ISSN 1063-7745, Crystallography Reports, 2010, Vol. 55, No. 6, pp. 964–970. © Pleiades Publishing, Inc., 2010.
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THEORY

Dedicated to the memory of B.N. Grechushnikov

Scaling in the Optical Characteristics of Aperiodic Structures with Self-Similarity Symmetry

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Received May 12, 2010

Abstract—The properties of diffraction gratings and multilayered systems constructed using 1D models of quasicrystals are considered based on numerical simulation. It is shown that there is a direct relationship between the self-similarity symmetry of quasicrystals and scaling in the characteristics of the above-mentioned optical devices. The degree of structural correspondence between the graphical representations of the geometric properties of crystals, light diffraction patterns of gratings, and the transmission spectra of multilayered systems is estimated. It is shown that certain types of self-similarity symmetry make the characteristics of aperiodic diffraction gratings highly stable to a change in the size ratio of forming elements.

DOI: 10.1134/S1063774510060106

Currently, many crystallographic studies are devoted to quasicrystals [1, 2]. Having both short- and long-range orders, their aperiodic structure does not satisfy the principle of translational symmetry [3]. This leads to the manifestation of a number of unique properties of quasicrystals, the analysis of which is important from both fundamental and applied points of view. Concerning applications, we should note the use of 1D models of quasicrystals in developing a new class of promising optical elements: aperiodic diffraction gratings and multilayered systems. Their properties radically differ from those of generally used periodic systems. One of the differences is that the optical characteristics of aperiodic systems are characterized by scale invariance (scaling) in many cases.

Although scaling (which manifests itself in self-similar properties of those or other physical dependences) has been considered for the above-mentioned optical elements in many studies (see, for example, [4–7]), the relationship of the observed self-similarity with the types of symmetry present in forming 1D structures has been insufficiently studied. In this paper we consider this problem based on the comparative analysis of the optical characteristics of diffraction gratings and multilayered systems, where the alternation of forming elements is determined by aperiodic sequences. One of the sequences used reflects the structure of the triad Cantor set, while the others are the Thue–Morse and Fibonacci sequences. These sequences are most often used to form quasi-periodic systems [6] composed of alternating elements of two types, A and B. All these systems possess self-similarity symmetry, which, like any other symmetry, should manifest itself in their optical characteristics [8].

Let us consider the properties of Cantor-like systems constructed based on a Cantor set. They can be represented as blocks of elements A and B corresponding to different complexity levels. The blocks of the first levels have the form $S_0 = A; S_1 = ABA; S_2 = ABABBBABA$, etc. A transition from each level to a higher one is performed by replacing elements: $A \to ABA$ and $B \to BBB$. The model of a 1D quasicrystal corresponding to these systems can be presented by putting the elements A and B into correspondence with segments of a certain length which separate the "atoms" forming a given quasicrystal. In this case, each fragment (composed of several successively located elements B) of the sequence is put into correspondence with one segment of a summary length. Figure 1a shows a quasicrystal fragment composed of 16 atoms for the case where the segments A and B are equal. The quasicrystals of this type are fractals; i.e., they have a pronounced self-similarity symmetry. Their structure, like that of the triad Cantor set, is characterized by the scaling factor $u = 3$ [9].

The number of atoms N in a quasicrystal and the total number $\tilde{N}$ of segments A and B are related as follows:

$$N \sim \tilde{N}^{D_1}, \tag{1}$$

where D_1 is referred to as the mass (or cluster) fractal dimension [9]. For the quasicrystal D_1 under consideration, it is equal to 0.63, i.e., coincides with the fractal Hausdorff–Besicovitch dimension of the Cantor set.

