Topology of Crystals Surf Ace Irradiated X-Ray Beams, by Sem and AFM Processing with Multiefractal Analysis

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Abstract – We investigate potassium sulphate crystals, grown up from solution by a method of slow evaporation at constant temperature. The structure of crystal surfaces was investigated by means of atomic-force microscope. The set of structural hills, at which steps there is a basic growth of a crystal are found on the crystals surface. The obtained structures are analyzed by a multifractal analysis method.

The knowledge of mechanical and optical properties of surfaces of a material enables to control the sizes and the shapes of nanostructures; it is possible to force to change the material properties: to raise a limit of fluidity or durability, a thermal capacity, electroresistance, diffusion ability of molecules are especially interesting and many other things. Properties of surfaces of ionic crystals, such as potassium sulfate, because of ionic character of interaction between atoms that leads to essential compensations effects on a surface of these crystals.

As objects to study we used crystals of potassium sulfate K_2SO_4 and crystals of potassium sulfate activated by thallium K_2SO_4:Tl. Crystals have been brought up from a solution by a method of slow evaporation at constant temperature.

The dynamic range and sensitivity of crystals of potassium sulfate, considerably was, depends on many parameters such as: a level of cleanliness used distillation waters, low percentage of other impurity in a chemical reactant, cleanliness experimental laboratories and etc. Concentration of containing substances in structure of potassium sulfate it has been prepared under the chemical directory.

The structure of surfaces of crystals was investigated with the help of atomic-force microscope Nanoscop IIIa (Veeco Inc., Woodbury, NY, USA).

Studying relief of the surface of crystal K_2SO_4:Tl we have found out bow-shaped lines on all surfaces (Fig. 1). The structure of paths and a branching of growing edges surface of impurity crystal substantially differs from a surface of crystal K_2SO_4. Here a little bit other structure of a surface is already seaming. On a surface of crystal K_2SO_4, it is distinctly visible each line (Fig. 2). Paths are straight lines contrary to the previous case.

Thallium, as an impurity which is included in a lattice at crystallization from a solution, plays an appreciable role in formation of paths thus, promoting the growth of new layers on a surface.

On the surface the set of hill-shaped eminences at which steps there is a basic growth of a crystal, is formed.

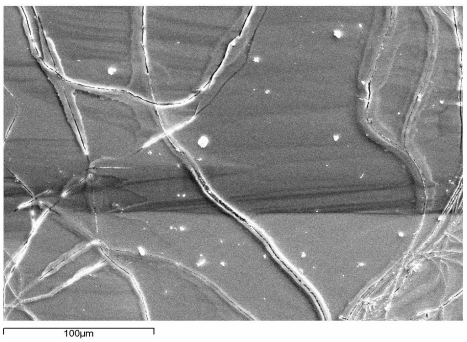


Fig. 1. K_2SO_4:Tl, electronic microscope (it is measured in GIN, Almaty)

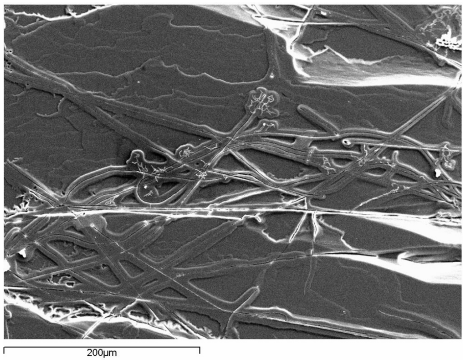
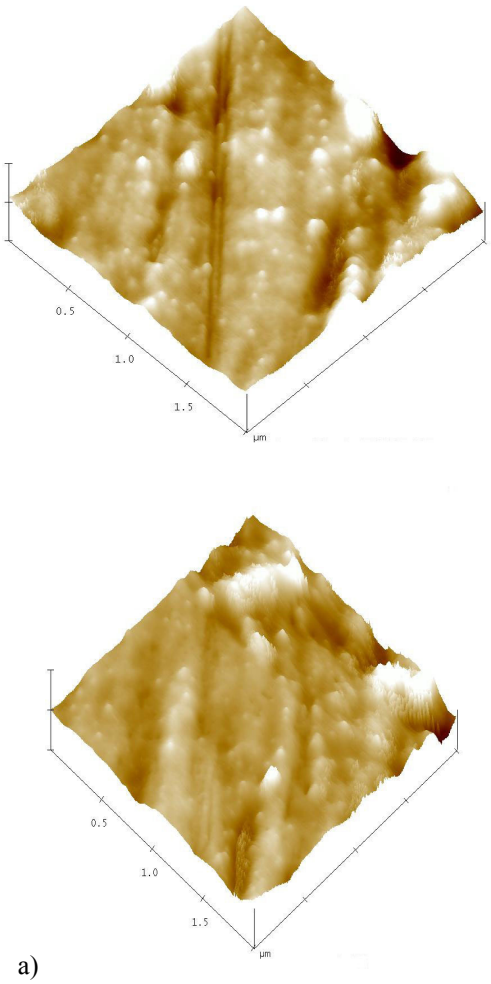


Fig. 2. K_2SO_4, electronic microscope (it is measured in GIN, Almaty)

On each path the outgrowth stages a crystal which is smoothly transformed to the big chains of lines is formed. The height of peak of each hill varies from 0, 5 up to 1, 5 µm.

