PRINCIPLES OF MODELING FOR COMPUTER-AIDED DESIGN OF WELDING MATERIALS

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ABSTRACT

A new concept of developing welding materials has been proposed. Physical-chemical processes that define the formation of the weld metal chemical composition, structures and properties, have been analyzed. The concept is taking into account the influence of the composition and properties of the welding materials on the process. Factors that define the performance of weld metal have been examined. Methods of mathematical modeling for development and optimization of electrodes, flux cored wires and other materials have been proposed. A general algorithm and a welding materials' computer-aided design (CAD) system have been created.

Keywords: Modeling, Computer-Aided Design, Welding, Materials

INTRODUCTION

The physicochemical processes that occur during fusion welding determine the course of a technological welding process and, consequently, its result, i.e., the composition, structure, and properties of the weld deposit. The investigation, analysis, and description of these processes should provide for the development of an optimal welding technology and modern welding materials, and the ultimate production of a weld deposit with the structure, composition, and properties stipulated by its service characteristics.

Fusion welding is a very complex process. Its complexity is primarily due to the formation of a weld pool, which is a multicomponent, multiphase system with a non uniform temperature field and complex mass- and heat-transfer processes. The mass-transfer processes on the metal–slag and metal–gas boundaries determine the chemical composition of the weld metal, and, consequently, they largely determine its mechanical properties. However, the properties of a weld, especially of a welded joint, are not shaped by the chemical composition of the metal alone. The type of crystallization in a weld has a great influence on its properties. The properties of the weld area and, to some extent, of the weld metal depend considerably on the temperature and thermomechanical cycles that accompany the welding process. This phase of the formation of a welded joint predetermines the mechanical properties of many alloy steels and alloys. A welding process can give rise to rates of heating and cooling in the metal due to heat transfer by a heat conduction mechanism that are often impossible to produce by surface heat transfer during heat treatment. The formation of a welded joint is accompanied by plastic deformation of the metal and the appearance of intrinsic stresses, which also influence the properties of joints.

The development of a metal welding technology, new welding materials, and processes for the heat treatment of welded joints should be based on clear scientific ideas regarding the course of welding processes. A theory is supposed to provide a correct description of the large set of phenomena that make up the essence of a welding process. However, for more than a century, the development of welding and hardfacing materials has been based on a system of empirical knowledge and the data accumulated and has depended mainly on the experience and training of the developers. There is no effective method that could be used to develop modern welding and hardfacing materials for various purposes on the basis of scientific theories. This is due to the large number of physicochemical and technological parameters that shape the composition, structure, and properties of the weld deposit. The processes and phenomena that occur during all the stages of different kinds of fusion welding can be described only by calling upon a long list of fundamental and applied sciences. In the current stage, it is not possible to devise a mathematical (formalized) description of the entire set of processes that occur during fusion welding and to devise a system for designing welding and hardfacing materials on its basis.

The lack of a scientific methodology for developing welding materials precludes ensuring the creation of welding materials with guaranteed service characteristics in a short time frame. The creation of a new approach for developing modern welding and hardfacing materials and a methodology for designing them on the basis of a complex physicochemical analysis of the interactions occurring during fusion welding between the liquid metal and the slag, the various structural transformations, and the thermally induced deformation processes occurring during the primary and secondary crystallization of the weld metal is needed.

Main points of the approach being developed

Welding materials perform their main function, which is to ensure the required strength characteristics and service properties of the weld metal, by participating in the welding process, which includes numerous different complex physicochemical processes that generally occur simultaneously. An analysis of the processes occurring during melting of the welding material and the metal being welded and during the formation of the weld bead and weld pool, an analysis of the crystallization of the molten metal in the weld pool, an analysis of the interaction of the weld metal with the environment, and an analysis of the service properties of the weld deposit and the welding material are needed. The result of applying a systematic approach and structural analysis to the problem of developing welding materials can be represented in the form of a sequence of steps that comprise the main points of the new approach:

- analysis of the environment, the working medium, and the loading of the working medium;
- establishment of the nature of the environment– working medium interaction;
- determination of the required structure of the weld metal;
- calculation of the primary structure and chemical composition of the weld metal;
- determination of the electrode formula of a special welding (hardfacing) material.

