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I. INTRODUCTION

It is known that any flat crystal surface is characterized by a certain density of free bonds possessing a fixed heat of adsorption and, on this basis, is a crystal defect. If the crystal is in a multicomponent medium, then, according to the second principle of thermodynamics, impurity atoms and molecules that lower the surface energy are deposited on such centers. Then it can be confidently argued that a limiting variant of Langmuir theory is always realized: the adsorption value approaches the monolayer capacity [1]. This state of the crystal surface in a multicomponent crystal-forming medium is characteristic of both equilibrium and nonequilibrium conditions. However, certain free energy thermodynamic fluctuations [2], irregularly and for a short period, are able to clear surface areas of adsorbate. Note that the distribution function of fluctuations on a homogeneous face surface can be described by Gibbs equilibrium theory [3]. The growth of the crystal face is possible only in these short intervals between desorption and secondary adsorption of impurities.

Crystal growth as a macroscopic phenomenon should be described by the equations of nonequilibrium thermodynamics. The mechanical-statistical solution to the problem of measuring macroscopic physical variables of the thermodynamic phase is well known [4]). Suppose the body is made up of *N* atoms. Then the size of the system can always be estimated at best to the accuracy of one atom. The relative error of measurements of any intensive thermodynamic variables cannot be less than $1/\sqrt{N}$. Thus, the locality limit for thermodynamic variables is at least the first tens of nanometers and partially overlapped by the field of thermodynamic fluctuations.

At the atomic level, some mechanisms of building particles embedding into the structure are implemented at the impurity desorption site, and objects with atomic scale in at least one dimension should be discussed. These are helical and combined dislocations, elementary steps, kinks of steps, two-dimensional nuclei, etc. After theoretical description of these mechanisms in the language of classical or quantum mechanics, a transition to thermodynamic description is necessary. But at this transition the problem of time inevitably arises – time reversibility in the laws of classical physics (CPT–invariance in quantum mechanics) and time irreversibility in thermodynamics. Note that the problem of time, as well as the problem of total adsorption of impurities on the growing face did not attract serious attention of the researchers of crystal growth [5, 6]. And, besides, the kinetic theories of growth widely used the Arrhenius equation [7], which has no strict theoretical justification for a nonequilibrium system. As a result, classical growth theories are internally inconsistent and abound in numerous empirical formulas and coefficients. However, the equations and phenomenological coefficients of nonequilibrium thermodynamics, in contrast to empirical coefficients, have a reliable justification in the principle of local equilibrium and the three principles of thermodynamics [3]

II. DISLOCATION IN A KOSSEL CRYSTAL

Let us discuss the helical dislocation as a defect of crystal structure, without the participation of which the growth of most crystals in nature does not occur [4, 5]. Consider a Kossel crystal [8] with a primitive cubic cell in which each particle inside the crystal contacts six neighbors and 20 more particles on the diagonals and use the Lennard-Jones potential:

$$U(r) = 4\varepsilon[(\chi/r)^{12} - (\chi/r)^{6}]. \qquad (1)$$

The equilibrium distance between particles in pairwise interaction is well known: $r_{min} = \chi\sqrt[6]{2} = 1{,}122\chi$. However, the minimum of interaction energy (1) of a surface particle is reached at

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a smaller distance $r_{min} = 1{,}085\chi$ from the nearest neighbor in the crystal. Inside the crystal, the bonds between particles become stronger and the internal energy decreases. In an ideal Kossel cubic crystal, the particles are at fixed distances r/r_{min} from each other [8]. For a surface particle, the first coordination hemisphere contains 17 neighbors and the second contains 57.

The Lennard-Jones potential serves only to illustrate model representations, since it has the necessary properties of the interatomic forces of attraction and repulsion.

It is easy to see that the main contribution to the bonding energy of a surface particle is made by the first coordination sphere. Taking into account interaction with particles of the second coordination sphere makes a correction not exceeding 8%, but always enhancing the binding energy of the particle with a crystal. To simplify further calculations, we will limit ourselves to the first coordination sphere only. We will also disregard the effect of adsorbed impurity, which additionally weakens the bonding strength of all surface atoms to the crystal. These two factors have a systematic but opposite effect.

