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HOMOGENEITY ESTIMATION MORPHOMETRIC MODEL FOR PARTICLE DISTRIBUTION ON EXAMPLE OF SiC DEPOSITED ON MULTILAYER STRUCTURE Fe/NiP

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The theoretical justification of the distribution for particles/defects homogeneity estimation criterion was done. The mathematical model was created on this basis and its object-oriented implementation was realized. It is shown that the use of object-oriented programming allows getting a sufficient clearness and simplicity of an object's general mathematical model, displaying in it as the object properties so and methods by which the model can operate. Adequacy of the proposed model and research method was verified experimentally on samples of silicon carbide SiC deposited on the multilayer structure of Fe/NiP.

Key words: homogeneity, morphometric analysis, morphometric parameters, object-oriented programming.

Здійснено теоретичне обґрунтування критерію для оцінки гомогенності розподілу часток/дефектів. На його основі створена математична модель і побудована її об'єктно-орієнтована реалізація. Показано, що використання об'єктно-орієнтованого програмування дозволяє з достатньою наочністю і простотою створити загальну математичну модель об'єкта, відобразивши в ній як властивості самого об'єкта, так і методи, якими він може оперувати. Адекватність запропонованої моделі та методу дослідження була перевірена експериментально на зразках карбіду кремнію SiC депонованого на багатошарову структуру Fe/NiP.

Ключові слова: гомогенність, морфометричний аналіз, морфопараметри, об'єктно-орієнтоване програмування.

Осуществлено теоретическое обоснование критерия для оценки гомогенности распределения частиц/дефектов. На его основе создана математическая модель и построена ее объектно-ориентированная реализация. Показано, что использование объектно-ориентированного программирования разрешает с достаточной наглядностью и простотой создать общую математическую модель объекта, отобразив в ней как свойства самого объекта, так и методы, которыми он может оперировать. Адекватность предложенной модели и метода исследования была проверена экспериментально на образцах карбида кремния SiC депонированного на многослойную структуру Fe/NiP.

Ключевые слова: гомогенность, морфометрический анализ, морфопараметры, объектно-ориентированное программирование.

INTRODUCTION

Semiconductor and composite materials deposition new technologies development, including nano- and micro- dimensional in-homogeneities, requires the development of modern research methods and models that provide detailed information about the homogeneity of particles/defects (P/D) distribution and other characteristics of their shape. It is convenient to use the morphometric approach to build such models. It is a proven instrument for study of objects' shapes in different fields of the science [1-3]. Modern research tools should have high spatial resolution, and must be nondestructive and noncontact. As an example, we can take a digital optical microscopy (DOM). DOM development caused the appearance of various image analysis methods and dedicated digital microscopes nowadays.

CONCEPTUAL PRINCIPLES AND METHOD

The development of the shape estimation and homogeneity of distribution of particles/defects rating criteria is one of important question that arises in the study of semiconductors and composite materials. It allows to rate the quality of materials and compare their actual parameters with expected. Table 1 shows the number of morphometric parameters [4]. They can be used in mathematical models of P/D homogeneity distribution estimation developments.

Let's make a detailed investigation of some of them, which we think could make comprehensive estimation of the form P/D – namely, numbers 3, 4, 5, 7, 8, 9, 11 (tabl. 1):

Table 1

1	P/D X,Y Coordinates	9	P/D Convexity
2	P/D Length, Width	10	P/D Convexity Area
3	P/D Perimeter	11	P/D Elongation
4	P/D Area	12	P/D Elongation Main Axes
5	P/D Gravity Center Coordinates	13	P/D Convexity Perimeter
6	P/D Inscribed and Circumscribed Circle	14	P/D Convexity Compactness
7	P/D Roundness	15	P/D Angle of Elongation Axes
8	P/D Compactness	16	P/D Additional Elongation Axes

– perimeter (P) [5]:

$$P=\sum_{i=1}^{n} d_i=\sqrt{(x_n-x_1)^2+(y_n-y_1)^2}+$$

$$+\sum_{i=1}^{n-1}\sqrt{(x_{i+1}-x_i)^2+(y_{i+1}-y_i)^2}\ ; \quad (1)$$

where n – quantities of polygon vertices.