Analysis of the environment. The environment is a system that has a complex influence on the working medium [1, 2, 3]. The passive and active states of the environment should be distinguished. The passive state is the state of the environment in which it does not interact with the working medium. The active state is characterized by its interaction with the working medium. In the step of analyzing the environment, we shall consider only the passive state. The following should be determined as a result of the analysis:

- the geometrical characteristics of the environment;
- the chemical composition of its components;

- the chemical and physical properties of the environment;
- the mechanical characteristics of the environment;
- the main physicochemical processes that occur in the environment in response to variation of the pressure, aero- or hydrodynamic conditions, temperature, and other factors.

A knowledge model of the environment in the form of a formalized description should be created on the basis of the analysis.

Analysis of the working medium. The working medium is the part, assembly, or product that is undergoing welding or the deposition of a protective coating to ensure that it can perform its functional purpose under the prolonged influence of the environment. A working medium can generally be of one of the following two types:

1. A working medium which is being restored after a failure caused by the external environment or on which a protective coating is being deposited so that it will withstand such failure during subsequent service;
2. A working medium that is being redesigned to increase its service life in comparison to previously employed analogs, if such exist, or because of the impracticality of manufacturing the entire working medium from an expensive material.

In the former case, the problem is simplified by the fact that we already have a definite knowledge set for the subject of analysis, including data on its service. In the latter case, we need to obtain and systematize knowledge about the working medium on the basis of its functional purpose. In either case, the knowledge obtained should contain information on the structure, composition, and properties of the working medium and the physicochemical processes that occur in it upon variation of the temperature, pressure, and volume. This knowledge must be formalized and represented in the form of a model.

Establishment of the nature of the environment– working medium interaction. In this stage of the design process, the knowledge that has been obtained about the environment and working medium are used to solve an extremely complex problem, more specifically, to determine the changes in the environment and the working medium that occur as a result of their interaction.

All of the experience previously gained from numerous diverse investigations of interactions between the working medium and the environment [1-11] allow us to assert the following:

- ❖ During such an interaction, the working medium is an open dynamic dissipative system, which exchanges mass and energy with the environment.
- ❖ During the interaction, the working medium and the environment undergo several transformations (structural, phase, chemical, etc.) as a result of the processes occurring in the boundary regions of the two interacting open dissipative systems, the frequency of such transformations increasing with the interaction time.
- ❖ The result of the interaction is failure of the surface or of the entire working medium.
- ❖ It is not possible to experimentally establish the sequence and completeness of the changes occurring in the working medium and the environment during the interaction.

On this basis, it may be concluded that to understand the processes occurring in the working medium under the action of the environment and to predict the results of the interaction, we must construct mathematical models that can be analyzed to establish the missing knowledge (the output parameters of the mathematical models):

$$\mathbf{Y} = \mathbf{F}\ (\mathbf{X}, \mathbf{Q}), \qquad (1)$$

where **Y** is the vector of values of the output parameters, **X** is the vector of values of the external parameters, and **Q** is the vector of values of the internal parameters.

The main difficulty in creating such a mathematical model is the establishment of dependences of type (1). A mathematical model having an explicit form generally cannot be created, and a system of ordinary differential equations or, as is most likely in our case, a system of high-order differential equations, which are quite difficult to solve even using computers, must be used. In such a case, a phenomenological model of the interaction must be constructed in the first step, and then it is successively transformed into a mathematical model (on the macroscopic level) by introducing a series of assumptions, restrictions, and simplifications. Such a model must undergo testing for equivalence, which is confined to the fact that the values of the *i*-th output parameter y_i do not exceed the permissible limits of definite range for it $[\mathbf{DR}]_i$:

$$y_i < [\mathbf{DR}]_i \qquad (2)$$

where $[\mathbf{DR}]_i$ is the vector of permissible values of the *i*-th output parameter y_i.

Thus, the mathematical model allows us to trace the evolution of the working medium during its interaction with the environment until the moment when it fails, i.e., the end of the working cycle.

