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USE OF COMPUTER PROCESSING BY THE METHOD OF MULTI-THRESHOLD CROSS SECTIONS FOR THE ANALYSIS OF OPTICAL IMAGES OF FRACTAL SURFACE MICROSTRUCTURE

I. Kolupaev
PhD, Associate Professor*
E-mail: 2read.kolupaev@gmail.com
O. Sobol'
Doctor of Physical and Mathematical Sciences,
Professor, Head of the Department*
E-mail: sool@kpi.kharkov.ua
A. Murakhovski*
E-mail: ostapvishna@mail.ru
T. Kol'tsova
PhD, Associate Professor**
Institute of Physical and Mathematical Sciences
and Information Technology
Immanuel Kant Baltic Federal University
Alexander Nevsky str., 14, Kaliningrad, Russian Federation, 236016
E-mail: annelet@yandex.ru
M. Kozlova**
E-mail: annelet@yandex.ru
V. Sobol'
Department of computer systems and software technologies***
E-mail: napster_199@mail.ru
*Department of Materials Science
National Technical University "Kharkiv Polytechnic Institute"
Bagaliya str., 21, Kharkov, Ukraine, 61002
Department of Technology and Materials Research*
***Saint Petersburg State Polytechnic University
Polytechnique str., 29, St. Petersburg, Russian Federation, 195251

Для кількісної оцінки розвитку фізико-хімічних процесів на поверхні в роботі апробований комп'ютерний метод аналізу багатопорогових перетинів зображень поверхневого рельєфу з 3-х мірним поданням зображення оптичної мікроскопії (в якості третьої осі Z використовується шкала інтенсивності). Показано, що заміна повнопрофільного аналізу на аналіз періодичної системи перетинів уздовж осі інтенсивності дозволяє зробити досить простим визначення фрактальної розмірності складних рельєфів поверхні, сформованих в нерівноважних умовах

Ключові слова: комп'ютерний аналіз, метод багатопорогових перетинів, шкала інтенсивності, фрактальна розмірність, іонно-плазмові покриття, графен

Для количественной оценки развития физико-химических процессов на поверхности в работе апробирован компьютерный метод анализа многопороговых сечений изображений поверхностного рельефа с 3-х мерным представлением изображения оптической микроскопии (в качестве третей оси Z используется шкала интенсивности). Показано, что замена полнопрофильного анализа на анализ периодической системы сечений вдоль оси интенсивности позволяет сделать достаточно простым определение фрактальной размерности сложных рельефов поверхности, сформированных в неравновесных условиях

Ключевые слова: компьютерный анализ, метод многопороговых сечений, шкала интенсивности, фрактальная размерность, ионно-плазменные покрытия, графен

1. Introduction

The functional properties of a material are largely determined by the statement of its surface. Therefore, methods developed now, create a specific structural state of the surface layers as a result of the surface modification and bring into play the thin films and coatings with the desired properties.

These processes are carried out under non-equilibrium technological conditions, and as a result, the structural type of material layers formed on the surface has a fractal (non-integer) dimension [1, 2].

2. Literature review and problem statement

The suggestion about the primary (original) chaos of fractal structures appropriates for describing on the basis of the dynamics of chaos [3] to purpose the apply of mathematical approach for analysis.

Such method was used in the evaluation of the friction surfaces [4], the surface condition after EDM [5], the physical characteristics of surface coatings growth [6, 7].

Practical conclusions based on the correlation of fractal dimension with standard technical characteristics: hardness, friction factor, material consumption, the optimal porosity of the coating, and the like, were obtained as an expected result of associating the computer processing and the experimental data.

This led to the development of a new direction in the science of materials – fractal materials science. So the basis for a quantitative description of dissipative structures formed under conditions far from equilibrium [8, 9] is reached.

For example, the consideration of changes of the "activity" of the etching process in aggressive environment, due to the structure of the material (discussed in ranges "macro-", "micro-", "nano-"), should be compared with the diffusion processes in the reagent, the duration of the process and a lot of other parameters.

Recently, much attention has been paid to the verification of the initial stages of growth mechanisms of deposition under nonequilibrium conditions.

This is caused by the requirement to control the condition (structural engineering), which allows achieving high (in some cases, unique high) functional properties [10, 11].

The definition of a fractal surface roughness changing depending on the physical and technological parameters of the process will show as expected the results necessary for prediction of the stability and reproducibility of generated properties and structural states of materials.

