Modeling and investigation of temperature fields at phase boundaries in powder mixtures undergoing melting and chemical transformation

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Abstract. An important component of the process of hardening parts by induction surfacing is the heating of hard alloy and flux particles in the surfacing charge. The article describes complex studies on measuring and modeling temperatures at phase boundaries in complex melting and thermoreactive powder mixtures. To register the temperature in the process of induction surfacing, it is proposed to use the XA-microthermocouple method and the method of thermal indication using SHS compositions. The data of numerical modeling and solution of the non-stationary problem of heat conduction in the selected model of composite contact materials are presented. The developed methods of complex registration of temperature in the process of induction surfacing make it possible to determine the melting temperatures of the surfacing charge and its individual components, as well as the surface of the part.

1. Introduction

Modern studies of multicomponent powder mixtures, the heating of which leads to the melting of individual components, the formation of alloys and coatings, chemical reactions and the synthesis of new substances, are impossible without knowledge of the temperature values and its distribution at the phase boundaries. Such information is necessary to control the processes of induction surfacing (IS), welding, self-propagating high-temperature synthesis (SHS), and many other technologies.

Among the various methods of surface treatment and coating [1–7], processes based on the chemical vapor deposition approach, in particular the boriding process, can be very promising, since this process can provide protection of various surfaces for parts made from various ferrous alloys [2–4, 8]. Matrix composites based on the Fe-B-FenB triple system are offered as a promising material for protective and hardening coatings.

Steel parts hardened in this way have good tribological properties, including resistance to abrasive, adhesive, fatigue and corrosive wear [9–15].

One of the main advantages of this type of hardening is that boride-hardened steels have extremely high hardness values (between 1600 and 2000 HV) [16–18].

Boring in the classical sense is a process of chemical-thermal treatment, diffusion saturation of the surface of metals and alloys with boron during heating and holding in a chemically active medium. This is a fairly common method for processing steel and derived materials. Often the surface subjected to saturation turns out to be two-phase: a region of a mixture of FeB, Fe2B borides and a transition region consisting of a solid solution of boron in combination with other elements contained in steel in α-Fe.
Upon detailed analysis, the internal structure of a layer of such coatings is represented by needles of borides, fused at the base. At the same time, such a coating structure has significant internal stresses that reduce their strength characteristics so much that relatively small impact, bending or compressive loads can lead to peeling or chipping of these coatings. Alternating loads and vibrations aggravate these processes that destroy the coating. In view of these circumstances, the method of the isothermal process of applying boron-based hardening compositions to steel parts has significant limitations in application for mass use in production and mechanical engineering.

In contrast to the classical approach, boriding using induction (HFC) heating has a number of advantages that should be noted. In particular, due to an increase in the heating rate, the rate of the coating formation process increases by tens of times. Also, reducing the borating time, coupled with the use of specialized fluxes, eliminates the need to create a protective gas environment. The short time required for induction heating leads to a reduction in the effect on the material of high temperatures, and also opens up prospects for combining the boriding process with subsequent heat treatment.

This combination of circumstances allows us to consider the boriding technique using induction heating as a promising approach to the creation of hardening coatings in the framework of conveyor technological lines in mass production, as well as for large volumes of parts creation per work shift.

An important component of the hardening process of parts by induction surfacing is the heating of hard alloy and flux particles in the surfacing charge [22]. At the same time, registration with an acceptable accuracy of temperature in the process of IS has certain technical and methodological difficulties. Firstly, the thickness of the coatings formed by the IS method varies within 1-3 mm, so the use of ordinary industrial and research thermocouples for this becomes impossible. Secondly, in the process of induction heating, the surface of the base metal emits a greater amount of energy (both in the form of heat and in a radiant way) than the coating being formed, therefore the pyrometric method of recording the temperature is also ineffective and reflects only the thermal state of the surface of the metal base. Third, due to the initial and constantly changing porosity of the deposited material, which is a multicomponent heterogeneous mixture, in the process of IS, all known contact thermometric methods give obviously irreproducible results [23].