Determination of the required structure of the weld metal. As is clear from (1), the output parameters depend on the influence of the environment and the properties of the working medium. In other words, the evolution of the working medium depends not only on the properties and characteristics of the environment, but also on its own structure and properties. Assuming that the external parameters are fixed, we can use computer modeling to perform virtual experiments with variation of the internal parameters and determine the output parameters, i.e., the result of the interaction of the working medium with the environment. Thus, by solving the optimization problem, we can determine scenarios for the evolution of the weld deposit of the working medium. The results of the solution include the optimal structure and properties of the layer deposited on the working medium. Behind the apparent simplicity of this approach there is a fairly complex sequence of approximations to the optimal solution. The solution of such a problem requires a large number of iterations with intelligent simplifications and restrictions and can be performed only with a dialog between an expert and an expert system based on mathematical models (1) and (2) and knowledge models of the environment, the working medium, and the nature of their interaction [1-11].

The required structure of the weld deposit determined as a result of such a solution is regarded in our approach as the secondary structure (we define structure as the phase-structure composition of a weld deposit of definite morphology). The basis for this terminology is the fact that the weld deposit undergoes two crystallization steps during its formation, viz., primary crystallization, during which the weld pool crystallizes, and secondary crystallization, during which solid-phase transformations of the cooled crystallized metal occur. The structures obtained at the conclusion of each crystallization step have corresponding names. Thus, we must next proceed from the secondary structure that we determined to determination of the primary structure and chemical composition of the weld deposit.

Calculation of the primary structure and chemical composition of weld deposits. The primary structure and chemical composition of a weld deposit can be calculated by solving the inverse problem, in which the input parameters are the structure and properties of the weld deposit obtained in the preceding step (the secondary structure). We construct the inverse problem by modeling the secondary crystallization process and the formation of the strengthening phases [12-15] using algorithms (1) and (2). The solution of this problem gives us the primary structure of the weld deposit and its chemical composition.

Calculation of the electrode formula. Knowing the primary structure and chemical composition of the weld deposit, we can calculate the electrode formula (composition) of a special welding material [16-22]. This is the concluding step of designing a new special welding material, and now we can move on to a test calculation or, more precisely, to verification and experimental confirmation of the design solution.

Verification of the design solution. The first step involves solving the direct problem. Its solution gives the structure and service life of deposits formed using a special welding material that has the electrode formula obtained as a result of the design solution. The result must satisfy condition (2). The direct problem is solved by computer modeling using an expert system, which serves as the core of a system for the computer-aided design of welding materials.

The second step involves the fabrication and full-scale testing of the welding material. It should be specially noted that the consumable is fabricated according to a technology that ensures obtaining the calculated electrode formula. The welding is carried out under the calculated conditions for the process on a mock-up of the working medium, which is subsequently loaded in a testing unit that simulates the influence of the environment. The testing is continued over the course of a calculated time cycle that determines the working cycle of the layers deposited (the lifetime of the working medium). This cycle is one of the output parameters of the mathematical model of the interaction of the environment with the working medium. If failure of the working medium occurs at the end or after completion of the working cycle, the testing is considered satisfactory. The results of designing in accordance with the steps described above should include:

- determination of the electrode formula of a special welding material;
- determination of the special features of the technological route for producing the consumable;
- the technology of the welding process;
- prediction of the chemical composition, structure, and properties of the layers deposited;
- determination of the length of the working cycle of the layers deposited.

Now we can formulate the main principles which must be followed to ensure the development of special welding materials:

- ❖ an individual approach to design, i.e., designing a special welding material for a specific working medium that operates under specific environmental conditions;
- ❖ creation of a knowledge base for the working medium, the environment, the interactions between the working medium and the environment, and the process occurring in the weld pool and during primary and secondary crystallization;
- ❖ mathematical and computer modeling of the processes occurring when the working medium interacts with the environment and of the processes that result in formation of the weld metal, i.e., the technological welding process and the crystallization processes;
- ❖ a systematic approach to the design process;

- automation of the design process based on a special system for the computer-aided design of welding materials, whose core element is an expert system;
- verification of the design work.

Development of a system for the computer-aided design of new welding and hardfacing materials.

