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Application of a Mathematical Model in Creating a Hard Alloy Tool That Combines Strength and Plasticity

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Abstract
The article discusses the use of a mathematical model in creating a hard alloy tool that combines strength and plasticity, the development of a multi-component alloy composition using methods of planning experiments and processing test results in materials science, the preparation of a multi-component metalloceramic material from local raw materials, and their physical and mechanical properties and their role in materials science.
The results of research on the use of a mathematical model in creating a hard alloy tool that combines strength and plasticity are presented. Using the steep ascent method to optimize the composition, a powder composition was determined that provided a level of stability and served as the basis for further research.
An alloy with a polydisperse composition is able to embody the required properties. It is assumed that large grains of the phase provide plasticity, and small grains provide high wear resistance of the alloy.

1. Introduction

The current state of the art in creating a hard alloy tool that combines optimal strength and plasticity is being analyzed and studied by scientists around the world. Many authors have dealt with this problem. The beginning of the 21st century is marked by the development of the technology of highly dispersed refractory materials. They are already used in all developed countries of the world in important areas of human activity (industry, defense, radio electronics, energy, transport, biotechnology, medicine, etc.) [1-3].

An analysis of the literature has shown that it is currently possible to obtain highly dispersed powders of many metals using modern methods. Analysis of research conducted in many countries indicates the real potential for using highly dispersed metal powders in the production of hard alloy tools, toolmaking, and other materials with high workability characteristics [4-5].

However, insufficient research has been conducted on the creation of hard alloy tools that combine strength and plasticity, and on the improvement and implementation of their mechanical properties, as well as on the creation of hard alloy tools based on highly dispersed powders of refractory metals, as well as composites. The goals and objectives of this scientific research work were formulated taking this into account [6-8].

The improvement and development of technological processes for obtaining hard alloys based on highly dispersed metal powders is directly related to the use of hard alloys, leading to a significant increase in the operational characteristics of tools and labor productivity [20].

One of the promising areas of improving hard alloys by changing the composition of alloys is the development of technologies that simultaneously provide properties such as toughness and wear resistance, strength and plasticity compared to standard hard alloys [9-11].

2. Methodology

In materials science, a multi-component alloy composition was developed using experimental design and test result processing methods.

Analytical studies and experiments are initially conducted to analyze processes and systems, improve them, and develop new technological recommendations. The main goal of analytical research is to obtain the equations necessary to calculate the process under study. This research area consists of constructing mathematical relationships (in most cases differential equations) that fully describe the process based on the general laws of physics and chemistry, and finding their solutions. Differential equations describe a group of processes that are essentially similar. But all processes are characterized by their nature, complexity, and a system of many interconnected indicators. For this reason, differential equations formulated to represent technological processes are difficult to solve using existing mathematical methods, or they are not always possible to solve. In such cases, additional experiments are conducted in laboratory conditions to determine the relationships between process variables. When differential equations of a particular process are processed based on similarity conditions and experimental results, empirical equations of a special nature are derived that can be applied only to specific conditions. Such analytical equations that relate technological indicators are subsequently used to perform engineering calculations of the process within the permissible limits of the indicator values [12-15].

Modeling is the process of replacing one object (the original) with another (the model) and studying the properties of the original by examining the properties of the model. The main goal of replacing the original with a model is to speed up, simplify, and reduce the cost of studying the properties of the original. The object can be any natural or artificial, real or imaginary system as the original. The purpose of the modeling concept is mainly to include models in the process of theoretical creation. Ideal models can be the initial stage of a theory or they can also be a model for interpreting a theory. Hypotheses can be constructed as the first steps in developing models. The researcher's inner intuition plays a large role in developing the initial model. Initially, a large number of models are put forward. However, as the research progresses, their number decreases. In the process of working with the model, an imaginary experiment is built. The criterion of adequacy is the reflection of certain aspects of the original object of experience in a model. Experimentation acts as the "referee" and a decision is made to retain or discard the results obtained using the model [16-17].

