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Investigation of the Properties of Powder Materials Using Computer Modeling

Viktoriya PASTERNAK[1,a*], Lyudmila SAMCHUK[1,b], Nataliia HULIIEVA[1,c], Igor ANDRUSHCHAK[1,d] and Artem RUBAN[2,e]

[1]Lutsk National Technical University, 75, Lvivska str., Lutsk, Ukraine, 43018

[2]National University of Civil Defence of Ukraine, 94 Chernishevska str., Kharkiv 61023, Ukraine

[a]Shyberko@ukr.net, [b]samchuk@gmail.com, [c]huliieva@lntu.edu.ua, [d]9000@lntu.edu.ua, [e]ruban_artem1979@ukr.net

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Abstract. Granulometric characteristics of structurally inhomogeneous materials based on full-scale mounds of a powder mixture of different fractional composition are established. Regularities of backfilling of powder particles of different shapes and sizes are revealed, and changes in the polydispersity of powder particles within each fraction are justified. It is proved that with a decrease in the average particle size of structurally inhomogeneous $AlCu_2$ materials in a single fraction, the size spread relative to this value of other particles increases. The results of calculating the porosity of backfills with particles of various shapes (round, triangular, and square) depending on the cross-sectional area of the lobules are presented. A three-dimensional diagram is constructed that shows the relationships between the fractional composition of powder particles, their average diameter, and the degree of inhomogeneity of homogeneous bronze $AlCu_2$.

Introduction

At the present stage of development of Mechanical Engineering Technology in a new and effective direction to expand the functionality of existing and create new approaches to the study of powder and heterogeneous materials, more and more attention is being paid to technologies for manufacturing structurally heterogeneous materials based on modern computer software [1, 2, 3]. Powder materials include a number of properties that need to be controlled in the process of manufacturing structurally heterogeneous materials, which include pressing density, quality and relationship of contacts with each other, grain sizes (particles), component content, shape and size of powders, etc [4, 5, 6]. Such structures are relevant for use in various branches of technology, in particular aircraft construction, mechanical engineering, materials science, which require the manufacture of products with increased operational properties at minimal financial costs, as well as reducing the cost of finished products [7]. At the same time, it is necessary to obtain all structural characteristics and properties at a qualitative level. To achieve the desired effect, you can use additive and traditional technologies for manufacturing powder materials, which allow you to form and manufacture products of complex configuration in a minimum period, introduce waste-free production of products for a wide purpose, save energy and materials, and reduce labour costs by reducing the number of technological operations [8, 9, 10]. As well, as apply the latest technologies and approaches that allow us to move from specific observation and statement of facts to predicting various properties of structurally heterogeneous materials, products, and processes using computer and information technologies [11, 12]. It should be noted that such products in most cases do not need finishing machining, which significantly reduces the cost of the finished product. However, a number of methods for studying powder metallurgy are evaluated ambiguously [13, 14]. On the one hand, in the manufacture of structural parts, it somewhat loses its position due to the significant energy intensity of obtaining raw materials and powders [15]. On the other hand, in the manufacture of products with unique properties, its role increases significantly and in many cases leads to heterogeneity of properties within materials, and does not make it possible to obtain structural characteristics at a qualitative level [16]. Therefore, when obtaining new structurally inhomogeneous materials with guaranteed properties, it is advisable to conduct experimental studies in the field of screen and granulometric analysis, which will allow us to estimate the distribution of particles of structurally inhomogeneous materials in size and shape (round, triangular, square), determine the fate of the dominant powder particle in each fraction, and also pay more attention to the porosity of the backfill of structurally inhomogeneous materials. Thus, the study of the properties of powder materials using computer modelling is an urgent task of materials science. It should be noted that the results obtained in these studies are phenomenological in nature and therefore require study that is more detailed.

Main Part

To determine the granulometric composition of structurally inhomogeneous materials, sieve analysis was used [17, 18], which consists in sifting materials after grinding through a set of standard sieves (Fig. 1) with holes of different sizes. This made it possible to select particles of structurally inhomogeneous materials for backfilling (Fig. 2, 3), the dimensions of which were justified by calculations in order to achieve such porosity of structurally inhomogeneous materials that would ensure optimal operability of the elements of plain bearing bushings. It should be noted that the sieves are installed on top of each other in descending order of the size of the sieves holes, from top to bottom. A certain amount of powder is placed on the top sieve and then the entire set of sieves is shaken on the Rotap device or manually for 10...15 minutes. There is a division into fractions that linger on sieves with grids of certain sizes. After separation, the fractions are weighed on each sieve and on the bottom (Fig. 1).