Considering quasicrystal atoms to be emission centers, one can calculate the distribution of the light field intensity for the far-field zone. This distribution, corresponding to the S_5 level, is shown in Fig. 1b (it cor-

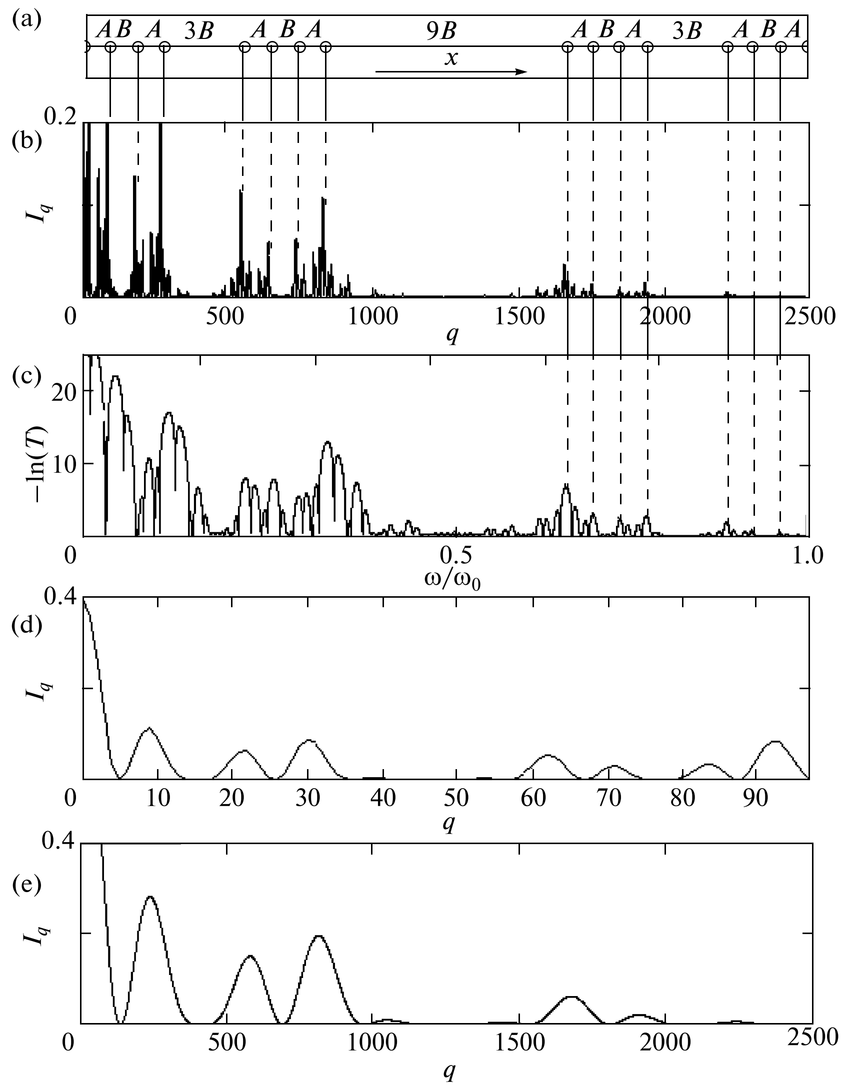

Fig. 1. Optical properties of the Cantor system: (a) a fragment of the forming-quasicrystal structure, (b) the diffraction pattern for the S_5 level (hereinafter the intensity I_q distribution is normalized to the maximum value), (c) the frequency dependence of the multilayered system transmittance T, (d) intensity distribution near zero spatial frequency, and (e) diffraction pattern for the S_4 level.

responds to the wave diffraction pattern from an aperiodic grating with infinitely narrow slits). The intensity I_q was calculated from the formula

$$I_q = \left|\sum_{n=0}^{N} e^{-iqsx_n}\right|^2, \qquad (2)$$

where $q = \frac{2\pi\alpha d}{\lambda}$ is the normalized spatial frequency (α is the diffraction angle, λ is the wavelength, and d is the size of forming elements), $i = \sqrt{-1}$, N is the number of emission centers, x_n is the coordinate of the nth center normalized to d, and s is the scaling factor. The calculations were performed on the assumption that q takes integer values and that $s = 0.001$.