Consider the model of a helical dislocation exiting to the crystal surface along the OZ axis at the point with coordinates *x*=0, *y*=0 (Fig. 1). The dislocation has a unit Burgers vector. Assigning the zero value of the z-coordinate to the upper boundary of the first atom – (½.½.0), we obtain coordinates of other three atoms located around dislocation: (–½.½.¼), (–½.–½.½), (½.–½.¾).

Suppose that the *z*-coordinate of any surface atom depends linearly on the angle of rotation of the radius-vector drawn from the dislocation axis to the center of the atom. Then at tetragonal symmetry of the crystal face the position *z* of surface atoms in the first quarter of the (*x*,*y*) plane can be described by the formula

$$z = \mathrm{arctg}(x/y)/2\pi \ - 1/8. \qquad (2)$$

In other quarters, if the coordinate system is rotated, *z* has to be further increased by ¼.

Using this expression in other quarters when rotating the coordinate system, *z* should be further increased by ¼. It should be noted that expression (2) does not lead to a minimum of the free energy of the crystal, but at *x*,*y*→∞, the dissymmetry of the nearest surroundings of any surface atom, expressed in values of Δ*z*, rapidly decreases and the dislocation effect disappears. This property of the formula reflects the physical phenomenon and allows the use of expression (2) for model constructions.

As a result the bonding energy of surface atoms in the first quarter is described by law 1 (Fig. 2). In the remaining quarters the bonding energy differs only for the first four atoms in the narrow region (Fig. 2) immediately adjacent to the dislocation axis at the given arrangement of atoms (Fig. 1).

It is obvious that the atoms located in the first quarter of the coordinate system are most strongly bonded, but the atoms in the fourth quarter are weakly bonded to the crystal surface (Fig. 1, Fig. 2). For an ideal surface without dislocation, the binding energy of any surface atom is about $U/4\varepsilon = -7.94$, which corresponds to a certain value of the equilibrium concentration of the surrounding crystal-forming solution.

For atoms 4 (Fig. 1), the relative reduction of the chemical potential is a rather large value $\Delta\mu_c/\mu_c = 0.28$. In the thermodynamic equilibrium state, the chemical potential of the crystal substance is equal to the chemical potential of the substance in solution [3] $\mu_c = \mu_s$, and the latter is defined by the Lewis formula:

$$\mu_s = \mu_0 + RT\ln(a), \qquad (3)$$

where μ_0 is the chemical potential of the building particles in the standard state in the saturated solution, a is their activity in the solution. If the chemical potential of the substance in the crystal decreases, the equilibrium solution corresponding to it will have a different (lower) concentration. Converting the relative change in chemical potential per molar number of atoms of type 4 we get:

$$\frac{\Delta\mu_c}{\mu_c} = \frac{\Delta\mu_s}{\mu_c} = \frac{RT\ln(a'/a_0)}{\mu_c} \approx \frac{RT\ln(c'/c_0)}{\mu_c} = \frac{RT\ln(\sigma'+1)}{\mu_c}, \qquad (4)$$

where $\sigma' = (c' - c_0)/c_0$ is the relative change in the equilibrium concentration of the solution for atom 4 (Fig. 1). Expanding the logarithm into Taylor's series and using standard Gibbs free energy of potassium sulfate formation under normal conditions ($\mu_c =- 1321\, J/(mol \cdot К)$) as an example, we obtain $\sigma' \approx -0{,}15$ for equilibrium conditions.

Thus, the equilibrium solution for the part of the crystal surface composed of atoms 4 should be considered as undersaturated, and atom 4, which is on the edge of the step, will be definitely removed from the crystal surface as a result of entropy fluctuations in the state of equilibrium. It will be followed by removal of atom 5, for which bond strength will immediately decrease after removal of atom 4, and then, clockwise, by other atoms (Fig. 1), for which the solution will also become undersaturated. However, the magnitude of the relative change in the chemical potential will decrease, as the distance to the dislocation axis grows, and eventually the process will cease. However, as the dislocation axis deviates, the magnitude of the relative change in the chemical potential will decrease and the process will stop. As a result, a funnel is formed around the dislocation – a "hollow core" (Fig. 3), theoretically predicted back in the 1950s [9, 10] and later observed in atomic force microscopes [11, 12].