Fig. 1. A series of sieves with different hole sizes and weighing weights of structurally inhomogeneous materials

Fig. 2. Full-scale powder bulk materials for forming structurally inhomogeneous materials (aluminum, d = 0,15-0,2 mm, P = 25%)

Fig. 3. Full-scale powder bulk materials for forming structurally inhomogeneous materials (copper, d = 045-0,63 mm, P = 20%)

The mass of this fraction is attributed to the sum of the masses of all fractions and multiplied by 100, which is the percentage of this fraction in the sample (%) [19, 20]:

$$A = \frac{a_1 \times 100}{a_1 + a_2 + a_3 + \ldots + a_n} (mcm) \tag{1}$$

Where a_1, a_2, a_3, a_n – fraction masses.

To determine the granulometric composition of powders, the standard scale of grids with square holes is adopted according to GOST 3584-53 [21, 22]. The screen number corresponds to the nominal size of the hole in millimetres [23, 24]. The results of the sieve analysis were calculated using the above formula (1) [25]. The powder fraction remaining on the sieve reaches 0,061 mm, in turn, it passed through a larger sieve of 0,080 mm, after which the fraction was obtained: 0,080 + 0,061. The average particle size of each fraction *d* was plotted along the abscissa axis of the graph (Fig. 4), which was defined as the arithmetic mean size of the holes of the positive and negative sieves. For example, in this case, the average particle size of the fraction is: 0,080 + 0,063 (mm), so we get:

$$d_{sr} = \frac{80+63}{2} = 72mcm$$

The content of fractions was plotted along the ordinate axis of the distribution graph (Fig. 4).

Table 1 shows the results of sieve analysis of homogeneous bronze, which showed that typical bulk structures of structurally inhomogeneous $AlCu_2$ materials allow us to judge the degree of their inhomogeneity and, accordingly, porosity.

Table 1. Results of sieve analysis $AlCu_2$

Sieve mesh hole size (mm)	Fraction content (%)	Average particle size (microns)
0,071	17.3	>71
0,063	15.6	67
0,056	18	59.5
0,05	19.6	53
0,045	13.8	47.5
Balance	15.7	<45
Sum	100	

The density of materials was studied by the pycnometric method, which made it possible to assess the effect of particles of different sizes and shapes on obtaining a uniform structure of bronze after its pressing and sintering. An exhaustive description of the granulometric composition of the initial components of the powder can be obtained from the experimentally established dependence (Fig. 4). This graphic representation of the granulometric composition of the powder of structurally inhomogeneous materials makes it possible to estimate the change in dispersion, the degree of grinding-the ratio of the average grain size of the starting material $AlCu_2$ to the average particle size of the crushed product, as well as specific energy costs. They also found that the degree of inhomogeneity (polydispersity) of structurally inhomogeneous $AlCu_2$ powder materials mainly depends on two parameters: 1) the average size of the dominant particles in a certain fraction; 2) standard deviation of $AlCu_2$ powder particle sizes from their average size. Thus, these results should be determined by constructing a Gaussian Curve based on a histogram of the distribution of particles of raw materials in a certain fraction (Fig. 4).

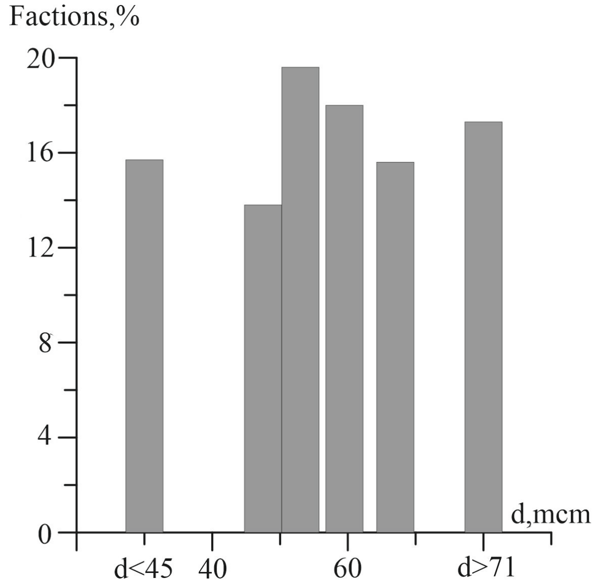

Fig. 4. Graphic representation of the granulometric composition of the powder $AlCu_2$

