Modeling of the chromium compounds synthesis in the nanocrystalline state

L S Shiryaeva and G V Galevskiy
Siberian State Industrial University, 42 Kirova Street, Novokuznetsk, 654007, Russia
E-mail: kafcmet@sibsiu.ru

Abstract. In this work, the technology of nanocrystalline chromium compounds by carbidization of chromium-containing raw materials with hydrocarbons in a plasma flow generated in a three-jet direct-flow reactor was selected as the object of study. The computer program was developed that implements a comprehensive multifactor model of the plasma synthesis process and allows multivariate engineering and research calculations of the effective carbidization parameters of chromium-containing raw materials.

1. Introduction
Computer modeling is one of the most effective tools of cognition, analysis and design, which are available to specialists responsible for the development and operation of complex chemical and metallurgical industries. The idea of computer modeling is simple and at the same time attractive, it allows the researcher to experiment with objects in cases where it is almost impossible or inexpedient to do this on a real object. Plasma synthesis is a complex metallurgical process for research. This is due to its short duration, high temperatures and the small volume of the carbide formation zone. Under such conditions, a model-mathematical approach seems to be very promising, involving the thermodynamic modeling of synthesis processes, the simulation of the interaction of streams of chromium-containing raw materials and heat carrier gas, and an experimental study with the method of the planned experiment.

Comparison of different technologies for producing powders of refractory compounds indicates that, to achieve the nanoscale, technologies based on the use of highly concentrated energy flows for gasification of raw materials and the formation of the target product during volumetric condensation from the gas phase are primarily demanded. Among such technologies, the plasma method is characterized by comparative ease of implementation and is the most studied and competitive [1-6]. The processes of plasma synthesis can conditionally be divided into three stages: 1) the evolution of the feedstock, including its movement in the flow of heat carrier gas, heating and phase transitions; 2) chemical reactions, i.e. synthesis itself; 3) the formation of a dispersed product (condensation, coalescence, crystallization, coagulation).

High speeds of the reaction media, which are 30-60 m/s in the channels of three-jet direct-flow reactors, depending on the operating parameters of the plasma torches and thereby contributing to a reduction in the residence time of raw materials at temperatures of its transition to the vapor phase (10-4 - 10-5 s), impose constraints on the completeness of the first stage, which, in the case of using dispersed raw materials, limits and determines the quantitative yield of the target product in this regard. In this regard, of all the factors affecting the degree of feedstock conversion, namely: the thermophysical and thermodynamic properties of the plasma and feedstock, the ratio of the mass flow...
rates of the plasma forming gas and feedstock, the initial plasma temperature, the design features of the reactor, specific energy consumption, the organization of the process of mixing dispersed feedstock with plasma, etc., – the main limiting factor is the heat exchange of a high-temperature gas flow with the particles of the processed material moving in it.

Therefore, high degrees of conversion of raw materials at the first stage of synthesis can be achieved with such hydrodynamic and energy parameters of the reactors that provide for a very limited time the supply of sufficient energy from the heat carrier to the dispersed raw materials for the required thermophysical and physicochemical transformations [7-9]. However, an experimental study of this stage of synthesis is difficult due to its short duration and the lack of diagnostic and monitoring tools that work reliably under such conditions and, as a rule, comes down to a model-mathematical one, which makes it possible, with a certain “idealization” of the process, to determine the effect on the transition degree of raw materials to the gas phase of the temperature and velocity of the gas flow in the raw materials input zone, consumption of reagents, input conditions and particle sizes of the raw material [1].

In the present work, as the object of study we selected the modeling technology for the production of chromium carbide by carbidization of chromium-containing raw materials with hydrocarbons in the plasma flow generated in a three-jet direct-flow reactor.

2. Modeling results
Technological options, parameters and indicators of chromium carbide synthesis (forecast) are presented in table 1. The calculation took into account possible losses of raw materials in the reactor in the amount of 4% and losses of synthesis products in the capture system in the amount of 5%. An analysis of the data in the table shows that the most promising is the technological option for producing carbide by carbidization of chromium powder, the technical and economic indicators of which are significantly higher than expected in other options.

| Reactor power, kW | 150 | 150 | 150 |
|-------------------|-----|-----|-----|
| Consumption of plasma-forming gas (nitrogen), kg/s | 9·10^{-3} | 9·10^{-3} | 9·10^{-3} |
| Initial temperature of the plasma flow, K | 5400 | 5400 | 5400 |
| Quenching temperatures, K | 2000 | 2000 | 2000 |
| Mass consumption concentration kg of raw material / kg of nitrogen | 0.10 | 0.12 | 0.15 |
| The degree of raw materials conversion to carbide | 0.96 | 0.96 | 0.96 |
| The yield of carbide, % of the mass | 91.4 | 90.0 | 91.8 |
| Productivity for chromium carbide, kg / h | 3.42 | 2.79 | 1.69 |
| The intensity of production, kg/h·m³ | 2011 | 1641 | 994 |
| Consumption of chromium-containing raw materials, kg/kg | 0.90 | 1.30 | 2.76 |
| Methane consumption kg/kg | 0.84 | 2.74 | 0.89 |
| Gas consumption – heat carrier, kg/kg | 9.47 | 11.6 | 19.70 |
| Specific consumption of energy, kW·h/kg | 43.85 | 53.76 | 88.70 |
| Cooling water consumption, m³/kg | 1.08 | 1.32 | 2.19 |

