{4}$$

Consequently, one would expect that probability distribution of many physical quantities on self-similar fractals follows the log-normal distribution. In support of this let us recall the real systems that exhibit fractal behaviour like isothermal aggregation [2], or stock fluctuations [3] with the log-normal statistics.

In real fractal systems we have somewhat different situation when compared to mathematical formulation. Contrary to mathematical fractals, for any real object in nature, fractal properties are observed only over a limited size range [4]. As pointed out by Mandelbrot, naturally fractal objects are self-similar above some lower cutoff ε up to some upper cutoff value ω [5]. Therefore, such fractals are referred to as truncated fractals. In the logarithmic scale this situation resembles finite crystals when after finite number of translations the crystal surface is reached. Evidently we can restore infinite translational symmetry when postulating the Born-von Karman boundary conditions. The same can be done for the fractals in the logarithmic scale. The periodic superstructures composed of truncated fractals with the Born-von Karman boundary conditions are sometimes called superfractals. Such superstructures have been used to model some antenna devices in fractal electrodynamics [6], [7]. Below we will use the term superfractal in somewhat different, more general meaning, which exploits their analogy with the well-known supercrystals [8], [9].

SUPERFRACTALS

The one to one correspondence between self-affine mappings of fractals and symmetries of ordinary crystals opens the way to define a more general class of hierarchical systems, that are the fractal counterparts of the modulated crystals (i.e. supercrystals) [8], [9]. Motivated by this idea let us to present the concept of superfractals. We assume that the basic distinction between fractal **G** and a superfractal **SG** relies on the symmetries of their self-dual spaces **G*** and **SG***, respectively. In the case of ordinary fractal **G** the **G*** is isomorphic with the lattice of an ordinary crystal, while for the superfractal its self-dual space **SG*** is isomorphic with a supercrystal. This means that in the latter case the members $\mathbf{x} \in \mathbf{SG}$ doesn't occupy sites predicted for the ordinary fractal but oscillate in a regular manner around sites of ideal structure. In other words the superfractal can be assumed as the geometrical object in which positions of its elements can be determined by superimposing modulation with the log periodicity b onto positions of conventional fractal with the log periodicity a. For better understanding of the idea of superfractal, let us remind the basic properties of modulated crystals (supercrystals). In the modulated crystals ions occupy positions, which show modulatory displacements from the lattice sites predicted by crystal structure according to the formula [10]

$$x_{n+1} = x_1 + na + \gamma \sin[(2\pi / b)(x_1 + na)] \tag{5}$$

where x_1 is the zeroth-order position of the chain. The shift modulations arise due to the presence of more than one ordering mechanism, each favouring different periodicity. It can be proved that modulation of the 1D crystal lattice along the line L can be obtained as an intersection of the 2D periodic structure (i.e. (1+1)D supercrystal) with the line L, provided that the line L is not parallel to a unit cell edge of the (1+1)D superstructure. The additional dimension is called the internal dimension of the modulated crystal. Thus, the modulated crystals can be assumed as the projection of periodic structure in the (n+k)D superspace (supercrystal) onto nD ($n \leq 3$) position space. By the analogy to the supercrystal we define the superfractal as the projection of an ordinary linear fractal within (n+k)D superspace, onto nD position space. We can easily find one to one correspondence between supercrystals and self-affine mappings on superfractals The only difference between superfractals and ordinary fractals can be summarized as follows: in superfractals **SG** the action of scaling mapping $\mathbf{S}^{(m,n,l)}{}_{SF} \in \mathbf{SG}^*$ transforms any point $\mathbf{x}= (\varepsilon, \eta, \rho) \in \mathbf{SG}$ according to the formula:

$$S^{(m,n,l)} : x = (e^{x_n}\varepsilon, e^{y_m}\eta, e^{z_l}\rho) \qquad (6)$$

where x_n, y_m, z_l are given by expressions of the type (5). Contrary to Eq. (6) the similarity transformation for ordinary fractal is given by Eq. (3). In Eq. (6) we have assumed that the coordinate axes are oriented along eigenvectors of the linear self-affine transformation. We should stress here that our results refer fractals contained both in the real as well as dynamical (spectral spaces) [11]-[13]. Moreover, it can be easily proved that both Hausdorff dimension and lacunarity of the superfractal are exactly the same as they are in the basic fractal structure.

APPLICATIONS

Invariance of the fractal structure under symmetry transformations $\mathbf{r}' \rightarrow \mathbf{R}_\alpha : \mathbf{r}$ leads to the expectation that various physical properties share this symmetry. As a matter of fact the rotational symmetry classifies different types of the anisotropy observed in physical systems.

Let us consider action of a symmetry element $\mathbf{O}_\alpha^{\,i}$ being a member of crystallographic group $\mathbf{O}_\alpha$, which characterizes symmetry of the dual space $\mathbf{G}^*$. By definition for any $\mathbf{S}^{(m,n,l)} \in \mathbf{G}^*$ we have $\mathbf{O}_\alpha^{\,i}\!:\!\mathbf{S}^{(m,n,l)} = \mathbf{S}^{(i,j,k)} \in \mathbf{G}^*$. Thus, we have $\mathbf{O}_\alpha^{\,i} :\mathbf{S}^{(m,n,l)} :\mathbf{G} \subset \mathbf{G}$ and $\mathbf{S}^{(m,n,l)} : \mathbf{G} \subset \mathbf{G}$, which means that crystal symmetry reflects the internal symmetry of the fractal **G**. We should stress here that we are dealing with the geometrical fractals rather than with the dynamical spaces [14]-[15]. Contrary to our case, the latter, characterized by the spectral dimension, often involve assumption of the connectivity condition [16]. Let us now focus our attention on the applications of the superfractals structures which in the log scale show sinusoidal oscillations superimposed onto log-periodicity.