The linear dimensions of such a formation cannot be established in the Lennard-Jones model, but one can use the thermodynamic model of a negative two-dimensional disk [9].

The random formation of empty space around a dislocation in a Kossel crystal, which is an open hollow cut disc of diameter r_1 and unit height coinciding with the size of the building particle b can be described using free energy fluctuations:

$$\Delta\Psi' = \frac{2\pi r_1 E}{b} - \frac{\pi r_1^2}{b^2}\Delta G, \qquad (5)$$

in which the first term is responsible for the emergence of an additional crystal surface along the side wall of the single-layer disk, and the second term is the change in internal energy due to the loss of particles that formed the crystal substance in the disk body, ΔG is the average change in the chemical potential of the crystal when one building particle is embedded in its surface structure, E is the bond energy between two surface particles. The bonding energy in the macroscopic sense determines the specific surface energy of the crystal, but in this case reflects the bonding between only two adjacent particles. Although formula (4) makes thermodynamic sense, all variables in it are not macroscopic. In addition, the variable ΔG per molecule is not the same as that for building particles inside the crystal, because it depends on a smaller number of bonds between the particles.

The conservation of the hollow disk on the crystal in equilibrium with the surrounding solution is determined by the known variation extremum condition

$$\delta(\Delta\Psi') = 0. \qquad (6)$$

The chemical potential of the equilibrium solution, but undersaturated with respect to the atoms on the edge of the step near the dislocation axis (Fig. 1, atom 4) differs by the value

$$\Delta G' = kT\ln(\sigma' + 1), \qquad (7)$$

and takes a negative value $\sigma' < 0$. As a result of the solution of the variational equation (5) we obtain the negative radius of curvature of the side walls of the equilibrium disk at the helical dislocation site (Fig. 3)

$$r'_1 = \frac{bE}{kT\ln(\sigma'+1)} \approx \frac{bE}{kT\sigma'} < 0. \qquad (8)$$

So, the value of the free energy as a result of the formation of the hollow disk is also negative and is

$$\Delta\Psi'_1 = \frac{\pi r_1 h_0 E}{b^2} < 0, \qquad (9)$$

which at thermodynamic equilibrium in the system indicates a natural process. In F.C. Frank [9] the sign of r'_1 is not discussed, but for the conditions of thermodynamic equilibrium the non-fluctuational nature of this disk and the sign are of great importance.

Let us note two opposing factors. On the one hand, the adsorbed impurity additionally weakens the connection of the atoms located at the edge of the step with the lower lying atoms. It occurs in the intervals between the fluctuations. So, the undersaturation value σ' for the atoms nearest to the dislocation certainly increases. But on the other hand, the lattice distortions quickly weaken and the value of the under-saturation decreases in response to digressing from the helical dislocation (Fig. 2). At the edge of the disk the undersaturation $\sigma' \to 0$. Thus, formula (6) represents some average value of the underdesorption index within the disk area, which is realized at the moments of impurities desorption.

Simultaneously, in deeper layers of crystalline matter, the second and subsequent hollow disks are formed in the dislocation core, but with a smaller radius (Fig. 3), because the binding force of atoms located at the edge of the non-growing step increases with depth. As a result, the equilibrium cone-shaped dislocation core at constant pressure and temperature, in accordance with the second law of thermodynamics, reduces the free Gibbs energy of the crystal by the value depending on chemical bonds of atoms, molecules and complexes in the crystal structure, the helical dislocation structure and on the impurity composition of the equilibrium crystallization medium by the value:

$$\Delta\Psi' = \sum \frac{\pi r_i h_0 E}{b^2} < 0. \qquad (10)$$

It is important to note that the dislocation core can persist only up to a certain supersaturation degree. So, in reality, the dislocation core can only be observed at minor supersaturation, for example, in AFM growth studies [11, 12].

III. CRYSTAL GROWTH RATE

Consider the growth of a crystal face with uniformly distributed growth steps running away from the dislocation core (Fig. 3). Evidence has been produced to prove the stability of uniformly distributed rectilinear elementary steps on the face of an equilibrium crystal [13]. The calculation is based on the Van der Waals interaction energy. Since most of the time the crystal face covered with adsorbate is in thermodynamic equilibrium with the solution [14], the structure of the surface even during crystal growth corresponds to the case described in [13]. Uniformly alternating steps on the flat face of the growing crystal are displayed through the surface interferometry (Fig. 4). The angle between the base surface of the octahedron face of potassium alum and the inclined flat face of the growing pyramid, which is a simple crystallographic form of tetragontrioctahedron, changes usually in the range from 10 to 20 angular minutes [14].