An even more difficult task is the experimental study of the non-stationary temperature field when composite contact materials (CCM) are produced by the SHS method, when the dimensions of the object under study are also much smaller than the dimensions of standard temperature sensors.

The solution to the indicated problems can be achieved in several independent ways:

- by minimizing the primary sensor that is sensitive to the temperature of the coating, metal base, charge and its individual components;
- by using temperature-dependent processes in materials (both existing in the system and introduced from the outside) for unambiguous, reliable and reproducible registration of the temperature reached in the system;
- by using numerical modeling methods to determine possible mechanisms of SHS-pre-reaction nature at the interface.

The purpose of this work was to develop complex methods for recording and modeling temperature at phase boundaries in a heated mixture of metal powders during its melting and chemical interaction between components.

2. Material choices and design
In order to increase the efficiency of means of production in the implementation of processes of diffusion saturation of the surface of metals and alloys with boron, we, based on the analysis of published studies, proposed a set of measures, including heating of steel subjected to strengthening by borating and saturating media with high-frequency currents (HFC), a combination of technological stages of diffusion borating of liquid and solid media, as well as the transfer of the diffusion process of borating into the chemical interaction between the elements Fe and B [1, 2], carried out on the surface of the materials under study.
The basis for this line of reasoning in the study of a new approach to diffusion saturation of the surface of metals and alloys with boron in the implementation of a controlled topochemical reaction Fe + B, was the study [24], in which a method of differential thermal analysis (DTA) was proposed. The authors of the work showed how the chemical interaction in an inert, rarefied atmosphere between iron (its oxides present on the surface of steel) and boron, which leads to the formation of iron borides, begins at temperatures of about 500-700 °C and ends with the formation of d-metal borides.

Samples of the charge for IS of the following composition, wt. %, were selected as research objects: hard alloy - 85, fused flux - 15. Hard alloy material is PG-US27 and PS-14-60 powders (0.5-1.5 mm), fluxes are industrial compositions of ASM (Rubtsovsk), TsSM (Astana), ZOR (Odessa) grades.

For the manufacture of microthermocouples, chromel and alumel wire 0.2 mm (GOST (State standard) 1790-77), placed in fiberglass insulation, was used. The splices were made by fusing wires with a DC capacitor welding with a carbon electrode.

For the manufacture of thermoindicator compositions, we used powders of PNE grade nickel, ASD-1 grade aluminum, and PTK grade titanium.

To simulate thermal fields in the SHS-responsive CCM system, the nonstationary heat conduction equation was solved by numerical methods in the Mathcad 2011 environment.

3. Experimental results
The temperature of individual components of the surfacing charge, the surface of the base metal and the surface of the melt at the hard alloy-air interface can be measured with an acceptable accuracy (up to 3-5%) using microthermocouples, provided that the size of their junction will be from 0.1 to 0.3 of characteristic dimensions of the investigated structural element. For this, we prepared and calibrated chromel-alumel microthermocouples (MTC).

In the first part of the study, to measure the temperature of powder materials, including a hard alloy for IS, the working junction of a thermocouple was welded under a microscope (MBS-10) to a separate powder particle, in which the heating temperature was measured.

Figure 1 shows photographs of hard alloy particles with thermoelectrodes attached to them, welded to one and two planes of the particle.

The proposed method provides the measurement of the heating temperature of the hard alloy, taking into account the basic requirements for contact temperature sensors [2].

![Figure 1. Scheme of fixing thermoelectrodes to one (left) and two (right) planes of the particle (x20).](image)

The temperatures of heating of the hard alloy were measured at the boundaries of the charge-base metal and charge-air. The results obtained are quite reliable, since the shape and chemical composition of the working layer do not differ from the shape and chemical composition of individual particles of the heated powder material [3].
Figure 2. Generalized graphs of surfacing charge heating at the boundaries: base metal - charge (1) and charge-air (2).

Figure 2 shows the characteristic curves of heating the surface of the melt (1) and the surfacing charge (2) recorded by a self-recording device.