The almost complete coincidence of the most significant peaks in the diffraction pattern with the position of the emission center indicates that the scaling factors u of the diffraction field and Cantor set should coincide and be equal to 3. It is of importance that the diffraction field has pronounced fractal signs. This confirms the fact that, in a wide range of spatial frequencies, the amplitude $A_q = \sqrt{I_q}$ of light oscillations obeys the relation

$$\sum_{q=0}^{Q} A_q \sim Q^{D_2}, \qquad (3)$$

where the calculated mass fractal dimension $D_2 = 0.62$ is very close to $D_1 = 0.63$. The maximum Q value, which determines the scaling range, is approxi-

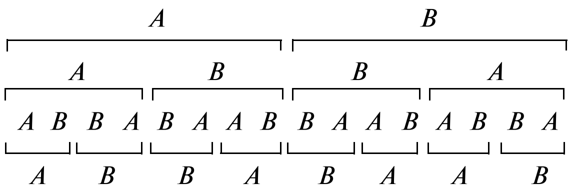

Fig. 2. Primary links of elements in the Morse–Thue system.

mately $Q_{\max} = 2200$ for the case under consideration. These estimates indicate that the self-similarity symmetry of the forming quasicrystal is directly related to the self-similar properties of the diffraction pattern. For the convenience of comparing the quasicrystal structure with the plots in Fig. 1, they are given with vertical reference lines passing through quasicrystal atoms. The good coincidence of these lines with the series of intensity distribution peaks in Fig. 1b indicates that the structure of the forming quasicrystal is directly reflected in the diffraction pattern.

To determine the generality of this structural correspondence, we also calculated the transmission spectrum of a dielectric multilayered system formed on the basis of the aforementioned law of alternating elements A and B, which determined the alternation of layers with different refractive indices in this case. This calculation was performed using the well-known matrix method [10, 11]. The spectrum in Fig. 1c is typical of equal phase incursions in layers. It corresponds to a system with the number of layers $J = 243$ (complexity level S_5) with the refractive indices $N_1 = 1.45$ and $N_2 = 2.3$. It can clearly be seen that the structure of the transmission spectrum also reflects the structure of the 1D quasicrystal. The above-mentioned self-similarity is especially pronounced in the range of frequencies ω close to the frequency ω_0, at which the phase incursions in the layers are close to $\pi/2$. An estimation of the fractal dimension of the plotted transmission spectrum in the above-mentioned frequency range gives $D_m = 1$, a value significantly differing from the corresponding dimension of intensity distribution in the diffraction pattern.

It is noteworthy that the self-similarity of optical characteristics also manifests itself in the similarity of their graphical representations related to different complexity levels of the system. In Fig. 1d this self-similarity is illustrated by the intensity distribution in the diffraction field on a larger scale. Here, the curve behavior is qualitatively similar to the plot in Fig. 1b. It is also similar to the behavior of the intensity distribution for the case where the emission centers correspond to the configuration of the S_4 level (Fig. 1e). The transmission spectrum of the multilayered system also exhibits a similar property. The transmission spectrum of the structure of the S_4 level (which is not shown) exhibits a structural similarity with the transmission spectrum related to the S_5 level.

Note that, although a change in the ratio of element sizes causes a change in the structure of the forming quasicrystal and characteristics of the optical elements, it does not violate (as the calculations showed) their structural correspondence.

Let us consider the properties of systems whose structure reflects the regularity in construction of the Morse–Thue sequences. These systems radically differ from the Cantor ones, because a Morse–Thue sequence does not provide any fractality of the forming quasicrystal structure. Morse–Thue systems can be constructed by combining blocks of elements determining different structural levels [6]. The recursive rule for combining blocks has the form $S_n = S_{n-1}S_{n-1}^{+}$; $S_n^{+} = S_{n-1}^{+}S_{n-1}$ for $n \geq 1$, where $S_0 = A$ and $S_0^{+} = B$. The corresponding blocks of structural levels can be written as $S_0 = A$; $S_1 = AB$; $S_2 = ABBA$; $S_3 = ABBABAAB$, etc. The transition to each higher structural level can be performed using the replacement rule: $A \to AB$, $B \to BA$. The number of elements in the block S_n is 2^n. The ratio of the number of elements A to the number of elements B is unity. A Morse–Thue system has a number of symmetries [12]. In particular, its structure is not violated when elements are removed from even sites (the level of the system decreases by unity). The system also remains the same when any two units of elements that can form the entire system are replaced by individual symbols. The latter property is illustrated in Fig. 2, which shows a series of the first elements of the system (the second row from below). The horizontal square brackets from below and above indicate the above-mentioned primary units in this series. The initial series can be obtained by redenoting them with the symbols A and B. Since a gradual increase in the sizes of primary units eventually doubles the number of elements they contain, we can assume that the self-similarity of the system under study (which is combined with the far-field correlations) is characterized by a scaling factor of 2.