During of process of scanning the surface of crystal K_2SO_4:Tl a photodetector, accepting the monochromatic beam of the diode laser, distinctly displays surfaces dislocations hills, performing back and forth motions (Fig. 3). The distance between hills for crystal K_2SO_4:Tl is 2 µm, for crystal K_2SO_4 – 5µm.

To record the good image during the scanning of the surface, we established the time of scanning 10 minutes on the average. In a case when scanning occurs quickly, danger of breakage of a measuring needle of cantilever raises.



a) b)

Fig. 3. K_2SO_4 (a) and K_2SO_4:Tl (b), (Atomic-force microscope).

That to possess the sufficient information, and to ascertain about laws defect formations in crystals, it was necessary to irradiate K2SO4 and K2SO4: Tl, with different time's duration. For samples homogeneously irradiated by Mb X-ray tube. The energy of excitation of X-ray irradiation was constant value at 17 keV.

For all crystals the time of exposition was about 5, 10 and 15 minutes. As for K_2SO_4, and so for K_2SO_4:Tl, time of an irradiation was identical, and after was created spherical hill-shaped eminences rather in the irradiated area on the surface of crystals.

Evident result of an irradiation of a crystal, has presented non-uniform complex structure. Up to an irradiation, all objects have been ground till the necessary sizes. The sizes of the investigated crystals is, were approximately identical on thickness – from 0.5 up to 1 mm, and on width and length varied – from 3x3, up to 6x6 mm. The area of a covering of an irradiation makes $\geq 1 см^2$ (Fig. 4):

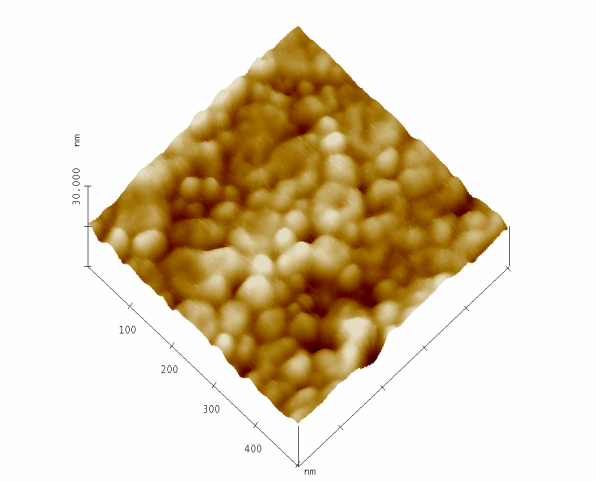


Fig. 4. K_2SO_4 after 15 minute X-ray irradiation, (Atomic-force microscope).

For the description of systems with the non-uniform, statistically ordered structure it is convenient to use methods of the analysis fractals of geometry. All regular fractals possess property of scale invariance, them the scaling structure is determinate by one scale multiplier. However in the majority of real cases as well as in our case, scale multipliers are non-uniform, and in a fractal there is a spectrum scaling. Such fractals structures is multifractals and are characterized by an infinite set of measures. The approach used for studying of these structures, besides geometry of an analyzed sample, allows establishing communication of its physical and chemical properties with parameters multifractals spectrum as so-called multifractals measures.

To multifractals parameters of system carry generalized fractals dimensions Renie and function of multifractal spectrum. The generalized dimensions Dq named also entropies Renie [1], are defined by ratio:

$$D_q = \begin{cases} \frac{1}{1-q} \ln \sum_{i=1}^{N} p_i^q & at \quad q \neq 1 \\ -\sum_{i=1}^{N} p_i \ln p_i & at \quad q = 1 \end{cases}$$

Where, qi – a parameter of singularly for the given weight pi. Sizes Dq are connected to functions of multifractal spectrum f (α) transformations of Legandre. The physical sense of function f (α) consists that it represents Hausford dimension of some homogeneous fractal subsets from initial set which brings the dominating contribution at set value q. A set of various values of function f (α) at different α represents a spectrum fractal dimensions of homogeneous subsets into which it is possible to break initial set.

