

Möbius function in modeling the fractal properties of colloidal structures

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The study of the structural properties of non-compact colloidal associates, as well as linear and branched polymers, is an important task of modern physical chemistry, since the structure at the nanoscale determines a number of important macroscopic features. Such systems often have fractal properties, that is, they exhibit scale invariance in a number of characteristics.

The development of the physics of fractal nanosystems determines an active interest in methods that make it possible to operate reliably at a level of (1-1000) nm. One of them is the small-angle scattering method, which analyzes the scattering of thermal neutrons or X-rays by material inhomogeneities, the size of which significantly exceeds the radiation wavelength [1].

The so-called phase problem somewhat limits the capabilities of scattering methods when solving the inverse problem on reconstructing the scatterer structure; therefore, complementary approaches, including direct modeling, are increasingly used in practice. Regarding fractals, a lot of algorithms for constructing deterministic [2] and stochastic [3] fractal objects have been proposed recently. The former are based on an exact repetition of the shape at different scales, while when using the latter, the scaling ratios are observed only "on average".

In this paper, we propose a new algorithm for constructing a fractal object, called the Möbius fractal, which is essentially on the verge between deterministic and stochastic fractals. The model is based on the Möbius function [4], which is defined for all natural numbers N and takes values $-1; 0; 1$, depending on the nature of the decomposition of the number N into prime factors. Within the framework of the developed algorithm, the values of the function $-1; 0; 1$ correspond to the directions left/straight/right in a plane. Thus, we get not a random walk, but, in a sense, a deterministic walk. On the other hand, the values of the Möbius function alternate randomly, thus ensuring the stochasticity of the procedure. The result of the construction is a rather complicated curve on the plane. It has self-intersections (thus, up to half of all the vertices of the figure are excluded). According to the correlation analysis, the fractal dimension of such a system is close to 1.8. The fractal dimension does not depend on the size of the system and does not depend on the range of natural numbers used in modeling, but is a global characteristic of this system.

In the given paper, a detailed analysis of the correlation functions of Möbius fractals in both real and reciprocal space is carried out, and prospects for the further use of these objects in describing the results of experimental methods of structural diagnostics of nanomaterials, including small-angle scattering, are outlined.

References

- [1] Pedersen J.S. // Adv. Coll. Inter.Sci. 70 (1997) 171.
- [2] Cherny A.Y. et al. // J. Appl. Cryst. 43 (2010) 790.
- [3] Tomchuk O.V. et al. // Colloids Surf. A 605 (2020) 125331.
- [4] Möbius A.F. // Journal für die reine und angewandte Mathematik 9 (1832) 105.

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