A fragment of a 1D Morse–Thue quasicrystal constructed based on the aforementioned rule for combining elements A and B is shown in Fig. 3a. In view of the relatively uniform distribution of atoms in this quasicrystal, its mass fractal dimension is unity. A grating with infinitely narrow slits put into correspondence with this quasicrystal will form a diffraction pattern that is shown in Fig. 3b (for a narrow range of spatial frequencies). The diffraction pattern was calculated using formula (2), in which the parameter d was taken to be the minimum distance between emission centers, the size ratio for the elements A and B was assumed to be $A : B = 1 : 1.67$, and the N value was taken as 233. The transmission spectrum of a multilayered system with the number of layers $J = 32$, formed

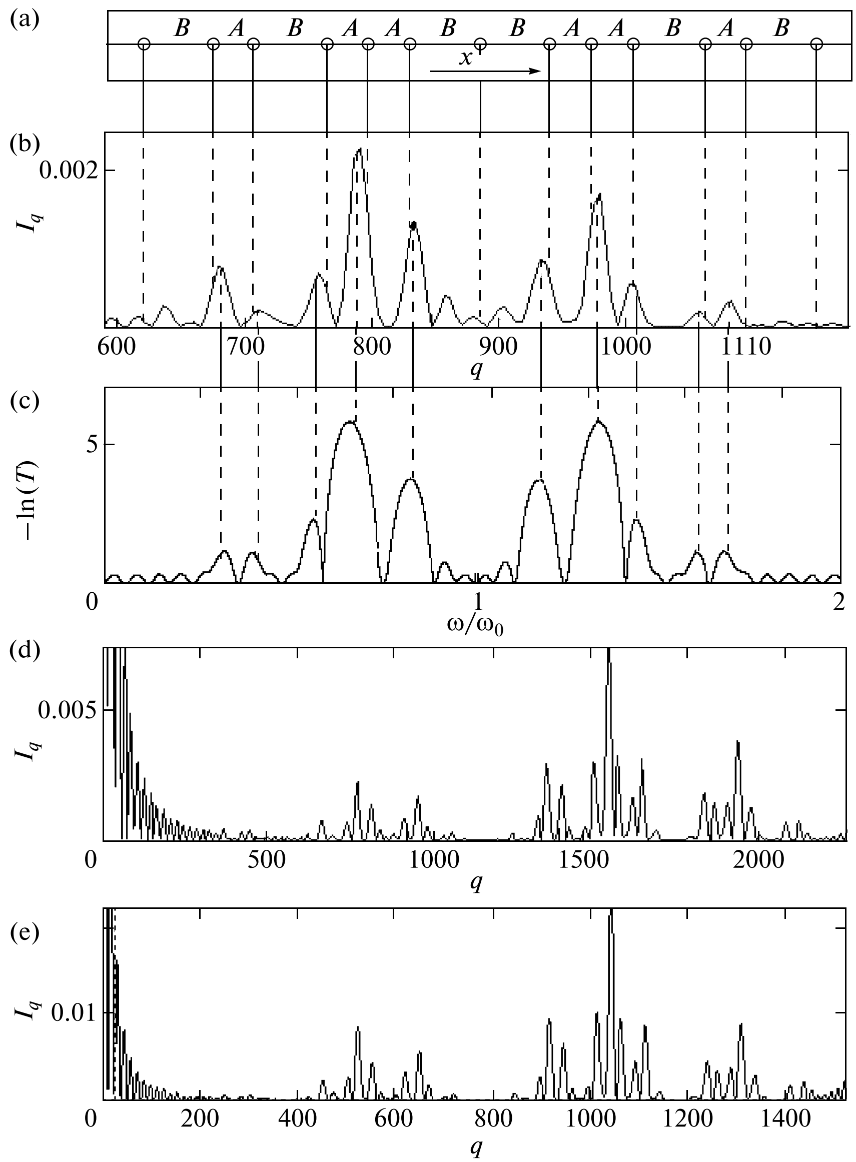

Fig. 3. Optical properties of the Morse–Thue system: (a) a fragment of forming-quasicrystal structure, (b) the diffraction pattern in a narrow band of spatial frequencies, (c) frequency dependence of the multilayered system transmittance T, and (d, e) the diffraction patterns in a wide band of spatial frequencies for $A : B =$ (d) 1 : 1.67 and (e) 1 : 3.

taking into account the rule for constructing this quasicrystal, is shown in Fig. 3c. The phase incursions in the layers, like in the previous case, were assumed to be equal. The above-denoted types of symmetry lead, as can be seen in the figures, to a certain structural similarity of the plots of optical characteristics and quasicrystal geometry. However, this similarity is less pronounced than in the previous case. At the same time, the degree of coincidence between the positions of diffraction peaks and the transmission maxima of the multilayered system is fairly high. This is also confirmed by the extreme value of the correlation coefficient between the distribution under consideration and the emission centers modeled by δ-like peaks.

Like Cantor systems, Morse–Thue systems also exhibit a self-similarity of optical characteristics. This is demonstrated in Fig. 3d, where the diffraction pattern is shown in a wider range of spatial frequencies. It can be seen that the intensity distribution consists of self-similar fragments which cover the ranges $624 < q < 1103$ and $1250 < q < 2205$ (the shapes of the envelopes of diffraction peaks in these ranges are fairly close). A comparison of the sizes of these fragments shows that the scaling factor of the diffraction pattern coincides with that of the Morse–Thue system and is $u = 2$.

We should emphasize the high stability of the intensity distribution shape near the central diffraction peak, which is demonstrated by the Morse–Thue system with a change in the sizes of elements A and B. This is confirmed by comparing Fig. 3d with Fig. 3e, which shows the diffraction pattern for the case where $A : B = 1 : 3$. It can be clearly seen that an increase in