Parameters Dq and f (α) enable to determine a degree of uniformity and orderliness of researched system. Parameter of uniformity it is possible to characterize probabilities pi fillings of vectorially identical sites of considered structure. The homogeneous system is characterized by parabolic function of multifractal spectrum f (α), determined by the above-stated set of probabilities. In this case square-law approximation of function f (α), executed by method the least squares, is authentic with factor R2 = 1. The above the degree of heterogeneity in system, the is more spectrum f (α) will deviate from parabolic, i.e. 0 <R2 <1. Hence, size R2 can be accepted for a parameter of uniformity of structure.

Parameter of orderliness Δ it is possible to determine difference D1-D∞ [2], where information dimension D1 characterizes a degree of infringement of symmetry of structure, and size D∞ it is connected to probability of a mistake in definition of required parameter. Then the more size Δ = D1-D∞, the above a degree of orderliness of system.

The above-stated parameters Δ and R2 allow allocating three basic such as distribution of elements of system to planes: chaotic, multifractal and monofractal. Chaotic distribution of elements of system homogeneously on the structure (R2 = 1) also is not ordered (Δ→0). Multifractal by definition it is not homogeneous (0 <R2 <1), but possesses some orderliness in an arrangement structural forming elements (Δ ≠ 0). Self-similar classical fractals (monofractals) are characterized by absolute uniformity (R2 = 1) and orderliness. As for regular fractals the spectrum generalized of fractal dimensions degenerates in one Hausford dimension D = D (q = 0) in this case to calculate parameter Δ in the above-stated way it is not obviously possible.

The ordered and chaotic distributions of elements in system are possible for distinguishing also, using concept entropy which in the first case always is less, than in the second. Information entropy S characterizes a level of self-organizing of structure and it is determined as average value of synergetic information got with probability pi, at a birth or destruction of structure:

$$S = -\sum_i p_i \ln p_i, \sum_i p_i = 1.$$

Thus, multifractal analysis (MFA) gives a set of statistical parameters which can be used for the quantitative description fractals structures.

Processing with the help of the program "Multifractal analysis" [2] static images of structures on a surface of crystals has shown the analysis, that at small increases (an electronic microscope, the size of the staff 50 microns) system of the paths arising on a surface of crystals, are more ordered in crystals without an impurity (Fig. 5):

K_2SO_4

samples	S specific	Δ	D0	R2
20	0.02792	0.20393	1.93509	0.5849
40	0.02868	0.26625	1.88831	0.8195
100	0.0281	0.22156	1.98096	0.72
200	0.02798	0.27173	1.97168	0.8159
average	0.02817	0.240868	1.94401	0.735075
max	0.02868	0.27173	1.98096	0.8195
min	0.02792	0.20393	1.88831	0.5849
+	0.00051	0.030863	0.03695	0.084425
-	0.00025	0.036938	0.0557	0.150175

K_2SO_4:Tl

samples	S specific	Δ	D0	R2
30	0.02848	0.22234	1.99438	0.8364
100	0.02913	0.15506	1.99943	0.8991
100–2	0.02904	0.14746	1.99343	0.7479
200	0.02818	0.17654	1.99625	0.9188
average	0.0287075	0.17535	1.995873	0.85055
max	0.02913	0.22234	1.99943	0.9188
min	0.02818	0.14746	1.99343	0.7479
+	0.0004225	0.04699	0.003558	0.06825
-	0.0005275	0.02789	0.002442	0.10265

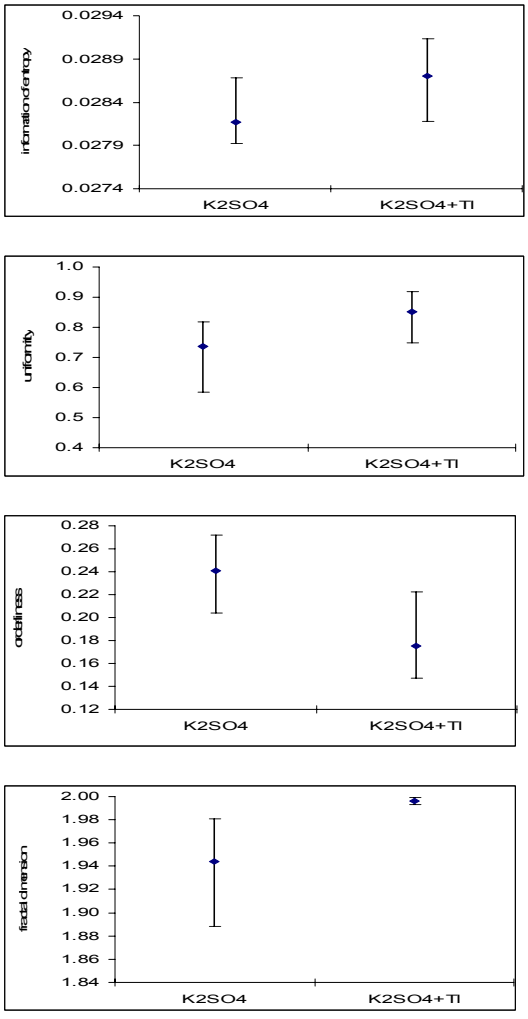


Fig. 5. Electronic microscope and multifractal analysis (Factors and their disorder, Almaty measurements in GIN 2004)