A design algorithm consisting of a sequence of design steps with a set of instructions and rules for each step from the creation of the data packages to the creation of the solution has been formulated on the basis of a structural analysis and the method developed. Structuralization of the problem with the links established, the feedback loops formed, the functional relationships, and the generation of the input and output parameters is presented in flow chart in Fig. 1 [23].

As can be seen, the methodology described is a closed system that is thickly covered by feedback loops and provides for the following:

- structuralization of each problem according to the customer's specifications;
- generation of data packages, instructions, and rules on its basis and ordering of them in the form of a statement of the problem for the expert system;
- solution of the problem with a dialog between the designer and the expert system;
- generation of a solution that includes the following:
    a) a prediction of the composition, structure, and properties of the weld deposit,
    b) the electrode formula of a welding material that ensures formation of the predicted weld deposit,
    c) the parameters of the welding process.

Automation of the design process was implemented by creating a special system [23-26] consisting of a large set of components that include methodical, linguistic, mathematical, programming, technical, information, and organizational software. The system includes several subsystems that solve different problems. In our case, the principal subsystem of the computer-aided design (CAD) system is an expert system, which serves as the main design tool.

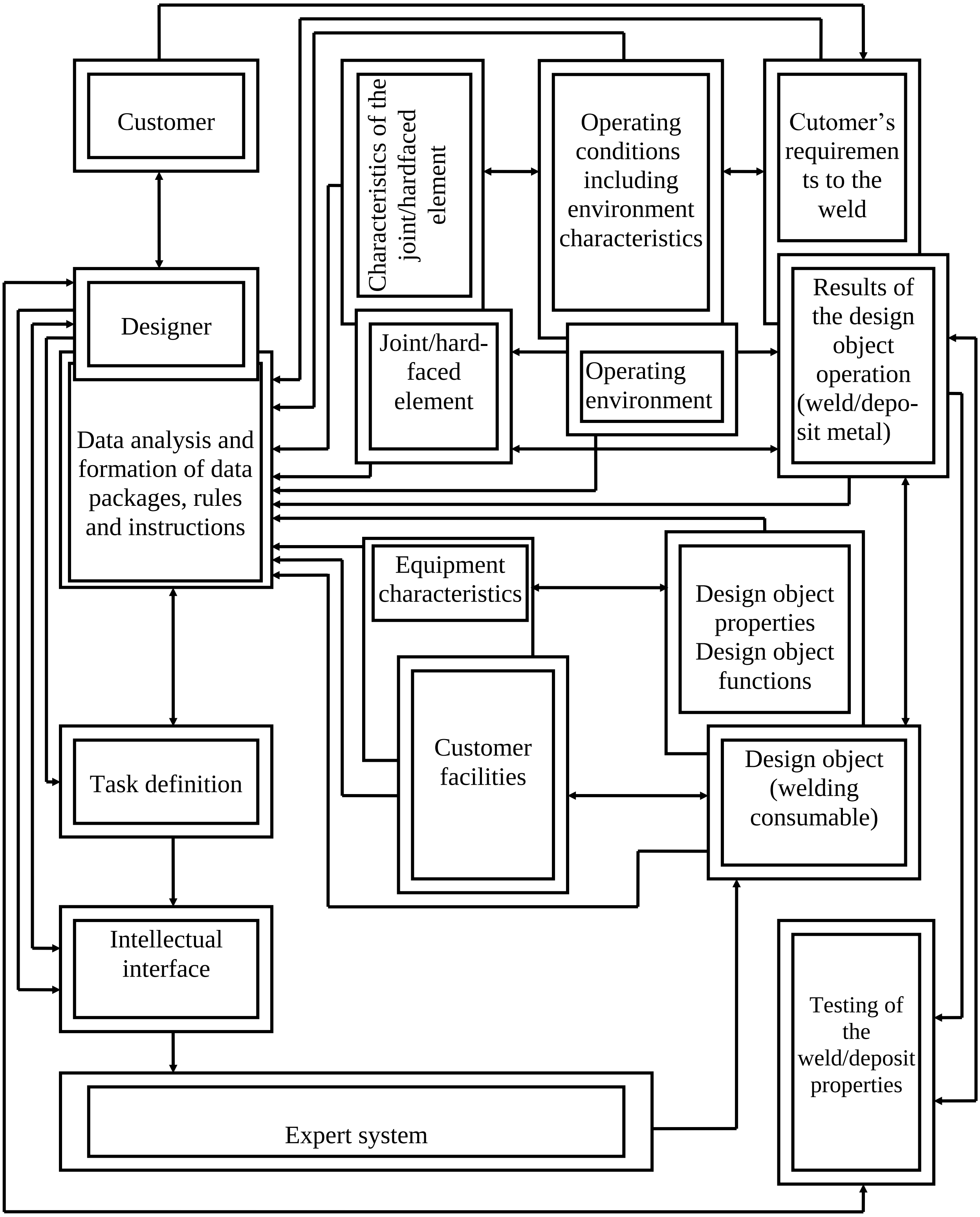

Fig.1 - Flow-chart of the method

A simplified version of the functional algorithm of the expert system is presented in Fig. 2.