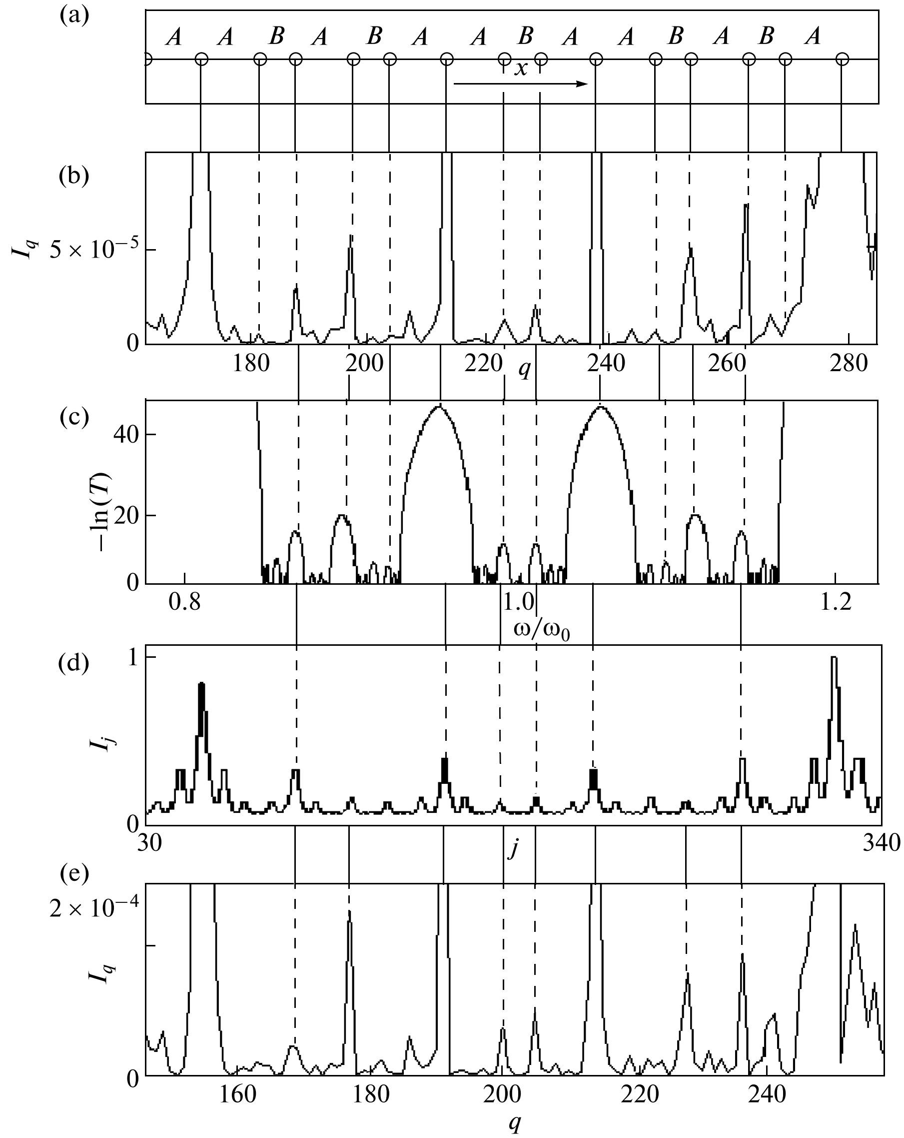

Fig. 4. Optical properties of the Fibonacci system: (a) a fragment of the forming-quasicrystal structure, (b) the diffraction pattern for $B : A = 1 : \tau$, (c) the frequency dependence of the multilayered system transmittance T, (d) the intensity distribution over layers (j is the layer number), and (e) the diffraction pattern for $B : A = 1 : 3.5$.

the size of element B by a factor of almost 2 does not cause any significant changes in the intensity distribution. The aforementioned property of this diffraction grating is apparently related to the presence of far-field correlations in the forming quasicrystal structure.

Let us now analyze Fibonacci systems. In this case, a block S_n of elements A and B satisfies the following recursive rule: $S_n = S_{n-1}S_{n-2}$ (for $n \geq 2$) [6]. The initial blocks have the form $S_0 = B$ and $S_1 = A$. Thus, the blocks of structural levels can be written as $S_0 = B$; $S_1 = A$; $S_2 = AB$; $S_3 = ABA$; $S_4 = ABAAB$, etc. At a transition to a higher structural level, the following rules are valid: $A \to AB$ and $B \to A$. It is noteworthy that, with an increase in the number of structural level n, the ratio of the number of elements A to the number of elements B in the block S_n tends to the golden mean $\tau \equiv \left(1 + \sqrt{5}\right)/2$.