After that, we analysed the effect of the area of particles of different shapes on the porosity of the SNM when filling in a square Hopper with a stable cross-section $S_b = 100cm^2$. The results of the analysis are shown in Fig. 5. In this case, the areas (*S*) of the lobules had the following values: $S_1 = 1cm^2$; $S_2 = 1mm^2$; $S_3 = 1mcm^2$. From the results obtained, it can be seen that due to the triangular shape of the particles, the porosity of the sample is the least sensitive to their area, and the most sensitive is in the case of square particles. Backfills with round particles have the highest porosity, compared to other forms of particles, with the same area.

Fig. 6 presents the results of calculating the porosity of hopper backfills with an area of $100cm^2$ by particles of various shapes (round, triangular and square) depending on the cross-sectional area of the *S* lobules.

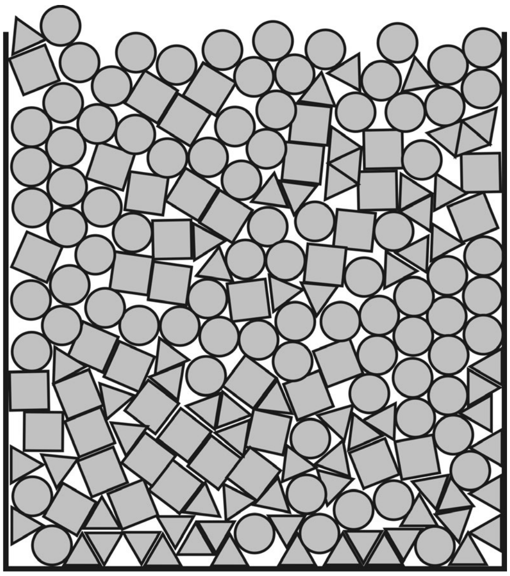

Fig. 5. Model powder backfill with particles of various shapes (round, triangular and square)

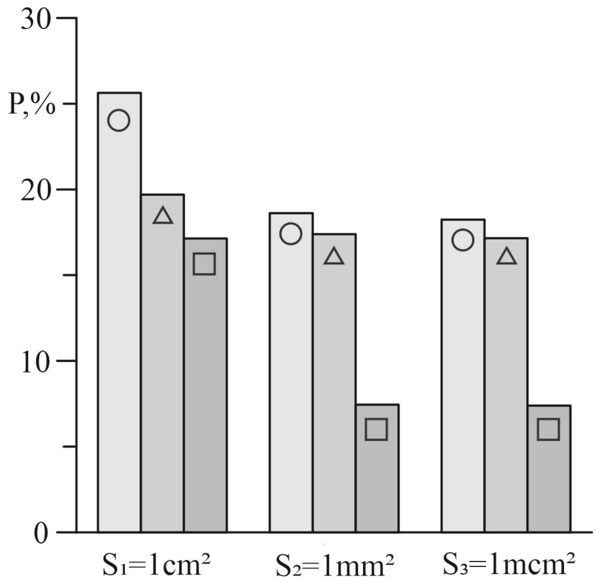

Fig. 6. Porosity dependence on the area of a square hopper

The results obtained confirm the good consistency of the porosity values determined using the Smart-eye application on experimental samples with those shown in Fig. 5, 6 based on the results of numerical calculations. The relative deviation did not exceed 7 %, which indicates the adequacy of the conducted studies and the reliability of the results obtained using them.

To obtain a more detailed description of the study of the properties of powder materials using computer modelling, we interpreted the results obtained based on the analysis of a three-dimensional diagram of a qualitative assessment of the granulometric characteristics of homogeneous bronze (Fig. 7). The three-dimensional diagrams shown illustrate the relationships between the fractional composition of the components of $AlCu_2$ powder particles, their average diameter, and polydispersity (Fig. 8). It should also be noted that the constructed three-dimensional diagrams allow us to roughly determine the polydispersity of the fractional composition of structurally inhomogeneous $AlCu_2$ materials, as well as the average size of powder particles in each fraction.