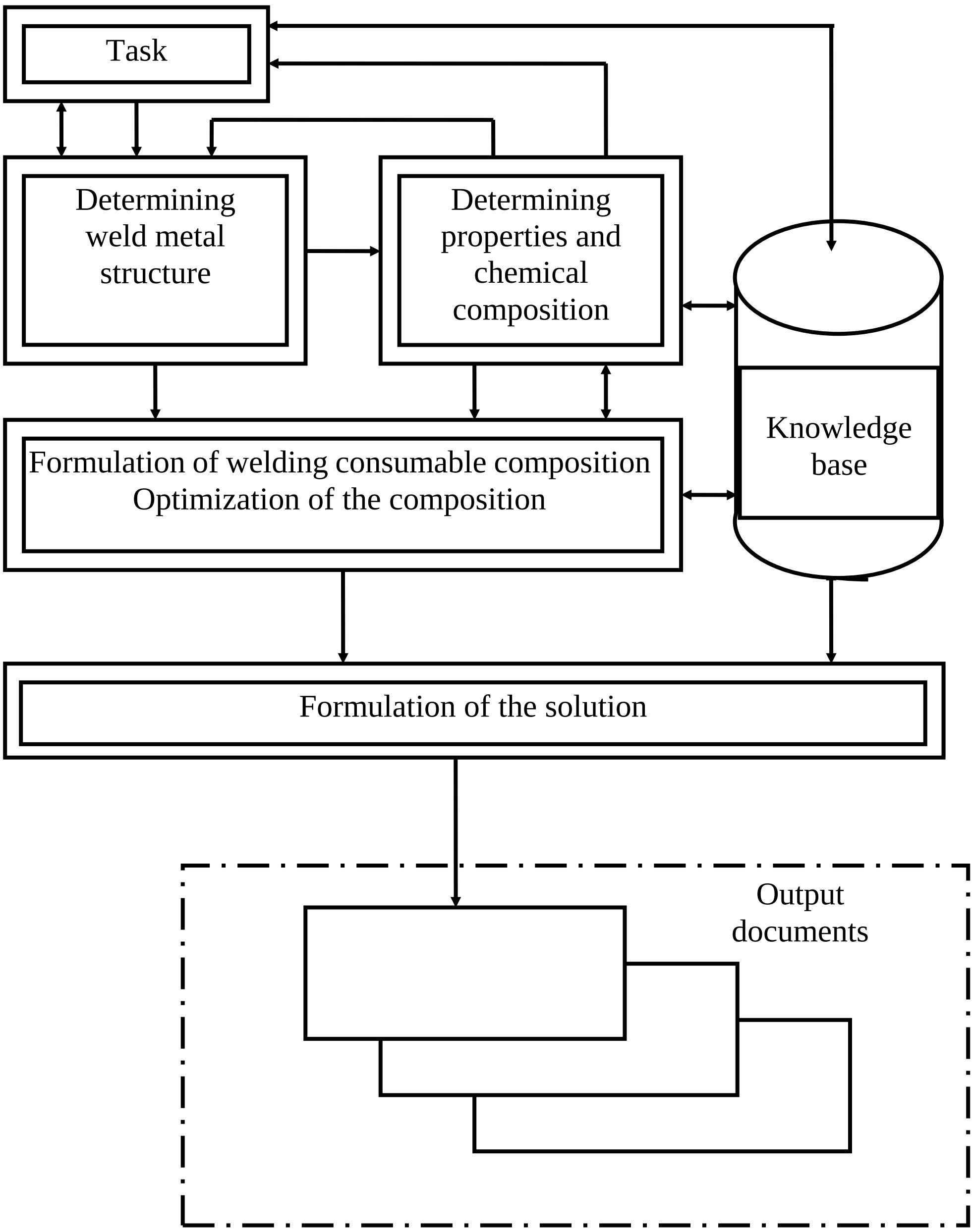

Fig. 2 - Functional algorithm of the expert system

Verification is a very important step that completes the formation of the design solution. Verification is a type of analysis, whose purpose is to establish the correspondence between two descriptions of the same object. The CAD system created includes structural and functional verification. During structural verification, the correspondence between the structure of the design object described in the technical specification and the structure obtained as a result of the design solution is established. During functional verification, the correspondence between the functioning processes, particularly the output parameters, assigned by the technical specification and by the design solution is verified. The verification system is a subsystem of the CAD system and ensures that a design solution with the smallest possible deviation of the structure and functions from those required by the technical specification is obtained.

The system developed for the computer-aided design of modern welding materials is an open system for individualized use, i.e., a system which is managed and supported directly by the developer of welding materials. Because of its open nature, the system provides for the possibility of constantly updating the knowledge bases and databases as the knowledge about the design object and the environment is improved and developed and for corresponding upgrading of the systems that manage these knowledge bases and databases. The system provides a significant reduction in the time needed to develop welding and hardfacing materials for the manufacture of complex welded metal assemblies and multifunctional hardfacing layers.

The proposed methodology has been successfully employed in the development of industrial batches of welding materials for various purposes, including:

- ❖ special electrodes for welding and hardfacing Ni_3Al alloys, which eliminate the typical cracking of these alloys under the effects of a welding cycle that creates thermal strains;
- ❖ flux-cored wires for the mechanized welding of galvanized steels at ultrahigh rates (up to 90 m/h) with guaranteed high mechanical characteristics. The wires ensure minimal gas and smoke production during welding;