Analysis of the events occurring in the region of impurity desorption *X* (Fig. 3) as a result of average free energy fluctuations at the crystal face leads in the first approximation to a formula determining the "instantaneous", on the macroscopic scale of measurements, normal growth rate of the crystal face region [14]:

$$v = \frac{\beta h_0 \sigma_f}{\kappa\, \mu_1 \mu_2 (1-q)\tau} = B\sigma_f. \quad (7)$$

Here: κ and β are kinetic coefficients determining the rate of settlement of kinks by adsorbate molecules and building particles. These coefficients depend on temperature and concentrations of impurity and building particles in the environment, but not on supersaturation (under-saturation) of the crystallization medium; $\sigma_f = (c_f - c_0)/c_0$ is the relative supersaturation of the solution at the surface of the desorbed face (away from the dislocation); $\mu_1 = l_1/b$ is the relative distance between kinks along one elementary step; $\mu_2 = l_2/b$ is the relative distance between steps.

To solve the time problem [15], the transfer theorem [16] was used. As a result, there are two additional macroscopic parameters in expression (7). Over the elementary, macroscopic time of stationary growth τ, an average of $1/(1-q)$ independent fluctuations occur (high dispersion value is $q/(1-q)^2$). *q* is a statistical parameter. Thus, the known fluctuations of the growth rate of the face can be easily explained by the large variability in the number of fluctuations for a fixed elementary time of stationary crystal growth.

The kinetic coefficients β and κ are close in magnitude because they reflect the competitive struggle of similarly sized building and impurity particles for the free kink.

Stationary crystal growth, while preserving the macroscopic flat face and the dynamic stepped surface topography at the molecular level (Fig. 3), entails additional conditions that were taken into account when deriving formula (7):

1. The number of fractures per unit face area at a given fixed supersaturation should be constant in time. That implies continuous generation of new rows of construction particles at the stage, compensating the phenomenon of fracture annihilation. The mechanism of this process is realized at the equilibrium transformation stage of the surface, represented by uniformly distributed elementary growth steps [13], as a result of small but frequent fluctuations of the free energy.
2. It is known that the mean value of the effective fluctuations of the free energy, relevant to the model outlined, depends only on the temperature of the thermodynamic system and is constant over time. Therefore, regardless of the nature of the surface topography, the number of kinks within the desorption section can be assumed to be constant. Hence, it follows that the size of the surface area affected by the average fluctuation is proportional to the surface density of fractures under the given stationary growth conditions.
3. If the average linear size of the desorption region is less than the distance between stages l_2, then, according to the solution of the problem similar to the Buffon problem in the probability theory, all kinks will be concentrated on a section of one step length within area *X*. Thus, as the distance between steps increases, the frequency of kinks will as you might expect grow to the natural limit $\mu_1 = 1$.

The frequency of steps μ_2 in the desorption region depends on the critical curvature of the elementary step adjacent to the helical dislocation r_2 (Fig. 3) [6]. To solve such a problem, let us again turn to the two-dimensional nucleus model (4). Suppose the crystal face is subject to the solution oversaturation σ_f. We obtain a positive value of the radius of curvature of the elementary step:

$$r_2 = \frac{bE}{kT\ln(\sigma_f + 1)} \approx \frac{bE}{kT\sigma_f} > 0. \quad (8)$$

As a rule, at the effective Burgers vector of dislocation h_0, an initial step quickly disintegrates into elementary steps at distances of the order of 100 nm from the dislocation [11, 12]. Therefore, the critical curvature can be calculated using the elementary step model (4).