– area (S) – polygon area – which is closed line without cross-self sections, given its vertices in order to bypass [5] and calculated by formula:

$$S=\frac{1}{2}\left|\sum_{i=1}^{n-1}(x_i+x_{i+1})(y_i-y_{i+1})\right|. \quad (2)$$

– center mass coordinates of a plane figure [5]:

$$\begin{cases} x_c=\dfrac{\sum_i\left(\dfrac{x_{i+1}-x_i}{2\cdot(x_{i+1}\cdot y_i-x_i\cdot y_{i+1})}\right)}{1{,}5\cdot\sum_{i=1}(x_{i+1}\cdot y_i-x_i\cdot y_{i+1})} \\ y_c=\dfrac{\sum_i\left(\dfrac{y_{i+1}-y_i}{2\cdot(x_{i+1}\cdot y_i-x_i\cdot y_{i+1})}\right)}{1{,}5\cdot\sum_{i=1}(x_{i+1}\cdot y_i-x_i\cdot y_{i+1})} \end{cases}. \quad (3)$$

– roundness (M_1) – defined as the ratio of inner circle radius of the particle to its outer circle radius (fig. 1a) [4]:

$$M_1=\frac{R_{\min}}{R_{\max}}, \quad (4)$$

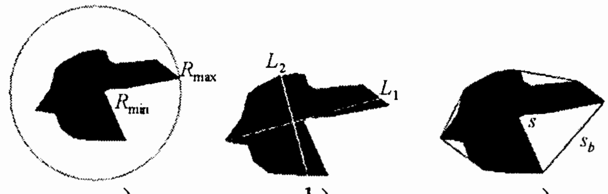

Fig. 1. a) – Roundness, b) – Elongation, c) – Convexity.

where, R_{min} – inscribed circle radius with center in gravity center, R_{max} – circumscribed circle radius with center in gravity center (fig. 1a).

In case $R_{min} << R_{max}$, we have $M_1 \to 0$. If $R_{min} \approx R_{max}$, then $M_1 \to 1$.

– compactness (M_2) – defined as ratio of area to its perimeter [4]:

$$M_2=\frac{4\cdot\pi\cdot S}{P^2}, \quad (5)$$

where, P – perimeter, S – area.

In case of huge P/D shape non-uniformity, P significantly increases at virtually constant S and respectively $M_2 \to 0$. When P/D shape is uniform, it is a circle, where $S=\pi R^2$ and $P=2\pi R$. Substituting these values in formula (6), we obtain $M_2=1$.

– elongation (M_3) – defined as the ratio between the length perpendicular to the P/D main axis (L_2) and length of the P/D main axis (L_1) (fig. 1b). The main axis is defined as the longest axis through the center of P/D gravity:

$$M_3=L_2/L_1. \quad (6)$$

If $L_2 << L_1$, then $M_3 \to 0$. If $L_2 \approx L_1$, then $M_3 \to 1$.

– convexity (M_4) calculated as the ratio between the P/D area S and convex body area S_b. An example of convex body can be stretched "rubber band" around the particle defect (fig. 1c):

$$M_4=S/S_b. \quad (7)$$

If $S << S_b$, then $M_4 \to 0$. If $S_b \approx S$, then $M_4 \to 1$. We use M_1, M_2, M_3, M_4 morphoparameters to analyze the P/D form as partial criterions, the rest – in other calculations of the samples' characteristics. As shown in 4 – 7, the values M_1, M_2, M_3, M_4 have the range from zero to one. If they tend to zero, the irregularity of P/D form is significant. With the approach to the one, shape form is close to the circle.

By grouping of M_1, M_2, M_3, M_4 we get a criterion for estimation of the P/D shape of semiconductor and composite materials non-uniformity, describing thus:

- total P/D form shape non-uniformity, the dynamics and magnitude of their changes based on the parameter M_1;
- detailed characteristic of the P/D compactness based on the parameter M_2;
- P/D elongation and their spatial orientation based on the parameter M_3;
- dynamics and the value of changing the shape as the ratio of peaks and gaps of P/D shape based on M_4.

Let's formulate a complex morphometric P/D shape evaluation criteria as follows:

$$F = \begin{pmatrix} M_1 \\ M_2 \\ M_3 \\ M_4 \end{pmatrix} \Rightarrow 1, \quad M_1, M_2, M_3, M_4 \in [0, 1]. \quad (8)$$

Calculated value of criterion F (8) is a vector that consists of four elements. If the value $F^T = (0, 0, 0, 0)$, that is corresponding to big non-uniform shape of P/D, while $F^T = (1, 1, 1, 1)$ shows that the shape is close to the circle.

