ABSTRACT

The master's thesis consists of an introduction, five chapters, conclusion, a list of references with 57 titles, 2 annexes and contains 20 figures, 2 tables. The full volume of the master's thesis is 105 pages, applications - 16 pages.

Relevance of the topic. The processes of interaction of metals with molecular gases are of great practical interest in connection with the problem of creating a new generation of heat-resistant materials for work in extreme conditions. Processes take place in open systems far from thermodynamic equilibrium and are characterized by diverse behavior. Computer simulation of these processes allows us to study the behavior of the gas-metal system without the need for experiments, which significantly reduces the cost and risk of research.

Relationship of work with scientific programs, plans, themes

Master's thesis was carried out at the Institute of Problems of Materials Science. I. M. Frantsevich NAS of Ukraine, within the theme "III-2-17; To study the regularities of compaction and the formation of a heterogeneous phase microstructure in the reaction liquid phase sintering of multicomponent metal systems; To create functional sintered materials with increased characteristics of electroerosive, wear - and heat resistance "

The goal is to develop a computer-integrated procedure for modeling the interaction of active molecular gases with the surface of metallic materials to establish mechanisms for the formation of functional properties, in particular heat resistance, under extreme operating conditions at high temperatures.

To achieve the goal, the following **research objectives** were formulated, which determined the logic of the study and its structure:

1. To study the regularities and features of the iron oxidation process in the region of thermodynamic instability of its oxides.

2. Experimentally study the nature of temperature changes

3. To compile a mathematical model of the process of iron oxidation in the region of thermodynamic instability of higher oxides.

4. Conduct a parametric identification of the mathematical model.

5. Develop a computer-integrated procedure for studying the oxidation of iron.

6. Develop a software module to support the procedure of computer-integrated calculation of the system under study.

The **object** of the study is the development of a computer-integrated procedure for modeling the interaction of active molecular gases with the surface of metallic materials to

establish mechanisms for the formation of functional properties in particular heat resistance under extreme operating conditions at high temperatures.

The **subject** of the research is the development of a procedure for computer-integrated studying of nonequilibrium and equilibrium metal reacting systems, their functional behavior under extreme conditions under the influence of high temperatures.

Research methods: experimental methods for determining the state of powder reactive systems, computer temperature monitoring system, mathematical modeling.

Scientific novelty of the results. The most significant scientific results of the master's thesis are:

• For the first time, a mathematical model with distributed parameters was used.

• For the first time, a software product was developed to resolve a model with distributed parameters

The practical significance of the results obtained is determined by the fact that the proposed software product provides the possibility of computer simulation of the oxygen-iron system under conditions of thermodynamic instability. This allows the values to simplify the process of system research due to the lack of the need for a real study of the object.

Approbation of the thesis results. The main provisions of the work were reported and discussed at 3 conferences.

Publications. Scientific provisions of the master thesis were published in 5 papers.

Keywords. MATHEMATICAL MODEL, COMPUTER-INTEGRATED CALCULATION, THERMODYNAMIC INSTABILITY, IRON OXIDATION, METHOD OF FINITE DIFFERENCE, GIR’S METHOD, MATHEMATICAL MODELING, MATLAB.