3. Computer program for the model implementation
Based on the results of theoretical and experimental studies, the computer program “Generalized Model of Carbide Formation in Plasma Synthesis” [10] has been developed, designed to conduct
multivariate engineering and research calculations of the content of chromium carbonitride and basic impurities in the synthesis products, their level of dispersion depending on the main technological parameters. Variable synthesis parameters are: the initial temperature of the plasma stream, the temperature of the quenching of the synthesis products, the amount of hydrocarbon for chromium carbidization, the concentration of hydrogen, atomic nitrogen in the plasma-forming gas. The calculation results are analyzed. The report is generated for each calculation option. The structural composition of the program includes: an internal DBMS, an interface for entering data, report output in Microsoft Excel.

The usage of software product makes it possible to carry out multivariate engineering and research calculations determining the content of chromium carbonitride and basic impurities, the level of dispersion and identifying the dependence of the content on the main parameters. To create a software product, the necessary information was collected on the development and development of the technology of plasma-metallurgical production of chromium carbonitride. A database has been created to store the necessary process data. Data from the database is transferred to the program, where it is used and processed.

The software makes it possible to calculate and present graphically the results of a study of the dependence of the content of chromium carbonitride in the synthesis products on the initial temperature of the plasma flow, the quenching temperature of the synthesis products, the amount of hydrocarbon for chromium carbidization, the concentration of hydrogen and atomic nitrogen in the plasma-forming gas.

The software product is based on the calculation of the content of chromium carbonitride in the synthesis products, carried out using field model data. The field model data obtained during the implementation of the plasma metallurgical production technology of chromium carbonitride are the values of the following synthesis parameters: the initial temperature of the plasma flow, the temperature of the quenching of the synthesis products, the amount of hydrocarbon for chromium carbidization, the concentration of hydrogen and atomic nitrogen in the plasma-forming gas.

When conducting the computational process, the listed synthesis parameters are input data. Data entry is carried out by changing the current value within the studied range under the supervision of a teacher, to whom the corresponding disciplines are assigned, which excludes the entry of incorrect data.

The content of chromium carbonitride in the synthesis products is described by the first-order equations. The result of the calculations is a graph that determines the nature of the dependence of chromium carbonitride content in the synthesis products and basic impurities on its conditions. Then an analysis of the results is carried out. Using a software product allows to be analyzed: the yield of chromium carbonitride and its associated phases; the dispersion level of chromium carbonitride; the effect of the initial temperature of the plasma flow; the effect of the amount of hydrocarbon for chromium carbidization; the effect of the concentration of hydrogen in the plasma-forming gas; the effect of the concentration of atomic nitrogen in the plasma-forming gas.

Based on the analysis, the following conclusions are made:
- on predicting the content of chromium carbonitride and impurities in the synthesis products depending on the main parameters (initial temperature of the plasma stream; temperature of quenching of the synthesis products; amount of hydrocarbon for chromium carbidization; concentrations of hydrogen in and atomic nitrogen in the plasma-forming gas);
- about the optimality of synthesis conditions and obtaining the required content of chromium carbonitride in its products;
- on the quantitative prediction of the chromium carbonitride dispersion.
A report is generated for each option.

The purpose of conducting multivariate engineering and research calculations is to optimize the formation of chromium carbonitride by determining the content of chromium carbonitride and basic impurities, the level of dispersion, and identifying the dependence of the content of synthesis products on its conditions.
The main tasks are: ensuring maximum yield of the target product; determination of factors affecting the composition of the product; search for effective control actions to obtain the desired content of chromium carbonitride in the synthesis products; development of user skills with the most common applications; independent performance by the user (student) of the work and the ability to control it by the teacher with mandatory user registration.

The program uses elements of an object-oriented approach and technology of traditional structural design. The program algorithm should provide calculation and graphical representation of the results of the study of the dependence of chromium carbonitride content in the synthesis products on its parameters. This software is installed on the computer using the Setup.EXE installation file. The main working window contains all the main bookmarks necessary for the user’s further work, with the help of which he selects chromium-containing raw materials and calculation options (figure 1).

![Figure 1](image_url)

The software product allows a report template in Microsoft Excel to be created, which presents the calculation results and the resulting graphical dependencies. An alternative output of the received information to a screen, printer or file located on an external medium is possible. The following is information on the content in products of plasma metallurgical synthesis of chromium carbonitride Cr$_{free}$, C$_{free}$, Cr$_2$O$_3$, N$_2$.

### 4. Conclusion

The developed computer program is a complete software product that helps to carry out multivariate engineering and research calculations to optimize the parameters of the plasma metallurgical production of chromium carbide, as well as research on the creation of new highly efficient processes using refractory nanocarbides, nanoborides and their compositions.

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