Ion-plasma condensates of quasi-binary boride systems with high mechanical properties [10] relate to one of the most promising materials for coatings, as well as the coating based on graphene [12, 13].

Great interest shown currently to graphene as a functional material, is supported with a number of it's unique properties (electronic, optical, mechanical and others. [14]). A technology of graphene synthesis on the copper substrate is regarded as one of the most promising methods of obtaining large area graphene coating in a composite system [15] for practical use.

3. The aim and the tasks of the study

The aim of the work was testing the computer analysis method based on multithreshold sections of the surface topography image (using the 3-dimensional representation of the image of the optical microscope, where the intensity axis is applied as the scale of real profile) for the quantitative estimation of the progress of physical and chemical processes on the surface during the deposition of films and coatings.

To achieve the set goal, the following tasks are to be solved:

– define possibilities of using computer processing by the method of multithreshold cross sections for the analysis of optical images;

– define the laws of formation of fractal structures on the surface of the growth of ion-plasma condensates of quasi-binary borides using computer processing of optical images of the surface;

– using the method of multithreshold cross sections to hold the control of uniformity, the fractal dimension of the boundaries and continuity of the coating system "graphene – copper substrate".

4. Materials and methods of the study

Ion-plasma coating solid solution diboride as the state of decay TiB_2-WB_2 quasi-binary system [2] with the thickness of range 0.3...1.7 mm was obtained by magnetron sputtering in an argon atmosphere.

The samples of the system "graphene – copper substrate" contained graphene layers grown by the CVD method in a mixture of methane gas, hydrogen and argon on a substrate of copper foil (Alfa Aesar, thickness 25 microns) at temperatures up to 1000 °C. At this temperature methane from the gas phase moves to the surface, diffuses through the boundary layer, adsorbs on the surface of the catalyst, and after its decomposition, produces the atomic carbon which diffuses to the surface of copper. Processes which occur on the surface largely depend on the substrate temperature and on the feed rate of carbon to the surface. The pre-annealing of copper substrate is a necessary operation prior to synthesis. The polished copper substrate was annealed in an argon/hydrogen mixture to restore perfect orientation of the surface of the copper grain growth.

The following algorithm was used for processing of the different stages of optical microscopy monitoring: after the initial treatment (monochromatization, contrast alignment, noise reduction, etc.) the conversion of initial data to a series of binary images based on the "multithreshold" technology [16] took place. The number of intensity levels and their relative positions are set in advance. Then a group of binary images representing the difference between adjacent levels (steps) are created (Fig. 1).

Author`s program for processing is written in the C++ language in the form of serial processing. That includes the regions of interest definition as well as the thresholds for calculating Hausdorff dimension.

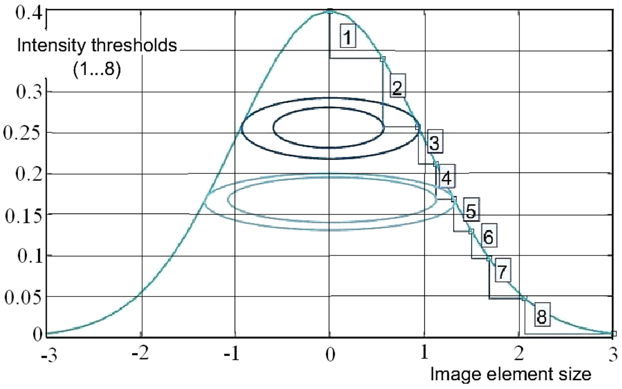


Fig. 1. Scheme of the formation of "intensity steps" on the selected picture element. 1...8 — the number of intensity levels when formatting a binary image.

Each of the "steps" is a fractal object much more simple for analysis compared to the "multifractal chaos". The standard technique for determining the Hausdorff dimension (Hausdorff-Besicovitch) applies for each step. A model [6], as proposed, compares the intensity of the image with the geometric height of the relief, and the idea, according to the Hausdorff dimension of stairs from the rapids, is to correlate this parameter and the geometry of the relief. The range of thresholds steps from 0 to 1, where "1" – corresponds to the maximum intensity of the image of the relief and the values of the thresholds are fractional numbers corresponding to the seven points of the sectional planes in the range of intensity scale [0, 1].

The “pixel size” directly related to the parameter “magnification” in the metallographic study is selected. Thus, the scaling is performed in assessing the applicability of fractal analysis.