Criteria of P/D shape irregularity (8) M_1 mostly decreases in response to the increasing size of peaks or failures form, M_2 – in response to increased local extreme form, M_3 – in response to overlapping symmetric peaks/gaps form, M_4 – in response to increasing of minor fluctuations or significant values changes. Thus we can flexibly define the limits to which the heading one or another component of the criterion according to the task (8). This enables to clearly define goals of leveling and implement adequate assessment:

$$F = \begin{cases} M_1 \to a_1 \\ M_2 \to a_2 \\ M_3 \to a_3 \\ M_4 \to a_4 \end{cases}, \quad M_1, M_2, M_3, M_4 \in [0, 1], \quad (9)$$

Where a_1, a_2, a_3, a_4 – values of partial limits for each component criterion F, $a_1, a_2, a_3, a_4 \in [0, 1]$.

Let's determine the plane figure's center of mass offset (3) $x_c; y_c$ relative to its geometric center $x_0; y_0$ by using binary image which was obtained by modern recording digital data tools. Homogeneity decreases with the offset increasing, i.e., homogeneity evaluation criteria can be represented as follows:

$$d = 1 - \sqrt{\frac{(x_c - x_0)^2 + (y_c - y_0)^2}{(x_{\max} - x_0)^2 + (y_{\max} - y_0)^2}}, \quad (10)$$

where $x_{\max}$; $y_{\max}$ – coordinates of the most distant point from the geometric center; x_c; y_c calculate according to the formula which defines the center mass of a plane figure:

$$x_c = \frac{\sum_{i=1}^{n} m_i x_i}{\sum_{i=1}^{n} m_i}; \; y_c = \frac{\sum_{i=1}^{n} m_i y_i}{\sum_{i=1}^{n} m_i}, \quad (11)$$

where x_i; y_i – points' coordinates, m_i – points' masses, n – points quantity.

As it is seen from the equation (10), the parameter d has ranges $0 \le d \le 1$. Thus, for an ideal homogeneous distribution of P/D evaluation criterion takes the value of homogeneity $d = 1$. In the case of high non-homogenous distribution $P/D - d \to 0$.

For calculations based on (10) and (11) let's present the binary image in the form of a plane figure which is consisting of individual points with a mass $m_i = 1$ at the points corresponding to the P/D and with a mass $m_i = 0$ of points not included P/D.

To improve the adequacy of the results for each sample, we need to increase measurements quantities of homogeneity m and calculate the average homogeneity and standard deviation for a series of experiments:

$$\bar{d} = \frac{\sum_{j=1}^{m} d_j}{m}, \quad \delta = \pm\sqrt{\frac{1}{m}\left(\sum_{j=1}^{m}\left(d_i - \bar{d}\right)\right)^2}. \quad (12)$$

Based on formulas (8), (9) and (10) we create a morphometric mathematical model of P/D form non-uniformity and homogeneity of their distribution in the semiconductor and composite materials and its object-oriented implementation, which allows realizing a detailed form evaluation and can be easily integrated into modern production systems.

The more detailed object description gives the higher degree of correspondence between him and his mathematical model. So there is need for describing and processing a large number of parameters and models communications that they influence on each other as well as the parameters and models relationships of other objects, because the object does not exist separate from the others.

Digital optical system for the analysis of P/D distribution homogeneity of semiconductor and composite materials is a complex subject. It is complex to construct model and implementation by using methods of linear or block (structural) programming. It is needed to do a lot of descriptive work, but formalized information will not properly classified, which greatly complicates further calculations which is associated with these parameters.

It is much easier to create the model based on object-oriented programming (OOP) [6 – 8]. It allows generating mathematical model of the object with sufficient clearness and simplicity, displaying the object properties as well as methods which can be operated. OOP properties allow using efficiently for systems simulation of *P*/*D* distribution homogeneity evaluation (HE) for semiconductor and composite materials.

Thus, based on the above, we should use the concept of simple technology to build mathematical models based on the OOP principles.

