Simulation of particle size distribution of mechanochemically activated charges of Al-SiC composite materials

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Annotation. In this work, 3D Spline models of the influence of silicon carbide content on the particle size distribution of the powder mechanochemical activated mixture Al-SiC were built. The formation of agglomerates in the process of mechanochemical activation (MCA) of a multicomponent Al-SiC mixture in a liquid medium of a saturated aqueous solution of boric acid has been established. The increase in the content of SiC in the charge increases the degree of agglomeration of the composite particles of the powder mixture in the process of MCA. Subsequent manual processing leads to the grinding of agglomerates and a change in the distribution of particle sizes from bimodal to unimodal distribution. The parameters of the constructed nonlinear model of the particle size distribution of mechanochemically activated Al – SiC powder blends (5–20 wt.%) Are determined. At the optimum content of silicon carbide (10% wt.), The relationship between the extreme values of the model parameters and the maximum hardness of the hot-compacted composite Al-SiC powder was established.

1. Introduction
Promising technologies for the production of powder and cast composite materials Al-SiC provide a solution to the actual problem of manufacturing valve seats of internal combustion engines [1]. An increase in the content (9% by weight) and a decrease in the size (115 μm) of SiC particles leads to an increase in the tensile strength values in tensile tests of the Al-SiC composite material obtained by injection molding technology [2]. Studies of the effect of the content (5-10% wt.) and the size of SiC particles on the mechanical properties of the powder composite hot-compacted material showed that a decrease in the particle size of SiC leads to an increase in hardness and compressive strength [3].

The SRSPU (NPI) has developed a technology for producing hot-compacted powder composite materials Al-SiC (0-20% wt.) based on mechanochemically activated charges in a liquid medium of a saturated aqueous solution of boric acid. The increased efficiency of mechanochemical activation has been shown, as compared with the mixing technology when producing hot-composit Al-SiC composite materials [4]. As a result of the research, the hereditary effect of the dispersion-agglomeration processes during the mechano-mechanical activation of the charge on the patterns of formation of hot-compacted low-porous aluminum-based powder materials was established [5-17].

Mechanochemical activation of powder blends in high-energy mills is accompanied by the formation of a new surface, an increase in the concentration of defects and chemical transformations. The accumulation of energy in a solid leads to a decrease in the activation energy of the subsequent chemical
transformation. The speed of a solid-phase reaction depends on the number and area of contacts between the interacting particles, and is also determined by the size distribution of the powder batch particles [18-21].

2. Purpose of the work
Construction of a particle size distribution model of mechanochemically activated Al-SiC powder blends.

3. Research methodology
Mechanochemical activation (MCA) of the powder mixture was carried out for 3.24 ks in a SAND – 1 ball planetary mill at a rotor speed of 4.8 s⁻¹ and a mass ratio of balls (d_b = 10 mm) and charge equal to 20. To form a protective layer on the surface of the powder particles, which prevents oxidation in the process of short-term heating of the molding in an air atmosphere, activated in a liquid medium a saturated aqueous solution of boric acid (20% of the mass of the charge) [4,22]. Powders of aluminum PA-4 and silicon carbide (black) SiC (0–20 wt.%) with irregular fragmentation of particles were used as starting materials [4]. The granulometric composition of the PA-4 powder (Figure 1) was investigated on a Microtrac Bluewave S3500 laser analyzer.

![Figure 1. The particle size of the powder PA-4](image)

The elemental analysis of the material of the mechanochemically activated charge particles was carried out using the EDAX Genesis 2000 KMS 30 microanalysis system coupled with the SEM FEI Quanta 200 (Collective Use Center “Nanotechnologies” of the SRSPU (NPI)).

To assess the degree of agglomeration of the charge in the MCA process, the average particle size of the charge d₀ was calculated after the mechanochemical activation of the Al-SiC powder batch and the subsequent manual pestle processing in the mortar d₁ based on the results of the sieve analysis of the particle size distribution of the charge [4]. The construction of 3D Spline models of particle size distribution of the powder mixture was carried out in Statistica.

4. Results of experimental studies
Analysis of the 3D Spline model of the influence of the silicon carbide content C_{SiC} on the particle size distribution of the powder mechanochemical activated mixture Al-SiC (Figure 2) showed that agglomerates (d₀ > d₁) are formed during the MCA multicomponent mixture Al-SiC. Elemental analysis (Figure 3) of the activated Al-SiC mixture (10% wt.) After manual processing showed that composite particles containing Al, C, O, Si are formed during MCA. The formation of agglomerates is accompanied by a continuous-sequential process of their dispersion-agglomeration-dispersion - ..., leading to a change in the average size of the powder particles d₀. Agglomeration of composite charge particles can be represented as a process of formation of compounds by topochemical reactions proceeding along the front of particle interaction, setting of particles on the contact surfaces, caricaturing
the material of soft particles with solid particles and cladding of solid particles with a layer of soft particle material [4].