5. The results of studies of the system TiB_2–WB_2 ion-plasma coating

The principal feature of the coatings – ion plasma condensates of the quasi-binary system TiB_2–WB_2, manufactured by magnetron sputtering in argon, consists in the appearance of the surface relief due to local peeling of the coating from the substrate. This phenomenon is caused by the relatively low adhesive bond between the growing coating and the surface region of substrate [17]. The stresses in the system “coating – substrate” due to the poor mechanical connection lead to flaking in places which can be determined in accordance with the theory of percolation when a strain energy dissipation [9].

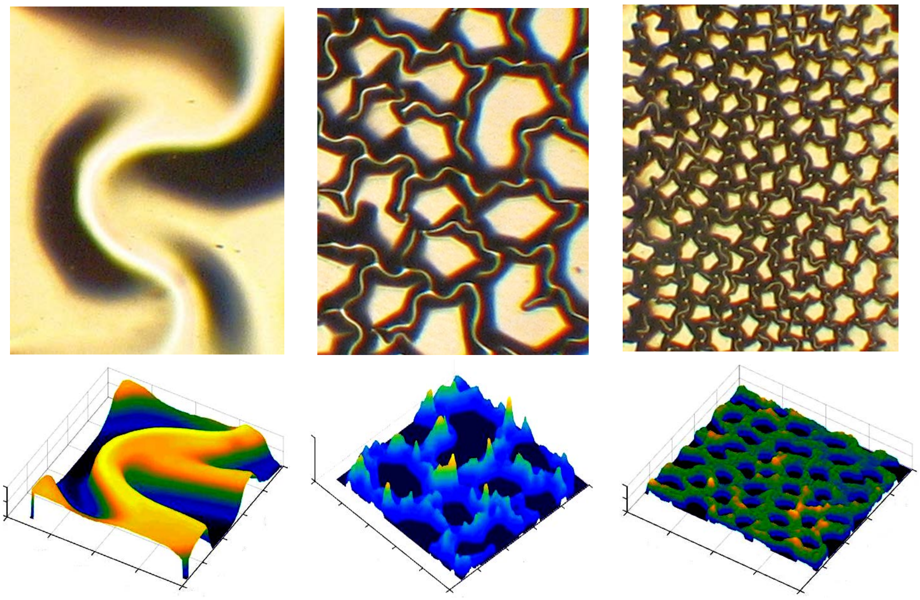
The formation of such structures occurs together with the decreasing processing temperature (starting with the deposition temperature from 500 °C to room level) and breaking vacuum conditions. The compressive stresses in the coating growth plane determine a convex shape of its elements (Fig. 2). The method of multithreshold sections allows in this case not only to define the dimension of heterogeneity but also to assess the level of the stress-strain state, which in turn determines the break between coverage and substrate and further formation of a 3-dimensional deformed structure as the result of self-organizational processes. Fig. 2 shows the three structure levels (in thickness) of these objects.

It’s visible that the high thickness of the coating (1.3 microns, Fig. 2, Series *a*) defines the formation of 3-dimensional structures with the largest cell size (about 20 microns) and with the highest fractal dimension of the contours (Fig. 3, curve 1). Reduction of the thickness of the coating to 0.7 microns (Fig. 2, Series *b*) results in the decrease of the average cell size to 10 microns; a coating thickness near 0.3 microns compared to the average cell size of about 3 microns.

As shown [18], the concentration of stresses near the interface of “coating – substrate” within a thin surface layer (80 microns) increases with decreasing thickness of the coating i. e. closer to the free surface of the sample. Thus, a decrease of the cell size by reducing the thickness may be associated with increasing levels of elastic stress-strain state in the coating.

As an addition to the general changes, a decrease in the results-tiered examination of fractal dimension (Fig. 3) with an increase in the stress-strain state was shown. The results of multilevel processing of intensity appeared the most informative for the highest thresholds levels (0.6 and higher).