Taking into account the natural limitation of the angular speed of rotation of the lower elementary step after the disintegration of the step height in the Burgers vector [6] in the first approximation we obtain the frequency of steps on the side face:

$$\mu_2 = \frac{2\pi r_2 h_0}{b^2} = \frac{2\pi h_0 E}{bkT\sigma_f}. \quad (9)$$

Thus, a quadratic dependence of the growth rate on supersaturation near the face surface appears when dislocation steps alternate uniformly:

$$v = \frac{\beta bkT}{2\pi\kappa\mu_1 E(1-q)\tau_0}\sigma_f^2 = A\sigma_f^2. \quad (10)$$

If the Burgers vector exceeds the elementary step twice, the step frequency also doubles (Fig. 4). Thus, as a result of impurity desorption at the given section of the face, the unit step (the lower step of the package of the Burgers vector) present at distances up to 100 nm from the dislocation exit will have a radius of curvature corresponding to the parameter of a two-dimensional nucleus. This case reflects the requirements of equilibrium thermodynamics at the moment of impurity desorption and ensures the safety of the step. In a series of fluctuations, the radius of curvature, r_2, may vary slightly near the mean value (8), which controls the stationary macroscopic growth rate (10).

Note that observations of crystal growth lead to the well-known nonlinear dependence of the growth rate on the magnitude of supersaturation in the stirred solution (Fig. 5). For a well-stirred solution, a linear dependence between the supersaturation of the solution away from the crystal and near the surface of the face is usually assumed:

$$\sigma_f = \vartheta\sigma. \qquad (11)$$

Within this assumption, let us discuss the empirical data (Fig. 5.). At the initial stage the dependence of normal face growth rates on supersaturation is close to quadratic, which follows from formula (10), but following some supersaturation ($\sigma > 0.06$) it becomes linear (Fig. 5, linear trend for alumina hexahedron).

This transition to linear dependence is caused by the face relief rearrangement. When supersaturation increases up to the mentioned transition, numerous macro steps are formed on the crystal faces. According to (8), the frequency of steps increases. In an isothermal stationary process, the average fluctuation entropy jump value remains unchanged, so the area affected by desorption phenomena X, which is accounted for by a macro step, also decreases. Thus, at high kink density and growth of supersaturation, the relief parameters μ_1 and μ_2 simultaneously tend to reach 1 and the limiting case comes – their dependence on supersaturation disappears. Thus, linear formula (7) in which B=*const* will be fulfilled (Fig. 5). For different simple crystallographic forms this transition occurs at different supersaturation values, which is caused by the structure of dislocations prevailing on the face.

IV. LINEAR ONSAGER REGIME

At small supersaturations the justification of the linear Onsager regime becomes an important problem. In the stationary mode of growth of an open thermodynamic system, a linear dependence between the coupled thermodynamic forces and thermodynamic fluxes should be observed [3]. Thus, the normal velocity of the face and the supersaturation of the solution near its surface at small deviations from equilibrium should be related by a linear function. But the experimental data (Fig. 5) and formula (10) obviously contradict this. This discrepancy is well known and is often mentioned in scientific literature [6].

Note that in the macroscopic description of the growing face, such as (111) (Fig. 4.), the echelon of elementary steps on it represents a new crystallographic form with a different Miller index. In Fig. 4, the faces of the trigonal pyramid of the right lower dislocation in the circled region represent a simple tetragon trioctahedron shape with Miller indices {45.45.46}. As the supersaturation increases, the step frequency (9) grows and the face indices continuously decrease (the frequency of bands in the interferogram should increase). Therefore, the boundaries of the nonequilibrium thermodynamic system change with increasing supersaturation. Onsager's postulates formally cannot be applied to such system. However, it is possible to change the physical model by fixing the boundaries of the system by a certain simple tetragontrioctahedron shape in a small oversaturation interval by the condition μ_2=*const*. Then, instead of equation (10), formula (7) with the constant coefficient B should be used in the thermodynamic analysis, and the linear Onsager regime comes into force.

V. SUPERSATURATIONS OF SOLUTION

In the described model we used values of relative changes of solution concentration: σ', σ_f and σ. The first two of which are difficult to measure in the experiment.

Note that even when the viscous crystallization medium is actively stirred, the relationship between σ_f and σ cannot be expressed as a linear relationship. However, assuming that all of the building substance diffusing through the viscous Newtonian boundary layer to the growing face of the crystal in the stationary growth regime is deposited on its surface, we obtain an additional equation for the growth rate:

$$v = \frac{D}{\rho}\frac{dc_f}{dx}, \qquad (12)$$

where D is the diffusion coefficient of the substance in solution, ρ is the density of the crystal.