A structural fragment of the quasicrystal reflecting this mathematical model is shown in Fig. 4a. It corresponds to the case where the sizes of elements A and B satisfy the relation $B : A = 1 : \tau$. The quasicrystal structure is not monofractal. However, it has certain self-similarity symmetry [13]. A contraction of the quasicrystal lattice by a factor of τ yields a lattice similar to the initial one. In this case, the position of each atom in the initial lattice will coincide exactly with the position of a particular atom in the contracted lattice. The self-similarity symmetry is related to another important property of the quasicrystal lattice. To clarify it, we should note that the serial numbers of elements A are set by the expression

$$n = \lfloor m\tau \rfloor, \quad m = 1, 2, 3\ldots, \tag{4}$$

and the serial numbers of elements B are set by the expression

$$k = \lfloor m\tau^2 \rfloor, \quad m = 1, 2, 3\ldots. \tag{5}$$

Here, $\lfloor x \rfloor$ is the largest integer that is no larger than x. When considering the sequence of serial numbers of elements A, one can easily see that, when all its terms are increased by a factor of τ (i.e., $\lfloor m\tau \rfloor$ is replaced with m), it is transformed into a sequence of numbers $\lfloor m\tau^2 \rfloor$ for elements B. Thus, we can conclude that the self-similarity in the structure of a forming quasicrystal is characterized by a scaling factor equal to τ.