The fractal dimension of the highest threshold slices in this system correlates with a radius of curvature of the dome-shaped places defined by deformation. As a result, the least deformed thick coatings (*a* – series) at a threshold of 0.6 demonstrate the Hausdorff dimension of 1.77; (*b* – series) with a greater deformation the dimension is 1.3, and for the thinnest and deformed coatings (*c* – series) the dimension is 1.2. It demonstrates much more at the threshold of 0.8: the results are 1.57, 1.15 and 1.04, respectively, for the (*a*), (*b*) and (*c*) series, (Fig. 2, 3).



a *b* *c*

Fig. 2. Selected images (magnification ×500), and their volumetric representation based on the intensity scale of optical microscopy of the TiB_2—WB_2 quasi-binary system coating, thickness: *a* — 1.3 microns; *b* — 0.7 microns; *c* — 0.3 microns

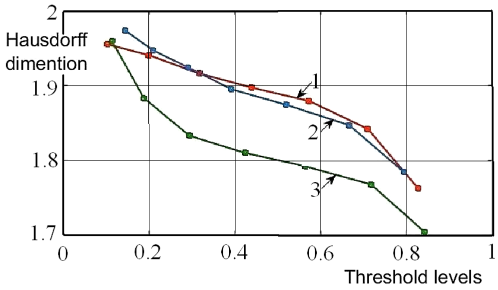


Fig. 3. The Hausdorff dimension of fragments selected as shown in Fig. 2.: 1 — series *a*; 2 — series *b*; 3 — series *c*

6. The results of studies of the systems “Graphene – copper substrate”

Colour changes of graphene domains should be taken into account during the rapid analysis based on data from optical microscopy systems “graphene – copper”, Fig. 4. This feature can become the basis for the analysis of “graphene multi-domain coating on copper substrate” system produced in the specific technological conditions. The idea of this method of analysis is the assumption on the optical properties of graphene layers [19, 20].

This gives reason to choose the colour as the primary characteristics of the image elements in the computer processing. In fact, the colour of domain relates to a copper substrate and varies depending on the coating elements, as it's observed by optical microscopy (Fig. 4). For the preliminary analysis, four variants of covering elements were selected. Every element could be selected interactively according to its colour. This choice is a local estimation of the relative "transparency" of graphene elements and based both on the reference data and the visual colour contrast of the image.

The proposed image processing method involves frequent confirmation of the free graphene layers property to change their transparency depending on the thickness and defects.

The range of thicknesses that are practically interesting (1…4 monolayers), the graphene coating should be as transparent as possible to observe the relief of the copper substrate within the analysis of images obtained through it. Furthermore, as shown in Fig. 4, graphene coating is not regular.

The colour has been chosen as the primary characteristic of the image elements at the processing. The following assumptions were made in the analysis of the images as the model ones. There are exactly four "options" of graphene coatings which determines the topography and different colours: (1) monolayers of graphene (mono- or diatomic thickness); (2) multilayer graphene domains; (3) areas of the amorphous carbon coating; (4) the free surface of the copper substrate (CuO_x layer).

Fig. 5 demonstrates the regular location of the selected fragments of colours in the RGB-color space (the axes of Fig. 5 show the intensity of each colour component in the RGB format).

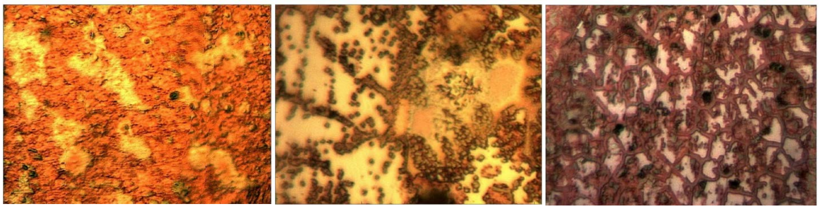
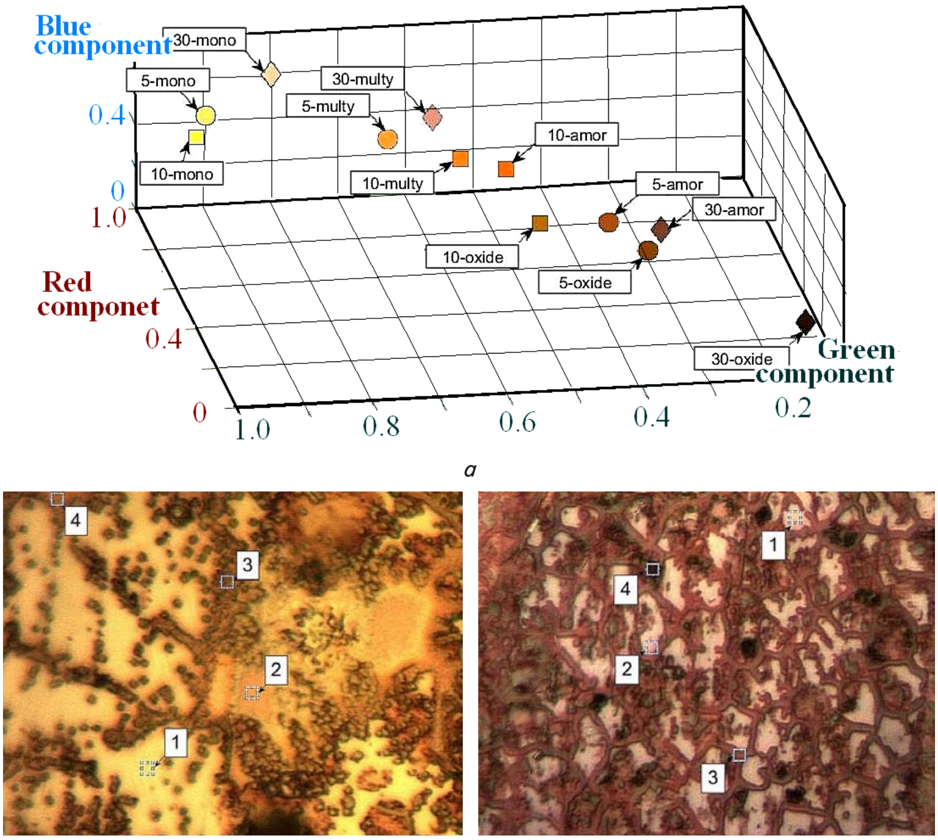