From expressions (10) and (11) in linear approximation of the boundary layer we obtain the relationship between supersaturations:

$$\sigma_f = \frac{1}{2\omega}\left(\sqrt{4\omega\sigma+1}-1\right), \qquad (13)$$

where $\omega = (A\delta\rho)/(Dc_0)$ is a dimensionless parameter, δ is the thickness of the boundary layer. From the data in Fig. 5, it is difficult to establish the value of the parameter ω. However, it is clear that at low supersaturation the boundary growth mode always tends to the kinetic mode ($\sigma_f \rightarrow \sigma$), while at high supersaturation – to the diffusion mode ($\sigma_f \rightarrow \sqrt{\sigma/\omega}$).

The situation is different when the growth rate depends linearly on supersaturation $0.06 < \sigma < 0.15$

(Fig. 5). Based on formulas (7) and (11), the growth mode will always be determined only by the value of the ϑ coefficient, which can be established empirically [14].

The case of natural convection is described in the model of the stationary boundary layer of the solution [17], when calculating the entropy production by the unit area of the growing face in the stationary mode:

$$\frac{d_i S}{dt} = K v, \qquad (14)$$

where K is the thermodynamic coefficient, linearly depending on supersaturation σ at stationary growth in a small deviation from equilibrium. In the extended version of the thermodynamic coefficient K, gravitation also provides its contribution. But the main component in K is always the first term $-\rho R \ln(\sigma + 1)$.

Expression (12) is obtained for the stationary regime of growth, at which the structure of the laminar boundary layer can be considered as linear. In this case, it is impossible to derive the dependence of entropy production density by the growing face of the crystal on supersaturation of the solution. However, it is noted that the thickness of the boundary layer is always a free parameter, which is determined only by the solution of the hydrodynamic problem of substance transfer in solution.

VI. CONCLUSIONS

It has been shown by the method of molecular dynamics that the equilibrium state in a gas is formed after an average of ten particle collisions [3]. In solutions, local equilibrium occurs in time of the order of 10^{-11} – 10^{-12} s. Thus, a interval of 10^{-2} – 10^{-3} s [14] between fluctuations leading to growth, is in stable thermodynamic equilibrium. During this time, the so-called "equilibrium" processes of alignment of the step distribution density on the dislocation pyramid [13] and the kink density on each step are realized as a result of minor fluctuations. It is important that entropy fluctuations differ in varieties – fluctuations of temperature, number of moles of a chemical component, volume, polarizability, magnetization, potential energy of the center of mass, etc. These varieties of fluctuations can also have different signs, are independent, equally probable, and are the source of such equilibrium surface transformations. Due to these numerous fluctuations, a stable stationary macroscopic structure of the growing face surface is formed under constant crystallization conditions on a large time scale (Fig. 4). Due to the equilibrium state of the face completely covered by adsorbate and "equilibrium" fluctuations of free energy, the habit of the stationary nonequilibrium and equilibrium crystal forms coincide, which allows a continuous transition from growth to equilibrium [18] and further to dissolution. But as dissolution begins, the macro structure of the dislocation pyramid changes [14].

An important feature of the approach to crystal growth through fluctuations of free energy and entropy is the separation of events occurring on a time scale of the order of 10^{-4} s during relaxation and "equilibrium" processes and events on a scale of 1 minute. Each separate fluctuation of free energy should be considered as an independent random event, the relaxation consequences of which are described by classical dynamics [14]. But the macroscopic kinetics of crystal growth is influenced only by the integral result of multiple relaxation processes. Such a model makes it possible, let us emphasize, to bypass, but not to solve the problem of time – its reversibility in Newtonian dynamics and irreversibility in macroscopic phenomena of the growth process.

Within such a two-level theory of crystal growth, it is possible to reliably justify equilibrium two-dimensional nucleation of two types as an integral part of the combined nonequilibrium dislocation mechanism of crystal growth. However, in contrast to the conclusions of the authors of [9-12], hollow dislocation nuclei exist in a limited range of supersaturation due to the equilibrium mechanism and have little effect on the growth kinetics of the face. Based on the combined growth mechanism, it is easy to explain the complex behavior of the crystal growth rate given an increasing degree of deviation of the crystal-forming system from equilibrium, and the occurrence of a hollow dislocation nucleus resulting from minor deviations from equilibrium, which do not contradict the equilibrium and nonequilibrium thermodynamics and circumvent the problem of time.