A mathematical model is a representation of a phenomenon, process, or object under study using mathematical expressions. Modeling the object under study involves creating a suitable mathematical model. To do this, the important aspects of the model are isolated and written using mathematical relationships [18-19]. After the mathematical model is built, its study is carried out using mathematical methods. The study of mathematical models is carried out using analytical, numerical, and simulation methods. Schematic representations of the construction and application of a mathematical model in materials science, as well as the construction of regression equations by conducting experiments, are shown in Figure 1. In an analytical model, the solution to the equation can be clearly visualized using mathematical tools. A numerical model can only find particular solutions for specific initial conditions and quantitative parameters of the model. A simulation model allows you to replicate a process and measure or determine the characteristics of interest.

Experiment planning includes the following steps:

1. Setting a goal;
2. Selection of optimization parameters;
3. Selection of factors affecting the optimization parameter;
4. Creating a linear plan;
5. Implementation of a linear plan and construction of a linear model;
6. The search for extremum;
7. Writing the domain of existence of an extremum.

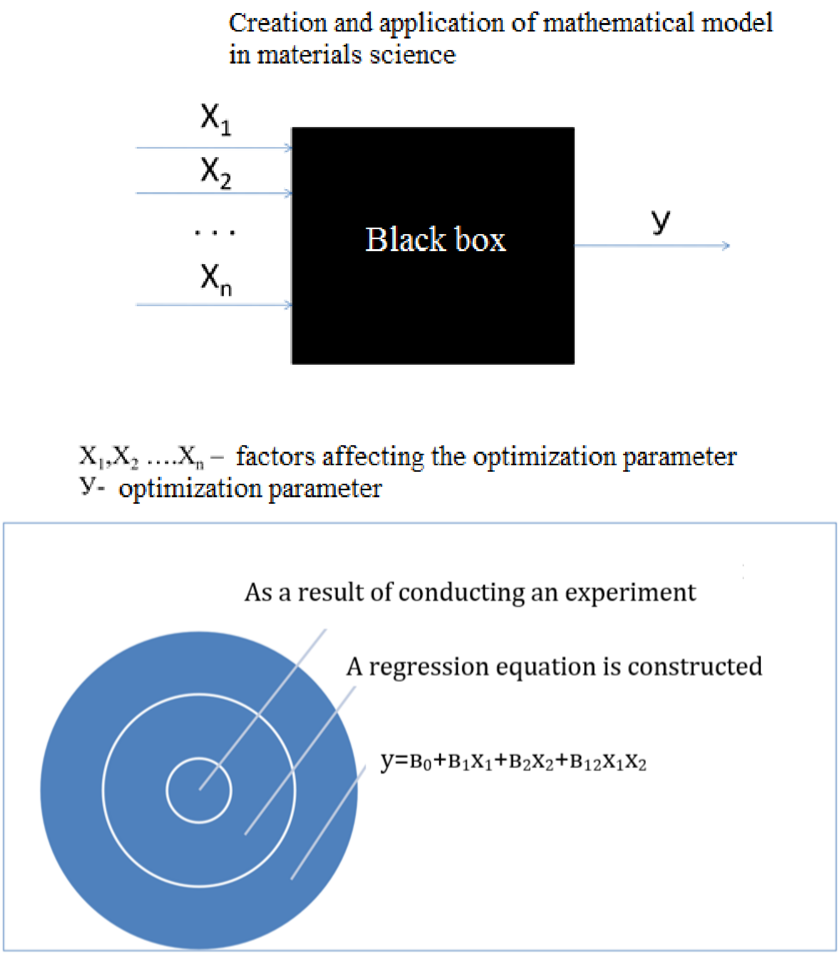

Fig. 1 *Schematic representations of constructing and applying mathematical models and constructing regression equations through experiments in materials science*

For example, it is required to find a nickel-based alloy with high strength by changing the amount of aluminum and tantalum elements in its composition. Let the strength of the nickel alloy, depending on the aluminum and tantalum elements in its composition, be as shown in Figure 2. Of course, the researcher does not know this in advance.