a *b* *c*

Fig. 4. Images of multi-domain graphene coating on copper substrate at the different synthesis conditions: *a* — 5 min; *b* — 10 min; *c* — 30 min (×800, size 1024×768, .*jpg)



a

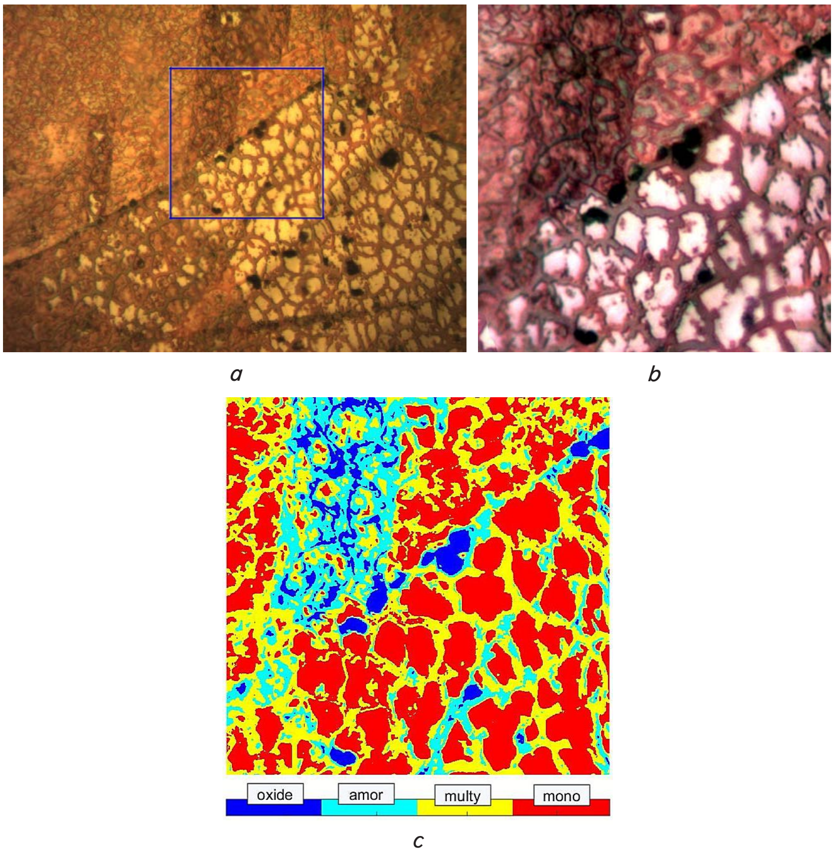
b *c*

Fig. 5. Colour selection of four supposed members of graphene coating: *a* — 3-dimensional representation; *b* — the picture of surface with the allocation of plots at coatings obtained at the technological deposition time for 10 min; *c* — deposition of 20 min (image regions of each type by interactive selection: 1 — monolayer graphene; 2 — multilayered graphene; 3 — amorphous carbon; 4 — copper oxide of substrate)

At the same time, the samples obtained at different process conditions (Fig. 4) show considerable variation. This does not add the certainty in the reliable identification of image elements.