- ❖ flux-cored wires for the mechanized hardfacing of high-speed tools with the guaranteed formation of a weld deposit having the properties of type A 600 M2 (SAE/ASTM USA) high-speed steel without subsequent heat treatment;
- ❖ flux-cored wires for the mechanized deposition of hardfacing layers that are resistant to shock-abrasion wear.

All the consumables developed have good welding-technological properties and displayed high values for the service characteristics of the weld deposit.

CONCLUSIONS

1. A systematic analysis of the purpose and functions of welding materials has been carried out, and a new approach to their development and design has been formulated on its basis.
2. It has been shown that an effective way to develop a new welding material is to solve the "inverse" problem of finding the electrode formula of the material as a function of the service characteristics of the weld metal.
3. The main processes occurring in all the stages of the formation of a weld and its interaction with the environment have been analyzed, and a conclusion has been drawn regarding the prospects of constructing corresponding models of these

processes, whose use could ensure obtaining the necessary data and knowledge for developing an electrode formula.

4. It has been shown that effective solution of a design problem requires a systematic approach to the design process and its automation on the basis of the creation of a specialized computer-aided design system. This permits an individual approach to design, i.e., the development of a specific material that has special functions for specific service conditions.
5. An efficient computer-aided design (CAD) system for welding materials, whose core component is an expert system that works with a knowledge system based on a phenomenological model of the nonequilibrium crystallization of a weld pool, has been developed for the first time. The CAD system for welding materials is organized as an open system for individualized use with the possibility of constantly updating and supplementing the databases and knowledge base as new data and knowledge are accumulated and developed.
6. Industrial batches of welding materials for various purposes have been developed, designed, and fabricated using the proposed methodology. The results attest to the high efficiency of the new method.

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