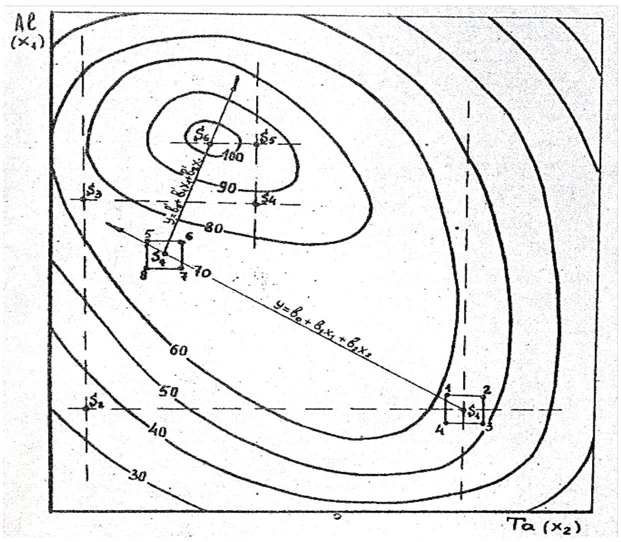

Fig. 2 *The strength of Ni-Al-Ta alloy depends on the Al-Ta content*

Let the researcher start the experiment at point S_1, based on some assumption.

Typically, an experiment involves changing the amount of one element while keeping the amount of the other constant. Starting the experiment in this way, it is clear from the figure that it will not be possible to find a composition with optimal consistency (S_6) at all. Moving the alloy in different directions around point S_1 does not significantly increase its strength. If the researcher moves to point S_2 in Figure 1, he can find an alloy with optimal strength. However, this path is very long (S_2-S_3-S_4-S_5-S_6). The same problem is solved using the mathematical design of research as follows. The researcher conducts four experiments around point S_1.

The result is a regression equation: $y=B_0+B_1X_1+B_2X_2$

Using this equation, the researcher determines the gradient of the effect of varying the amount of aluminum and tantalum elements in the alloy on the strength of the alloy. By conducting several additional experiments around point S_7, the steepest ascent method finds point S_6 by linear approximation in the direction of the gradient of the response function. To find a nickel-aluminum-tantalum alloy with optimal strength, it was enough to conduct two series of experiments. This method was proposed in 1953 by the American chemist and mathematician Boks.

Regression equation: $y=B_0+B_1X_1+B_2X_2+B_{12}X_1X_2$

$$b_i = \frac{\sum_u^N = 1X_{iu}Y_u}{N} \quad (1)$$

The coefficients of the regression equation are checked for significance using the Student's t-test. For this purpose, the confidence interval for the regression coefficients is found. The variance of the regression coefficients:

$$S_{bi}^2 = \frac{S_y^2}{N} \quad (2)$$

S_{bi}^2 - variance of determining regression coefficients

S_y^2 - Variance of tests determined in parallel

N – number of experiments

We find the confidence interval of the regression coefficients based on the Student's criterion:

$$\Delta b_i = \pm t_{aN} S_{bi} \quad (3)$$

Regression coefficients are meaningful if the absolute value is equal to or greater than the confidence interval:

$$|b_i| \geq \Delta b_i \quad (4)$$

S_{bi} - standard deviation,

To check the adequacy of the model, the adequacy variance is calculated:

$$S_{ad}^2 = \frac{\sum_u^N = 1(y_u^{his} - y_u^{eks})}{N-K-1} \quad (5)$$

Then, the model is checked for adequacy using Fisher's criterion:

$$F\frac{his}{f2;f1} = \frac{S_{ad}^2}{S_y^2} \quad (6)$$

According to Fisher's criterion, a model is considered adequate if the following conditions are met:

$$F^{his} < F^{jad} \quad (7)$$

3. Research Results

The results of the scientific research conducted confirm that polydisperse alloys are capable of embodying the required properties. It is assumed that the large grains of the phase provide plasticity, while the small grains provide high wear resistance of the alloy. As the proportion of fine grains in the alloy increases, the hardness, compressive strength, and ductility limits increase. The bending strength limit is almost independent of the change in the ratio of large and small grains in the alloy and mixture, only decreasing slightly when the amount of small grains increases. When the fine particles in the mixture increase to 40%, the plastic deformation limit practically does not change, and when it increases to 60%, the plastic deformation limit decreases slightly (by 10%). Analysis of the data obtained shows that alloys with a ratio of large and small fractions of 60:40 have some useful value in terms of combining plasticity and wear resistance.