![Spline graph a)](image_a)

![Spline graph b)](image_b)
**Figure 2.** 3D Spline model of the effect of SiC content on the particle size distribution of the powder mechanochemical activated mixture Al-SiC

a) after MCA; b) after the MCA and subsequent manual processing in a mortar

**Figure 3.** Elemental analysis of composite particles of mechanochemically activated mixture Al-SiC (10% wt.)

The increase in the content of SiC in the charge increases the proportion of agglomerated composite particles of the powder mixture in the process of MCA. Subsequent manual processing leads to the grinding of agglomerates and a change in the distribution of particle sizes from bimodal to unimodal distribution. The single-modal size distribution of agglomerated Al-SiC particles can be described by the Rosin-Rammler equation in a double logarithmic scale, reduced to a linear form [4, 23] and taking into account the passage values \( p \) of the powder mixture with dimensions greater than \( X \)

\[
\ln \left( \ln \left( \frac{1}{p} \right) \right) = \ln \alpha + \beta \cdot \ln X, \quad (1)
\]

\[
y = a + b \cdot x, \quad (2)
\]

where

\[
y = \ln \left( \ln \left( \frac{1}{p} \right) \right), \quad x = \ln X, \quad a = \ln \alpha, \quad b = \beta,
\]

\( \alpha, \beta \) – parameters of the Rosin-Rammler equation

\[
F(X) = \alpha \cdot \beta \cdot X^{\beta-1} \cdot \exp(-\alpha \cdot X^\beta), \quad (3)
\]

The results of studies of the mechanochemical activation of multicomponent mixtures conducted at the SRSPU (NPI) showed that dependence \( y(x) \) can be described by a logistic function [24]

\[
y = a + b \left( \frac{x}{c} \right)^d, \quad (4)
\]

The values of the \( (a, b) \) parameters of the linear and \( (a, b, c, d) \) nonlinear model (4) were calculated using the standard Table Curve 2D package. The assessment of the degree of compliance of the
constructed models with the results of experimental studies was assessed using the coefficient of
determination \( r^2 \) (Table 1.2).

Analysis of the calculated values of the coefficient of determination \( r^2 \) showed an increase in the degree of compliance with the results of experimental studies in the transition from linear (2) to nonlinear logistic (4) models \( y(x) \) for the entire range of \( C_{SiC} \) values studied. Linear models (2) cannot be used to describe the particle size distribution of mechanochemically activated powder blends of Al-SiC with

Table 1. The values of the parameters of the linear (2) and non-linear (4) models for the charge after the MCA.

| \( C_{SiC} \), % wt. | Values of parameters of a linear equation \( y = a + b \cdot x \) | Values of nonlinear equation parameters \( y = a + b \left(1 + \left(\frac{x}{c}\right)^d\right) \) |
|-------------------|-------------------|---------------------------|
| \( 5 \)            | \( -2.62 \), \( 0.61 \), \( 0.960 \), \( 2.79 \) | \( a \), \( b \), \( c \), \( d \), \( r^2 \) |
| \( 10 \)           | \( -1.970 \), \( 0.428 \), \( 0.938 \), \( -8.988 \) | \( -9.575 \), \( 2.714 \), \( 1.878 \), \( 0.976 \) |
| \( 15 \)           | \( -1.804 \), \( 0.317 \), \( 0.969 \), \( -3.838 \) | \( 10.1 \), \( 2.259 \), \( -2.985 \), \( 0.985 \) |
| \( 20 \)           | \( -1.244 \), \( 0.224 \), \( 0.938 \), \( -2.509 \) | \( 4.156 \), \( 3.828 \), \( -1.162 \), \( 0.943 \) |

Table 2. The values of the parameters of the linear (2) and non-linear (4) models for the charge after the MCA and the subsequent manual processing in the mortar.

| \( C_{SiC} \), % wt. | Values of parameters of a linear equation \( y = a + b \cdot x \) | Values of nonlinear equation parameters \( y = a + b \left(1 + \left(\frac{x}{c}\right)^d\right) \) |
|-------------------|-------------------|---------------------------|
| \( 5 \)            | \( -2.229 \), \( 0.695 \), \( 0.866 \), \( -1.59 \) | \( a \), \( b \), \( c \), \( d \), \( r^2 \) |
| \( 10 \)           | \( -3.607 \), \( 0.905 \), \( 0.849 \), \( 0.039 \) | \( 3.748 \), \( 4.088 \), \( -6.94 \), \( 0.976 \) |
| \( 15 \)           | \( -3.203 \), \( 0.778 \), \( 0.581 \), \( 0.385 \) | \( 103.43 \), \( 11.51 \), \( -5.877 \), \( 0.891 \) |
| \( 20 \)           | \( -2.699 \), \( 0.624 \), \( 0.524 \), \( 0.188 \) | \( 18,135 \), \( 6,119 \), \( -38,56 \), \( 0.917 \) |

an increased SiC content (15-20% wt.). Dependences (5) of the effect of \( C_{SiC} \) on non-linear parameter values

\[
a, b, c, d = f(C_{SiC})
\]

models (4) \( y(x) \) are extreme. It has been established that with an optimal SiC content of 10% by weight, ensuring the production of hot-composite Al-SiC composite material with a maximum hardness (371 HV) [4], extreme values of parameters \( a, b, c, d \) are observed (table 1.2) for a nonlinear particle size distribution model powder mechanochemically activated charges.

5. Conclusions

Based on the studies, a nonlinear model of the particle size distribution of mechanochemically activated Al – SiC powder blends was constructed. The hereditary effect of mechanochemical activation on the formation of the mechanical properties of the hot- compacted Al-SiC composite material has been established.

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