The log-periodic oscillations in the DLA structures, rupture, earthquake, and financial crushes with amplitude of the order of 10% have been reported [17], At present the most evident example of application of the superfractals comes from the studies of statistical properties of DNA sequences in the bacterial chromosomes [18]. Numerical studies of correlations between the DNA coding regions of bacterial chromosome of the *Borrelia burgdorferi,* shows long-range correlations and log-periodic modulations of the type (6) along the whole

chromosome. This result can be extended onto other bacterial chromosomes. The fact that in log scale the sinusoidal modulation is superimposed onto conventional log-periodicity indicates the geometrical structure of bacterial chromosomes should be modeled
by the type-I superfractals rather then by simple fractals.

A fractal system with log-periodicity were used to describe the stock [19], [20] or crude oil [21] market microstructure. The appearance of sinusoidal modulation superimposed onto log-periodicity were found in the economic data and interpreted as the precursor effect of financial crisis or speculation bubble. In our nomenclature we can ascribe such behaviour as the the superfractality. There is other indirect proof that the superfractals can be useful in quantification of DLA surface dendritic aggregates The analytical study of the instability of the planar cracks which bear strong resemblance to the equivalent result in the dendritic DLA [22]. Analytical study of the planar cracks contains solutions of the stress concentration around wedge tip, which show oscillatory corrections to the conventional power law result. Consequently, there arises oscillatory modulation of the major sidebranch lengths. By the analogy one would expect an oscillatory contribution the correlation functions in the planar DLA systems. Since the superfractals are nothing but idealization of a physical system that has an oscillatory component of some correlation functions one can expect that the DLA precipitates can be adequately modeled by the superfractals.

DISCUSSION AND SUMMARY

The analysis outlined above places the symmetry of linear deterministic fractals within common framework of the solid state symmetry. This agrees with our intuition, as a direct consequence of the ubiquitous self-similarity, fractals can be created by simple transformations. Generally, any affine transformations are combinations of just shifts, rotations, scalings and shears. In our considerations we have reduced to the scaling transformations only. The identified symmetry offers a different perspective on the variety of fractals patterns. The remarkable point is that although we have continuum of the self-similarity scales, the symmetry of the fractals can be classified according to the finite number of symmetry groups elaborated by crystallographers. This offers not only better understanding of hierarchical systems but indicates general way how to detect and classify the patterns of complex systems. From practical point of view symmetry results in the reduction of complexity and may even allow to discover novel structural properties of hierarchical systems. Along with the fractals for which symmetry of their self-affine transformations is isomorphic with the symmetry of conventional crystals there arises concept of superfractals.

These hierarchical systems show position modulations of their components with respect to that expected for conventional fractals. The symmetry of self-affine transformations of the superfractals can be directly related to the symmetry of supercrystals. We expect that the idea of superfractals can stimulate methods of characterization of fractal structures. In numerical calculations of fractal characteristics most of the numerical procedures become ineffective when applied to the structures that exhibit modulations of the structure [23]-[26]. Such situation arises always when intimate relation between self-similarity and fractality is broken. This is just the effect we expect in the case of incommensurately modulated fractals (superfractals). We should mention that the term superfractal was previously used in description of systems that are periodic structure of fractal units [6] that model some antenna devices in electrodynamics [6], [7]. The difference between these two superstructures relies on the fact that the superfractal by Jaggards [6] show real space periodicity while our definition assumes the log periodicity. Although meaning of the term superfractal is somewhat different, but we believe it wouldn't lead to misinterpretations. As we have mentioned above the probability distribution of some quantities on simple self-similar fractals is often described by the log-normal distribution (4). In the superfractals one would expect oscillatory deviations from the log-normal function but in average the log-normal distribution should be preserved. The set of eigenvalues and eigenvectors of the self-similar mapping (1) of the fractal G determines the symmetry group of the self-dual space $\mathbf{G}_s^*$. With infinitesimal change of the scaling parameters there can arise abrupt change of the crystallographic group that describes the symmetry of a fractal. Conventional measure of the complexity of fractional statistical systems is the Shanon or excess entropy [27]. As we know [28] any symmetry of the system results in the reduction of the excess entropy. Thus, proper identification of the symmetry gives us a new tool which allows us to predict abrupt changes in entropy when infinitesimal change of the scaling factors changes the symmetry of the system. This agrees with the Landau theory, which relates the symmetry changes with the phase transitions. In view of this we can predict when minimal variation of the fractal parameters can generate significant changes of its statistical or thermodynamical parameters. We believe that the possible area of applications of the result obtained covers also the statistical mechanical systems, computation-theoretic problems or hierarchical networks [29].

In summary, we have proved that the set of injective scaling transformations of a 3D fractal is isomorphic with a conventional crystal lattice. Basing on the proved isomorphism we have introduced a new family of hierarchical systems - superfractals, which are isomorphic with the
modulated crystals (supercrystals). Finally we have given extensive study of the results obtained pointing some real physical systems that exactly exhibit the superfractal behaviour.

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