Based on the results of the conducted scientific research, a multi-component Mo-TiC-Ni-W-Fe hard alloy composition was developed for the production of the inlet box cage roller № 25 of the SPS-2, 300 mill of Uzmetkombinat JSC. In addition to the main elements Mo and TiC, elements such as Ni, Fe, and W were added to the composition to improve technological and operational characteristics:

1. Molybdenum (Mo) – when included in the alloy, it provides elasticity, fire resistance, and corrosion resistance;
2. Titanium (Ti) – provides the alloy with heat resistance, mechanical strength at high temperatures, corrosion resistance, and allows for the optimal ratio of plasticity and strength characteristics;
3. Nickel (Ni) – when included in the alloy, the necessary processability and plasticity are achieved, it has good pressability, and during the sintering process it provides density, viscosity, mechanical strength, and corrosion resistance (for parts used at high temperatures);
4. Iron (Fe) – when included in the alloy, it increases the processability by restoring oxides on the surface of titanium carbide particles and strengthens the tool by combining titanium with molybdenum;
5. Tungsten (W) – when included in the alloy, it provides hardness and fire resistance, corrosion resistance, strengthens the molybdenum base and increases the hardness of the alloy.

Initial studies showed that it was not possible to create eutectic alloys of this composition by baking powder compositions. The baked alloy did not meet any of the parameter requirements. Therefore, the development of the replacement alloy was carried out, on the one hand, in the direction of increasing the TiC content, and on the other hand, in the direction of introducing additives of refractory metals that improve the technological and operational characteristics of the alloy. The alloy was evaluated by comparing two characteristics: flexural strength (σ_m) and Rockwell hardness (HRC). It is known that these characteristics are well combined with the hardness and refractoriness characteristics that determine the workability and durability of the tool during hot pressing. Therefore, σ_m and HRC was taken as an evaluation criterion when determining the optimal composition in the development of the alloy. Figures 3 and 4 show a graph of the dependence of the calculated values of the bending strength σ_m on the change in the amount of TiC and Ni.

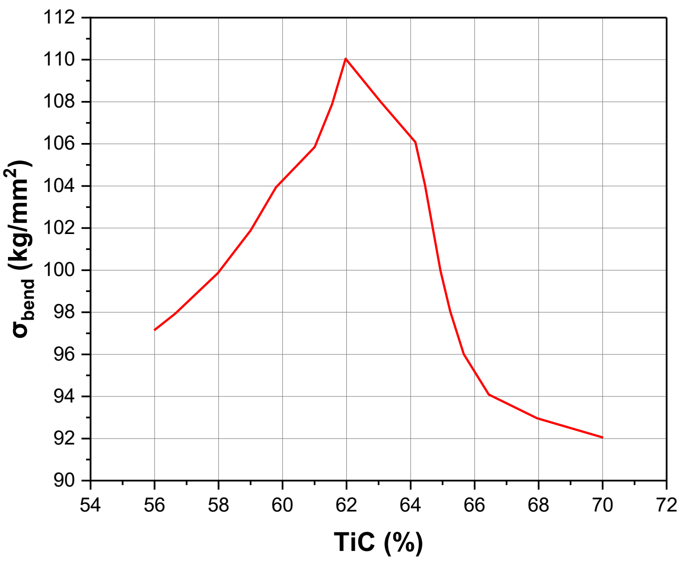

Fig. 3 *Dependence of calculated values of bending strength σ_m with changes in the amount of TiC*

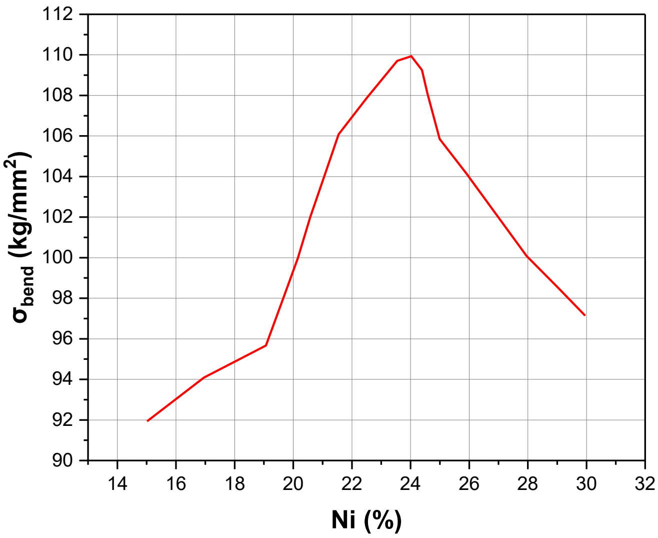

Fig. 4 *Dependence of calculated values of bending strength σ_m with changing Ni content*