Fig. 2 shows an appropriate object-oriented morphometric model of *P*/*D* distribution homogeneity evaluation for semiconductor and composite

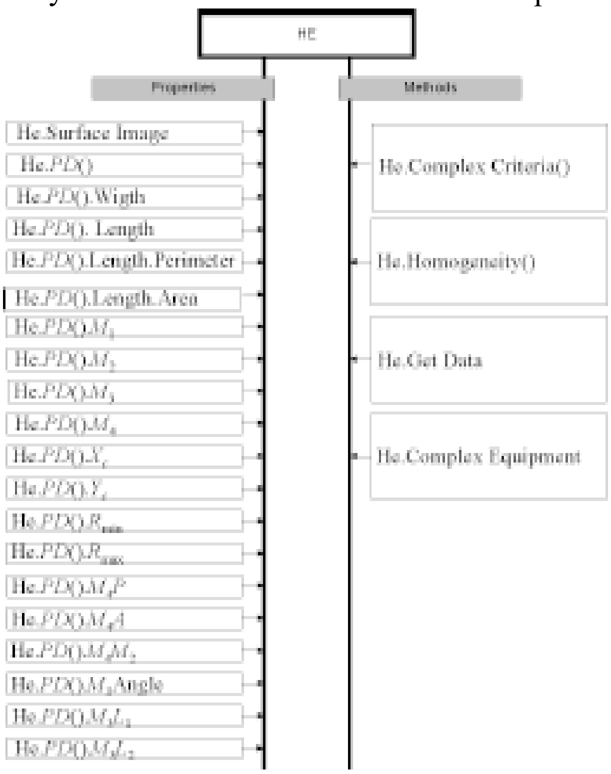

Fig. 2. Object-oriented morphometric model of P/D distribution homogeneity evaluation for semiconductor and composite materials.

Tabl. 2 presents a detailed description of properties and methods of HE class.

Based on the proposed HE model we built a digital optical-mechanical system for P/D distribution homogeneity analysis of semiconductor and composite materials.

Table 2

Name	Description
HE.SurfaceImage	Surface image
HE.PD()	The set of identified particles/defects
HE.PD().Width	The particle width
HE.PD().Length	The particle length
HE.PD().Length.Perimeter	The particle perimeter
HE.PD().Length.Area	The particle area
HE.PD().M_1	The particle roundness
HE.PD().M_2	The particle compactness
HE.PD().M_3	The particle elongation
HE.PD().M_4	The particle convexity
HE.PD().X_c	Gravity center (*X* coordinate)
HE.PD().Y_c	Gravity center (*Y* coordinate)
HE.PD().R_{min}	Inscribed circle radius
HE.PD().R_{max}	Circumscribed circle radius
HE.PD().M_4P	Convexity perimeter
HE.PD().M_4A	Convexity area
HE.PD().M_4M_2	Compactness convexity
HE.PD().M_3Angle	Rotation angle of elongation axes
HE.PD().M_3L_1	Main elongation axis
HE.PD().M_3L_2	Additional elongation axis
HE.ComplexCriteria()	The particle form evaluation (8)
HE.Homogeneity()	Material homogeneity evaluation (12)
HE.GetData	Getting information about surface
HE.ControlEquipment	The control parameters of optical-mechanical system

EXPERIMENTAL RESULTS AND DISCUSSION

We made a study of *P*/*D* distribution homogeneity for SiC particles deposited on the multilayer Fe/NiP structure for practical constructed model's adequacy confirmation.

Studies were conducted on the digital optical video microscope – IntScope [9] at 100× optical zoom with coaxial metal – halide light source. Typical images of the surface were selected for the analysis (fig. 3a) and made their binary equivalents (fig. 3b).

The analysis of SiC particles distribution homogeneity and the detailed form calculations were done for the deposited silicon carbide SiC on the base of offered mathematical model. Calculations

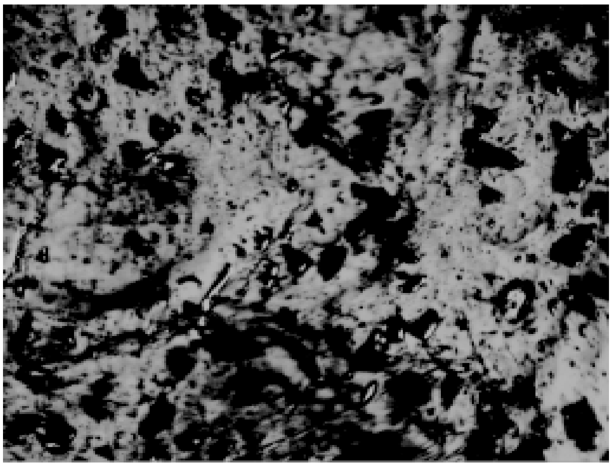

Fig. 3a. Sample image (100× magnification).