The experiments have shown that as the size of the hard alloy particles increases, the depth of penetration of the base metal decreases with unchanged surfacing modes. When surfacing a charge with a hard alloy particle size of 0.5-1.2 mm, the penetration depth was 0.40-0.50 mm. When surfacing particles of 2.0-3.0 mm, the penetration of the base metal was 0.30-0.35 mm, this is explained by the fact that a current is induced in large particles and heats them. Therefore, with an increase in the thickness of the deposited layer, it is advisable to increase the granules of the hard alloy.

It was also found that the intensity of heating of the hard alloy in the surfacing charge decreases as its fraction decreases. By means of the MTC, the heating temperature of the surfacing charge can be measured along the height of its filling at almost any point, including on its surface (charge-air boundary and in contact with a part, charge-part boundary).

However, in practice, it is also necessary to control the heating temperature of the surface of the part during the IS process. Traditional methods of temperature registration (thermocouple, pyrometer) have not found application in production due to the complex hardware design in the first case, and in the second - a large measurement error.

We measured the temperature of the part surface heated by high-frequency currents using two types of thermal indicators (TI): thermit mixtures, as well as mixtures of titanium, nickel and aluminum powders, which react with each other according to the SHS reaction [8].

The SHS process in the studied metal mixtures is clearly visible (Figure 3), since there is instantaneous heating and ignition of the entire TI sample.
Figure 3. Ignition of Ni-Al thermal indicator.

To calibrate the investigated Ni-Al and Ni-Ti TIs, a tungsten-rhenium MTC with a diameter of 0.2 mm was used, which was welded to a metal plate using capacitor welding, and a TI pellet was placed outside the mediocre proximity to the MTC and then the sample was heated in an inductor. On the temperature curve of heating the TI, a characteristic temperature spike is clearly visible, upon ignition of the powder mixture, which corresponds to the occurrence of SHS in it in the thermal explosion mode. The total temperature measurement error with such a hardware design of the method using a software and hardware complex did not exceed 3.5-4.5%.

Thus, the developed methods of complex registration of temperature in the process of induction surfacing make it possible to determine the melting temperatures of the surfacing charge and its individual components, the surface of the part, to study the features of thermal processes in the case of IS and allow, in the process of moving the part in the HF inductor, to determine the temperature fields on the surface to be hardened, and also promptly correct the operating modes of the HF generator.

For the second part of the study - numerical modeling and solving the non-stationary problem of heat conduction in the chosen CCM model, we will take some assumptions:

- we will assume that the sintering processes in each cell develop similarly;
- volumetric electrical power does not change during the synthesis of CCM;
- the temperature changes in the range of 20-1500 °C;
- lateral losses are realized due to convective exchange.

Taking these assumptions into account, the formulation of the problem is reduced to solving the well-known non-stationary heat equation:

\[
\frac{d}{dx} \left( K_{xx} \frac{d\varphi}{dx} \right) + \frac{d}{dy} \left( K_{yy} \frac{d\varphi}{dy} \right) + \frac{d}{dz} \left( K_{zz} \frac{d\varphi}{dz} \right) = \lambda \frac{d\varphi}{dt} \quad (1)
\]

Figure 4 shows the temperature profiles along the axis of the CCM cell, it can be seen that the temperature profile has a maximum at the junction of the copper fiber-powder mixture, a plateau in the powder mixture until \( t = 6.0 \) s and a second maximum located in the center of the powder workpiece through 8.0 s heating.
4. Conclusion
1. Complex methods of temperature registration in the process of induction surfacing based on the use of microthermocouples and SHS thermal indicators have been developed.
2. When registering the temperature by the microthermocouple method, it is possible to fix the melting temperatures of individual components of the charge and the temperature at the interfaces.
3. When registering the temperature by the thermal indicator method, the errors did not exceed 4.5%.
4. The calculation of the temperature field in the pre-reaction period in the electrosynthesis of CMC with allowance for contact phenomena has been carried out.

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Figure 4. Temperature profile along the axis of the CCM cell (after 1 second SHS).
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