To establish the relationship between the symmetry of quasicrystal self-similarity and the characteristics of the corresponding optical elements, we calculated, like in the previous cases, the diffraction pattern (Fig. 4b) and transmission spectrum (Fig. 4c) of the grating ($N = 731$) and multilayered system ($J = 610$), which reflect the forming quasicrystal geometry. These figures indicate a high degree of structural correspondence between the graphical representations of the crystal geometry and the optical characteristics. An analysis of the optical properties of Fibonacci systems revealed that the aforementioned structural correspondence is typical of another characteristic: the distribution of radiation intensity over multilayered system layers (Fig. 4d). The plots in Fig. 4 have self-similar signs. For example, Fig. 4b exhibits a qualitative similarity of the intensity distribution in two ranges of spatial frequencies: $171 < q < 213$ and $213 < q < 239$. The ratio of the widths of these ranges is close to τ; hence, the golden mean ratio τ also determines the scaling factor for the diffraction pattern. Note that the strongest diffraction peaks in the above-mentioned ranges are located (with respect to their boundaries) at the golden mean points.

With a change in the relative sizes of elements A and B, the light diffraction pattern from a Fibonacci grating significantly changes. However, in some ranges of spatial frequencies near the central diffraction peak, the shape of the intensity distribution is similar, regardless of the ratio of the forming-element sizes. This fact, which is indicative of the important role that far-field correlations play in the structure of the forming quasicrystal, is illustrated by Fig. 4e. The diffraction pattern in Fig. 4e, which corresponds to the case where $B : A = 1 : 3.5$, is similar to the diffraction pattern shown in Fig. 4b.

Apparently, the similarity between the light diffraction patterns from gratings and the transmission spectra of the multilayered systems should be additionally clarified. This fact, strange at first glance, can be easily explained. The calculations show that partial rays diffracting from a grating to form a certain diffraction peak are equivalent (with respect to the difference in their phases) to certain sets of rays at the multilayered system output, the interference of which determines the occurrence of one maxima in the transmission spectrum. Obviously this correspondence will be observed if the sequences of forming elements in gratings and multilayered systems coincide.

To make sure that the above-mentioned regularity is characteristic of only systems with pronounced self-similarity symmetries, we performed similar calculations for systems whose geometry is determined by the Rudin–Shapiro sequence [14] (similar in properties to a random sequence). As one would expect, the calculation of the optical characteristics of these systems showed that they lack self-similar signs. This indicates that the above-mentioned regularity is typical of only systems with pronounced self-similarity symmetries.

We performed additional calculations which showed that the above data on gratings with infinitely narrow slits can be applied to aperiodic gratings of other types that have slits of finite size (amplitude gratings) or a certain profile (phase gratings). Note also that the self-similar signs observed in the characteristics of the types of optical systems under consideration hardly depend on the specific mechanism of interaction with radiation. One can make sure of this by analyzing the results of [15], where light diffraction from a metal Fibonacci grating was considered based on the vector method taking into account the polariton effects. An additional confirmation of these conclusions can be found in [16], where the X-ray reflection spectra of a multilayered system with metal layers, which was also constructed based on the Fibonacci principle, were calculated.

In summary, we can conclude that the results of this study gain deeper insight into the phenomenon of the light transmission through a structure having self-similarity symmetry. The principle of structural correspondence considered on the basis of numerical simulation is not universal; nevertheless, it can be a good landmark for explaining the relationship between the scaling characteristics of aperiodic optical systems and light waves transmitted through them from the general point of view. The revealed effect of the stability of a light diffraction pattern from gratings with a certain type of self-similarity symmetry can be used in practice in optical devices and laser systems based on such gratings.

ACKNOWLEDGMENTS

This study was supported by grant NSh-4408.2008.2 for the Support of Leading Scientific Schools.

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Translated by Yu. Sin'kov