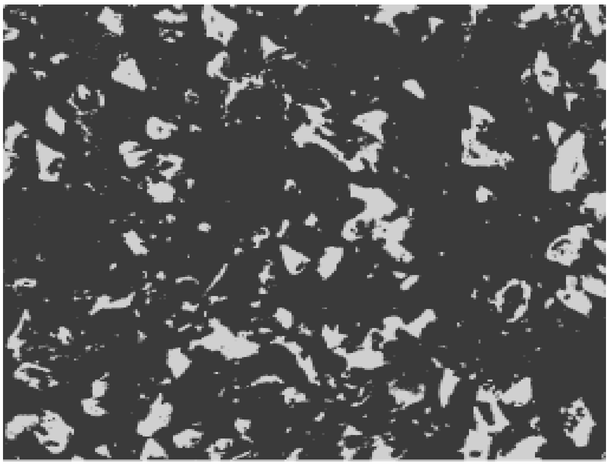

Fig. 3b. Binary equivalent of the sample image.

show that for the studied samples $\bar{d}$= 0.98. This testifies that the distribution of SiC particles deposited on multilayer structure of Fe/NiP is close to homogeneous.

Fig. 4 shows particles distribution charts based on elongation (fig. 4a) and the compactness (fig. 4b). Profiles analysis of the particle distribution has showed their approximation to the hyperbolic form and allowed to get series of results:

- Area of most of particles varies 0,5 – 2,5 мм^2
- Analysis of the area distribution shows that the number of particles with small size is much higher.
- Analysis of the elongation distribution shows that most particles of silicon carbide SiC elongated with
- ratio S between the main and additional axis of elongation.
- Analysis of the compactness distribution shows that the number of round particles is smaller. Existing peak of particles quantity in the range 0,3 – 0,7 indicates that most SiC particles have a complex form.

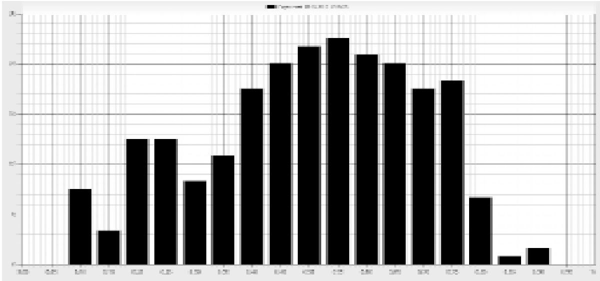

Fig. 4a. Silicon Carbide SiC particles quantity distribution by elongation.

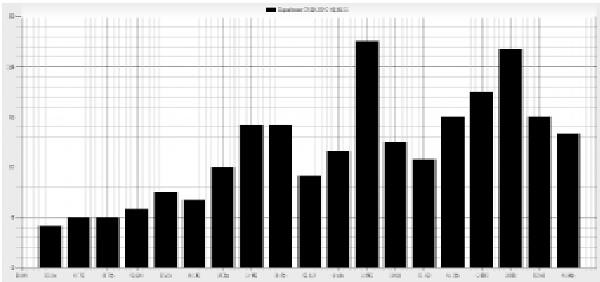

Fig. 4b. Silicon Carbide SiC particles quantity distribution by compactness.

CONCLUSIONS

Morphometric parameters showed the new ways of materials *P*/*D* form characteristics analysis. They describe shape, reflecting a common non-uniform shape as well as the relationship between different characteristics on the different stage of investigation. Based on their analysis we can conclude that the detailed computerized evaluation of *P*/*D* distribution homogeneity and shape non-uniformity is advisable to do by use of morphometric parameters.

1. Morphometric parameters are a convenient tool to evaluate *P/D* distribution, which allows constructing informative computerized assessment tools of quality estimation for semiconductor and composite materials and, consequently, improving the production process.
2. The proposed criterion for assessing the *P*/*D* distribution homogeneity of various materials allows estimating their distribution including spatial displacement and the mass of different components (optional) that enables characterization of the complex multicomponent composite materials in details.
3. Developed morphometric object-oriented model of *P*/*D* distribution homogeneity of semiconductor and composite materials evaluation that includes information about the object of investigation, the criteria for assessing and managing the installation allows to create a software package based on new technologies and integrate it into the management system.

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