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Figures

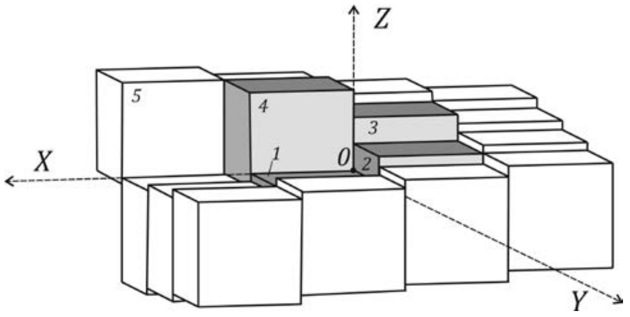

Fig. 1: Location of surface atoms on the edge of tetragonal symmetry around the helical dislocation. The first layer of the nearest 16 atoms is shown. Atoms directly in contact with the dislocation are highlighted in color.

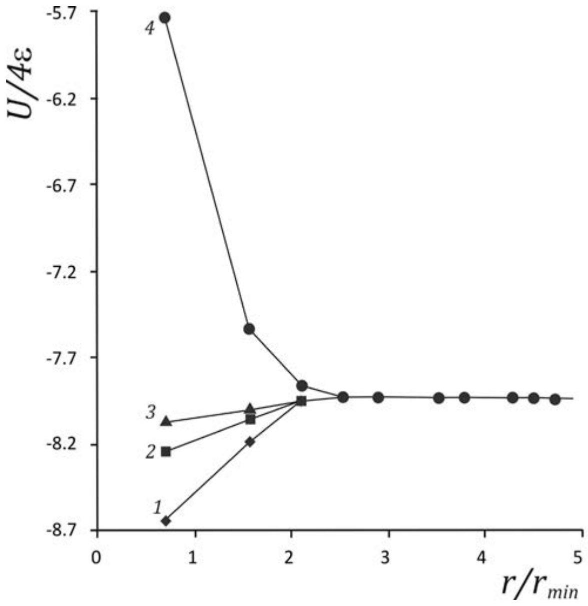

Fig. 2: Dependence of atom binding energy on the distance to the dislocation. The number indicates the atoms closest to the dislocation, located in the corresponding quarter of the coordinate system (Fig. 1)