At the big increases (atomic-force microscope, the size of the staff of 500 nanometers and less) the system of hills and peaks is more ordered in crystals with an impurity (Fig. 6):

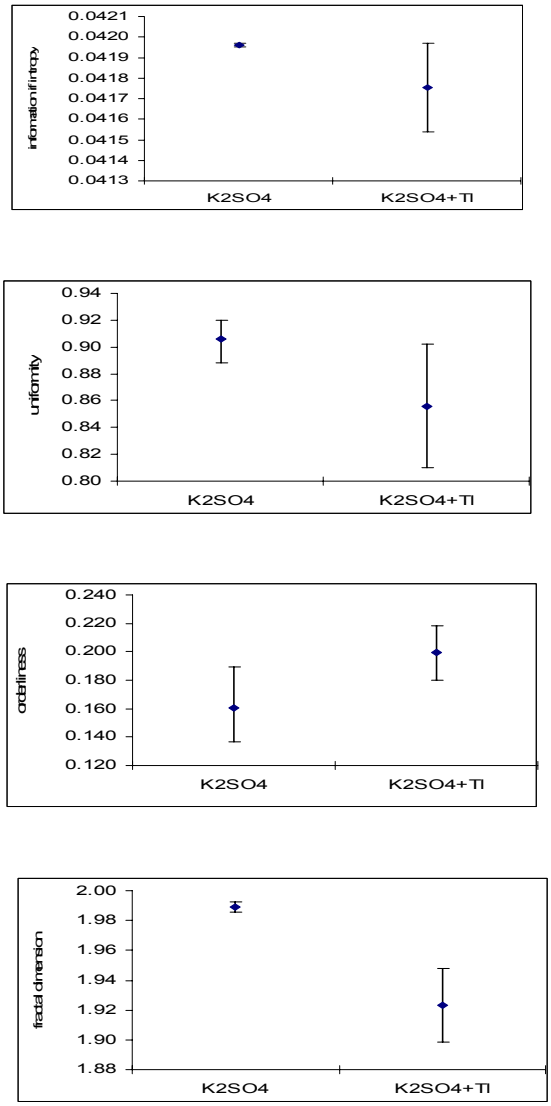


Fig. 6. Atomic-force microscope and multifractal analysis (Factors and their disorder, measurements in Switzerland, 2005–2006)

K_2SO_4

samples	S specific	Δ	D0	R2
1	0.04196	0.15512	1.98945	0.888
2	0.04195	0.1895	1.98593	0.9199
6	0.04197	0.13649	1.99247	0.91
average	0.04196	0.16037	1.989283	0.905967
max	0.04197	0.1895	1.99247	0.9199
min	0.04195	0.13649	1.98593	0.888
+	1E-05	0.02913	0.003187	0.013933
-	1E-05	0.02388	0.003353	0.017967

K_2SO_4 :Tl

samples	S specific	Δ	D0	R2
7	0.04154	0.18	1.89844	0.9018
8	0.04197	0.2184	1.94815	0.81
average	0.041755	0.1992	1.923295	0.8559
max	0.04197	0.2184	1.94815	0.9018
min	0.04154	0.18	1.89844	0.81
+	0.000215	0.0192	0.024855	0.0459
-	0.000215	0.0192	0.024855	0.0459

At the big increases (atomic-force microscope, the size of the staff of 500 nm and less) the system of hills and peaks is more ordered in crystals with an impurity (Fig. 5).

We assume that the explanation of this distinction at different increases speaks different mechanisms of occurrence of structure a surface of crystals. In scales 50 microns of a path, which width about 1 micron, are caused by indemnification of breakage of communications between atoms on a surface. It we explain practically constant width of paths. In this case the impurity which are taking place on a surface of a crystal, incur a part of such indemnification, reducing, thus, orderliness of superficial structure (the impurity settles down irregularly).

In scales of structure of 500 nanometers are sensitive to defect taking place by a line and at its presence correlate with its field. In this connection the surface of crystals with an impurity is more ordered.

Thus, of multifractal analysis shows different ratio orderliness structures on a surface of the activated and pure crystals, and allow putting forward the assumptions explaining this divergence.

References

[1]. Renyi A., On measures of entropy and information // Pal Turan (Hrsg): Selected Papers of Alfred Renyi. – 1961. – Vol. 2, – P. 1956–1961.

[2]. Vertjagina E.N., Vestnik KarGU. 2005. – P. 33–36.