More certain results are obtained when a selection of colours occurs in the Lab colour space use. One of the main properties of the Lab colour model is the independence from the device, in this way the interactive mode is eliminated and the process becomes more objective.

An example of a colour analysis of the optical image on the basis of assumptions about the four components of the graphene layer on a copper substrate made above is shown in Fig. 6. This technique makes the morphological analysis of the elements of each type available.



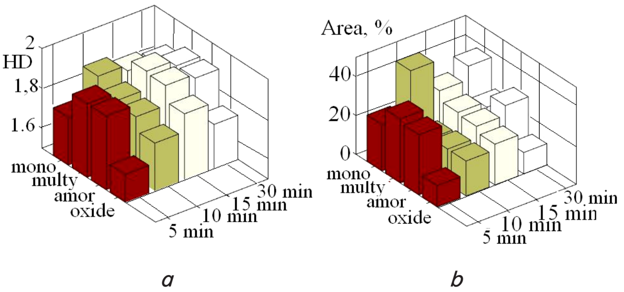
a *b* *c*

Fig. 6. Highlighted elements in the images in the model of the four components of the topography of the graphene coating on copper; *a* — selecting graphene area (technological parameters 800 °C, 10 min); *b* — an optical image; *c* — the selected items according to the assumptions made

The morphological characteristics (the area (A), the equivalent diameter (ED) and Hausdorff-Besikovitch dimension (HD)) were analyzed according to model and segmentation available.

The first of these options (area) represents the size of a single selected item, regardless of its form. The second (equivalent diameter) gives an estimate of the shape of the selected region by comparing it with the form of the equivalent circle. The third parameter (the Hausdorff-Besicovitch dimension) assesses the spreading of boundaries. Changes of this parameter from 1 to 2 gives the estimate of the dimension of the object: from the one-dimensional (line) to two-dimensional (plane).

The results of such processing are shown in Fig. 7. A comparison of the data is given in the relative form to be able to offer practical advice on the selection of optimal technology.



a *b*

Fig. 7. The four components of "graphene coating on a copper substrate" depending on the technological time of CVD process: *a* — variation of the Hausdorff dimension; *b* — the relative area

Synchronous analysis of each of the selected elements of the structure of graphene coating during its evolution makes it possible to propose a model of the growth mechanism of the graphene coating on copper.

7. Discussion of the results of work on the formation and development of the surface relief in the chemical-thermal process of carbon deposition on a copper substrate

Simultaneous and comparative analysis of each of the selected elements of the structure of the poligraphene coating during its evolution makes it possible to offer a consistent growth mechanism of graphene coating on copper. This mechanism clarifies put forward earlier assumptions about the growth kinetics of poly-graphene coatings based on optical microscopy data.

The mechanism (4Colours) proposed takes into account mentioned previously discussed and assumptions about the growth kinetics of poly-graphene coverage, but try to rearrange it based on their own observations by means of optical microscopy.

The change in the number of layers of graphene in the areas of multi graphene domains takes place with increasing thickness of the coating under conditions of increasing the exposure time of the process. 4C – the mechanism is based on a real assumption that the roughness of the substrate has a "double scale": the size of the regions plane (111) Cu (and possibly other crystallographically perfect) and typical block sizes of polycrystalline copper. That is defined as "micro" and "nano" or if otherwise formulated scale: "micro" and "sub micro."

Scheme covering as proposed underlying 4C – the mechanism is presented in Fig. 8.

According to the 4C proposition, the formation places of amorphous graphene islands (Fig. 8) are determined by surfactants defects in the substrate. The number and activity of these centers are quite expectedly affected the previous chemical and thermal processing. The following formation of the graphene layer begins in the case of "acceptable" conditions stimulating the growth of graphene, particularly if the orientation of the substrate was coherent (Fig. 8). Spreading of mono- or multi graphene cover (domain) is controlled by diffusion of carbon atoms at the domain perimeter.

Domain delivered in this way can move in front of their growth layer of amorphous carbon formed on its perimeter randomly. When this layer reaches a critical size, domain growth in the plane is hindered in the local area of the perimeter. Given the increase in the plane domain over a certain size or in preventing migration of impurity atoms on the perimeter of the domain, carbon atoms begin the formation of an additional layer of graphene (multi-graphfene). Such layer is formed on the previous boundaries of the domain that stay in contact with the amorphous carbon. The surface of the graphene is no doubt about the optimum crystallographic orientation.