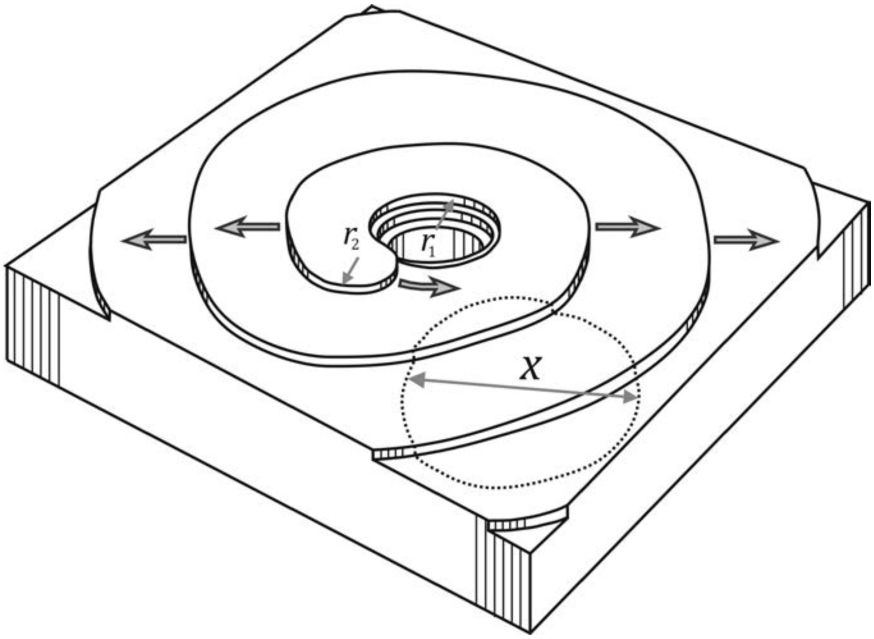

Fig. 3: Structure of the dislocation pyramid on the growing crystal face

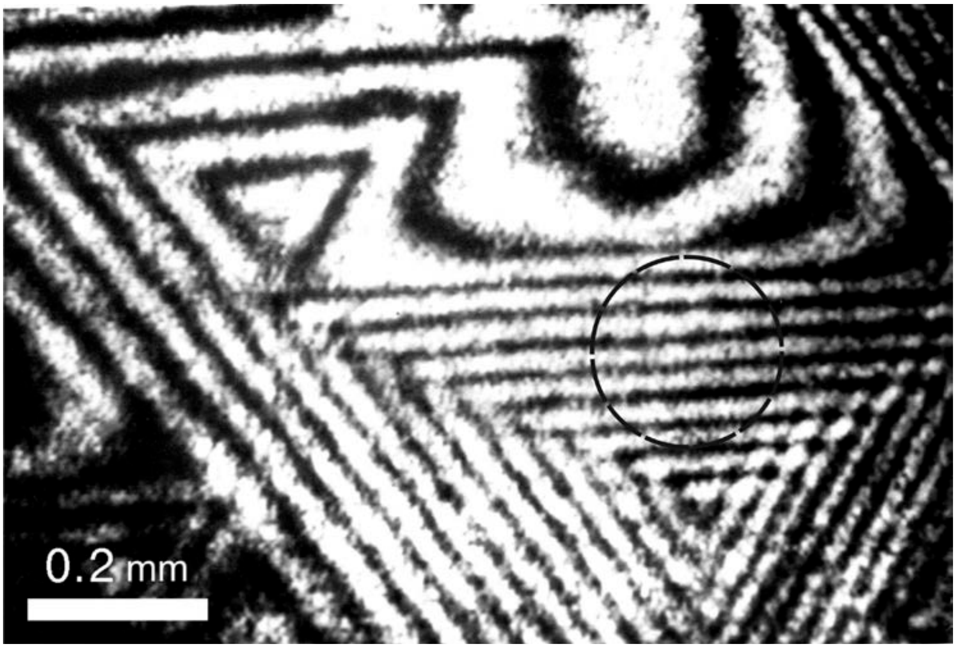

Fig. 4: Interferogram of the growth pyramids of two helical dislocations differing twice by the Buergers vector. The frequency of interference fringes is proportional to the frequency of elementary steps on the surface of the face (111) of alumina. The more active lower pyramid absorbs the upper one.

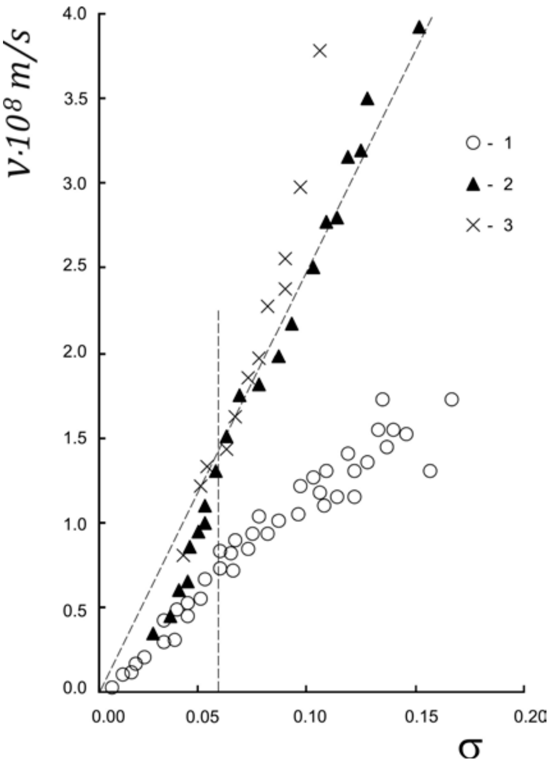

Fig. 5: Kinetics of growth of the crystal faces of alum-potassium alum in aqueous solution at active agitation, obtained with a Michelson interferometer. $T = 20°C$. 1 – faces {111}, 2 – {100}, 3 – {110}.