The composition optimization was carried out using the mathematical design of experiments method. As a starting point for the development, an alloy with a fully controllable characteristic value (σ_m=900 MPa, HRC=80) was selected with a composition of 60% TiC, 4% Fe, 20% Ni, 4% W and the rest molybdenum Mo.

Table 1 *Optimization plan for the composition of freshly sintered alloy with steep ascent method*

№	Experiment №	TiC, %	Ni, %	W %	Fe, %	σ_{bend} kgf/mm²
		X_1	X_2	X_3	X_4	y
1	Bi	+5	+2			-
2	Bi*		-	-	-	-
3	Step	1	-	-	-	-
4	№ 1	56	22	3,5	3,5	-
5	№ 2	57	22	3,5	3,5	-
6	№ 3	58	22	3,5	3,5	110
7	№ 4	59	22	3,5	3,5	-
8	№ 5	60	22	3,5	3,5	-
9	№ 6	61	22	3,5	3,5	-
10	№ 7	62	22	3,5	3,5	115
11	№ 8	63	22	3,5	3,5	-
12	№ 9	64	22	3,5	3,5	-
13	№ 10	65	22	3,5	3,5	-
14	№ 11	66	22	3,5	3,5	106
15	№ 12	67	22	3,5	3,5	-
16	№ 13	68	22	3,5	3,5	-
17	№ 14	69	22	3,5	3,5	-
18	№ 15	70	22	3,5	3,5	98

When optimizing the composition, the composition of the powder composition was determined using the steep ascent method, which provided a strength level of σ_m=1150MPa and HRC=84 (Table 1) and was taken as the basis for further studies. The optimal composition of the powder composition includes 60% TiC, 4% Fe, 20% Ni, 4% W, and the rest is molybdenum Mo.

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4. Conclusion

Based on the conducted theoretical and experimental studies and the analysis of the results obtained, complex scientific, technical and technological methods and guidelines were proposed, which allowed expanding and developing scientific research, as well as identifying further ways of developing high-tech processes in mechanical engineering, which are of great importance for all sectors of the economy. The following conclusions were presented as a result of research on the use of a mathematical model in the creation of a hard alloy tool that combines strength and plasticity:

1. The current state of methods used in materials science was analyzed by world scientists.
2. The composition of a multi-component alloy was developed using methods of planning experiments and processing test results in materials science.
3. The results of the conducted scientific research work confirmed that polydisperse alloys are capable of embodying the required properties. It is assumed that large grains of the phase provide plasticity, and small grains provide high wear resistance of the alloy.
4. Optimization of the composition of a multi-component alloy was carried out using the method of mathematical design of experiments.
5. A newly baked alloy with the Mo-TiC-Ni-W-Fe system prepared by powder metallurgy from powders of refractory metals was obtained.
6. The scientific significance of the research results is the selection of a mathematical model, the size and nature of which depend on the effectiveness of the formation of the structure.
7. Patent No. IAP 06458 of the Intellectual Property Agency of the Republic of Uzbekistan on metalloceramic material was obtained on 30.04.2021. The developed new metalloceramic material made it possible to produce new types of import-substituting devices from local raw materials.

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

The authors confirm contribution to the paper as follows: ***study conception and design:*** *Alisher Rasulov, Akmal Allanazarov;* ***data collection:*** *Alisher Rasulov, Malokhat Tukhtasheva;* ***analysis and interpretation of results:*** *Alisher Rasulov, Shokhrukh Tlovoldiyev[1], Kamol Khakimov, Shokhbos Botirov;* ***draft manuscript preparation:*** *Alisher Rasulov. All authors reviewed the results and approved the final version of the manuscript.*

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