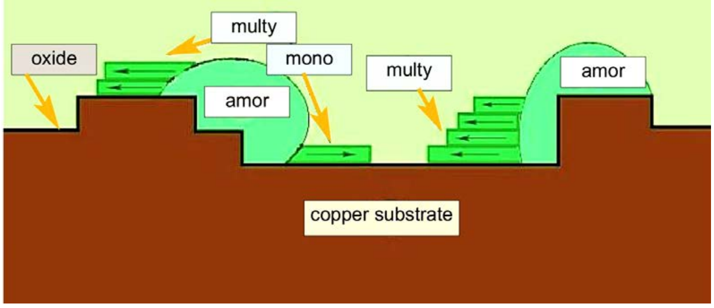


Fig. 8. The scheme of the mechanism of formation and evolution of graphene coating relief as 4C — mechanism represent

8. Conclusions

1. The multithreshold method of image analysis proposed and applied in the present study is based on an assessment of the fractal dimension of relief elements rather than the entire surface “as a whole”, which makes the processing procedure effective in the images of any origin (not only optical microscopy data, but also scanning electron microscopy).

2. The development of the relief of the coatings obtained by magnetron sputtering is determined by the orderly separation under the action of compressive stresses. The coating thickness increases, the average size of the “cells”, formed as a consequence of the self-organized ordering, increases too. The fractal dimension of the “cells” in the intensity sections of higher threshold value reduces (the transition from two-dimensional to one-dimensional scale) as a result of the thickness decrease and the compression stress increase.

3. The proposed method of analysis of the colour optical image is based on the assumption that the four components of the graphene layer on a copper substrate allow realizing the morphological analysis of the elements of each type. Simultaneous analysis of each selected type of elements of the graphene coating during its evolution makes it possible to construct a physical model of the formation of a graphene coating in practical technology.

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ANALYSIS OF BEHAVIOR OF SOLUTIONS' SUPPORT FOR NONLINEAR PARTIAL EQUATIONS

K. Stiepanova
PhD, Lecturer
Department of Higher Mathematics, Economic and Mathematical Methods
Simon Kuznets Kharkiv National University of Economics
Nauky ave., 9-a, Kharkiv, Ukraine, 61166
E-mail: stepanova.ekaterina@hneu.net

Розглядається початкова задача про розподіл температури на нескінченності для напівлінійного параболічного рівняння другого порядку, що містить член поглинання. Проводиться аналіз поведінки носія розв'язку задачі Коші для зазначеного вище диференціального рівняння в частинних похідних. Доведено, що при певних умовах на параметри задачі спостерігається стиснення носія

Ключові слова: розв'язок, задача Коші, диференціальне рівняння в частинних похідних, носій

Рассматривается начальная задача о распределении температуры на бесконечности для полулинейного параболического уравнения второго порядка, которое содержит член поглощения. Проводится анализ поведения носителя решения задачи Коши для указанного выше дифференциального уравнения в частных производных. Доказано, что при определенных условиях на параметры задачи наблюдается сжатие носителя

Ключевые слова: решение, задача Коши, дифференциальное уравнение в частных производных, носитель

1. Introduction

Partial differential equations of the second order of parabolic type are more common in the study of processes of heat conduction and diffusion. As you know, the process of heat distribution in space can be fully described by temperature u(x, t), where $x\in\mathbb{R}^n$. If the temperature is not constant, then there are heat flows which are directed from places with higher temperature to places with the lowest temperature. We consider thermal processes in a fairly large range of temperature changes, leading to quasi-linear heat equations. So let's write divergent parabolic equations in general form:

$$u_t = \operatorname{div}\left(k\left(u,u_x\right)\nabla u\right)+F\left(x,t\right),$$

where

$$\operatorname{div} A\left(x\right)=\sum_{i=1}^{n}\frac{\partial A_i}{\partial x_i}$$

for

$$A\left(x\right)=\left(A_1\left(x\right),\ldots,A_n\left(x\right)\right);$$

$k\left(u,u_x\right)$ – the coefficient of the thermal diffusivity;

$$\nabla u=\operatorname{grad} u=\frac{\partial u}{\partial x_1\ldots\partial x_n};$$

$F\left(x,t\right)$ – the density of the heat sources (flows).