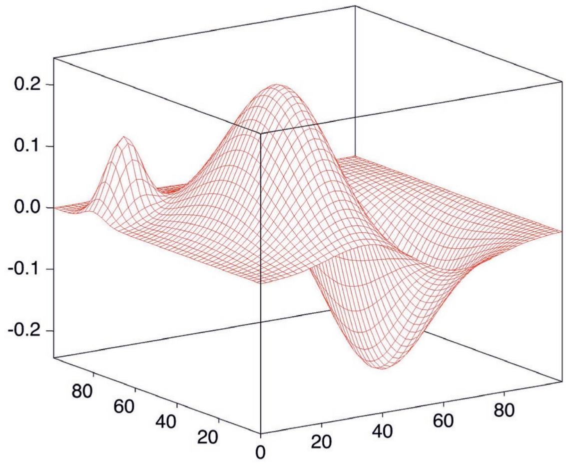

Fig. 7. The surface of a three-dimensional diagram for qualitative assessment of granulometric parameters characteristics of homogeneous bronze $AlCu_2$

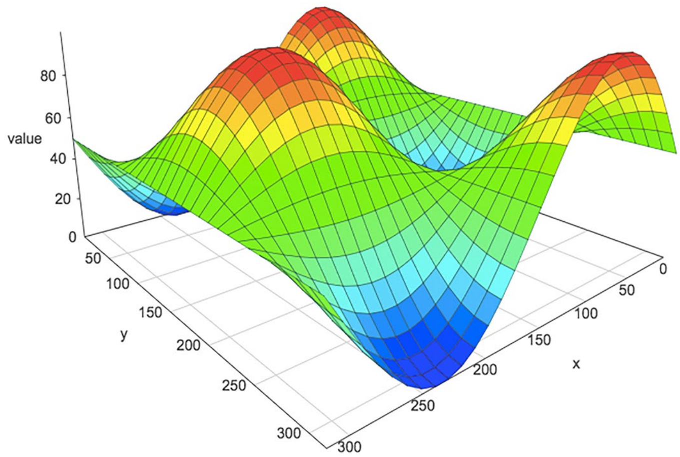

Fig. 8. Three-dimensional diagram for qualitative assessment of granulometric parameters characteristics of homogeneous bronze $AlCu_2$

The obtained results of experimental studies establish the quantitative distribution of $AlCu_2$ powder particles by size and shape in the corresponding fraction. It is shown that with a decrease in the dispersion of powder particles of the initial components of $AlCu_2$, its size spread increases. In addition, the presence of a significant number of non-spherical (non-isometric) particles of $AlCu_2$ powders was revealed, which is most expressed in the dispersed fraction (+0,125-0,1). As a result, it was found that the polydispersity of such a powder could reach no more than 20-25%.

Conclusion

The results of the study made it possible to establish the quantitative distribution of $AlCu_2$ powder particles by size and shape in the corresponding fraction. The use of round, triangular, and square particles is investigated and justified. The diameter of powder particles of structurally inhomogeneous materials depended on the pH of the medium, and mainly ranged from 0,15 mm to 0,63 mm. It is proved that due to the triangular shape of the particles, the porosity of the sample is the least sensitive to their area, and the most sensitive is in the case of square particles. Backfills with round particles have the highest porosity, compared to other forms of particles, with the same area.

The simulated three-dimensional diagram for a qualitative assessment of the granulometric characteristics of homogeneous bronze $AlCu_2$ of the SolidWorks software environment allows us to solve structural and simulation problems in the following areas:

1) determine the quantitative distribution of $AlCu_2$ powder particles by size and shape in the corresponding fraction;

2) forecasting the regularities of the formation of the structure of materials, taking into account the size and shape (spherical, ellipsoid, non-isometric) of the structural elements of the SNM charge;

3) establishing correlations between the components, structure and properties of the SNM;

4) determine the optimal conditions for modelling the composite formation process, depending on the nature of heterogeneity and load conditions.

Based on the obtained experimental data, optimal conditions for the chemical equilibrium of the initial components of $AlCu_2$ are justified and a qualitative assessment of the granulometric characteristics of homogeneous bronze $AlCu_2$, which is characterized by its homogeneity of structure and polydispersity, is obtained. It should also be noted that the constructed three-dimensional diagrams using computer modelling allow us to determine the relationships between the fractional composition of the components of the structurally inhomogeneous $AlCu_2$ material, as well as the average size of powder particles in each fraction. It should also be noted that the results obtained make it possible to predict the general behaviour of structurally inhomogeneous materials using computer and mathematical modelling at all stages of obtaining new materials.

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