Thermophysical model of electron beam boriding of carbon steel St3

D E Dasheev, N N Smirnyagina, A E Lapina and A S Milonov

Institute of Physical Materials Science SB RAS, 8 Sakhyanova Str., Ulan-Ude, The Republic of Buryatia, 670047, Russia

E-mail: dasheevdorzzo@gmail.com

Abstract. The work aims at developing a thermophysical model of electron-beam boriding of carbon steels. The main attention focuses on the physicochemical processes of the formation of iron borides occurring in the treatment zone by the electron beam. A thermodynamic study of phase equilibria in the systems Fe-B-C-O has been performed. On the basis of numerical calculations of temperature fields it is shown that temperature and time conditions of heating and cooling of steel determine the nature of structural transformations. Strength characteristics of iron boride layers have been determined. Then these layers obtained by different methods and using various source components have been thoroughly compared with each other during the analysis.

1. Introduction
Surface treatment of materials and coatings carried out in various ways with the aim of modifying the structure, improving strength and other properties, increasing service life, etc. [1–2]. Typical examples of high-temperature technological processes are laser and electronic technologies of welding, cutting, heat treatment, arc welding and other methods of joining materials, plasma coating and surface treatment technologies, etc. Treatment with the help of concentrated energy flows, under the influence of which a locally and globally heterogeneous structure is formed, belongs to a promising direction in this industry. The use of an electron beam as a heating source can significantly expand the possibilities of surface modification of alloys and metals. The formation of the structure and properties of the surface layers occurs directly during treatment and is the result of a variety of irreversible processes. For example, during electron beam treatment, heating and melting, redistribution of alloying elements are observed. In turn, changes in phase and chemical composition, as well as time-varying heterogeneous temperature field entail the appearance of mechanical stresses of different physical nature. Traditionally, mathematical modeling in this area is reduced to the calculation of the form of efficient energy sources, melting and crystallization processes under high-energy conditions, the phenomenon of sputtering of the surface layer or the hydrodynamics of melts [3–5].

The article deals with the construction of a mathematical model of thermal fields arising from the action of an electron beam on the sample. This article describes thermodynamic study of Fe-B-C-O phase equilibrium in a high vacuum. Thermal processes at electron beam treatment of different power have been analyzed and simulated.
2. Mathematical model

Various mathematical models are described in detail in [3–5]. The study of thermal processes in materials treated with highly concentrated electron fluxes is based on the solution of thermal conductivity problems:

\[ \rho c \frac{\partial T}{\partial t} = -\nabla \cdot J + \lambda \nabla T, \]

where \( c, \rho, \lambda \) – heat capacity, density and thermal conductivity, depending on temperature and coordinates.

Depending on the nature of the impact, the sources are volumetric and surface, stationary and moving, distributed and point [6].

The nature of the distribution of energy in the electron beam can be described by a Gaussian curve (figure 1) with a maximum in volume:

\[ q(x, y, z) = q_0 \exp \left[-(x^2 + y^2)k_1 - (z - h)^2k_2 \right], \]

where \( q_0 \) is the maximum power density of the heat source (determined by the current and voltage), \( k_1 \) is the concentration coefficient of the electron flow (similar to laser radiation), \( h \) is the position of the maximum heat release in the bulk of the material. You can determine the effective radius of the electron beam \( R_1 = 1/(k_1)^{1/2} \) and effective area of energy dissipation or electron penetration into the volume \( R_2 = 1/(k_2)^{1/2} \). Then, provided \( T = kt^* \gg R_2 \), where \( k = \lambda/(cp) \) is the coefficient of thermal diffusivity, \( t^* \) is the time characteristic of the process (for example, observation time), \( xT \) is the characteristic thermal scale, the energy source associated with the electron beam can be considered superficial. So, if the electron beam power density does not exceed \( q_0 \sim 10^5–10^6 \text{ W/cm}^2 \), the heat source can be considered surface. Surface treatment using an electron beam is carried out in scan mode. For frequencies above 50 Hz, the effective heat source is distributed and is characterized by a constant density \( q_0 \).

\[ \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho T(x, y, z) dx dy dz = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x, y, z; \tau) q_0 dx dy dz \]

where \( G \) is the Green function of this problem.

Integrating by spatial coordinates \( x', y', z' \) we obtain

Temperature at \( x, y, z \) coordinates [7]:

\[ T(x, y, z; \tau) = \frac{q_0}{c_p(4\pi\alpha \tau)^{1/2}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz G(x, y, z; \tau) \]

Figure 1. Scheme of energy input to the sample surface.

Temperature at \( x, y, z \) coordinates [7]:

\[ T(x, y, z; \tau) = \frac{q_0}{c_p(4\pi\alpha \tau)^{1/2}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz G(x, y, z; \tau) \]

where \( G \) is the Green function of this problem.

Integrating by spatial coordinates \( x', y', z' \) we obtain
\[ T(x, y, z, \tau) = \frac{q_0}{16c_0(4\pi\alpha\tau)^{3/2}} \times \int_0^\tau \text{erfc} \left( \frac{h(k_2)^{1/2} \left( 1 + \frac{Z \tau}{h_0} \right)}{\left( 1 + \frac{\tau}{\tau_0} \right)^{1/2}} \right) e^{-\frac{l^2}{4d^2(\tau + \tau_0)(\tau + \tau_1)^{1/2}}} d\tau, \]

where \( \tau_0 = \alpha k_1/4; \tau_1 = \alpha k_2/4. \)

From the equation it follows that the maximum temperature lies at the point with \( z = h, r = 0. \) Temperature at this point:

\[ T(x, y, z, \tau) = \frac{q_0}{16c_0(4\pi\alpha\tau)^{3/2}} \times \int_0^\tau \text{erfc} \left( \frac{h(k_2)^{1/2} \left( 1 + \frac{Z \tau}{h_0} \right)}{\left( 1 + \frac{\tau}{\tau_0} \right)^{1/2}} \right) \times 10^{(\psi(h_0)(h_0/\tau_0)^{1/2})} d\tau. \]

In conditions when \( \tau_1 \leq \tau_0, \tau \leq \tau_1. \)

3. The analysis of thermal fields and phase equilibria

The thermodynamics of phase equilibria in Fe-B-C-O systems has been studied in order to optimize conditions for forming functional layers on the surface of titanium and iron-carbon alloys as a result of electron-beam boriding in vacuum [8]. The crystallization fields of all possible phases have been defined, as well as temperature and pressure influence on its behavior has been determined (figure 2). Thermal properties and the character of Fe2B and FeB boride dissociation have been simulated depending on the total pressure in the system. Thus, the temperature and pressure influence on its behavior was determined. For example, an interaction of Fe2O3 with various boronizing components (B2O3, B4C, B) at pressure of 10^5 Pa begins at temperature of 1300–1600 K, as well as at pressure of...
10^{-2}–10^{-3} \text{ Pa} the temperature falls down to 850–900 \text{ K}. It is found that in mixtures with B\textsubscript{4}C and B the phase transformation should originally occur in condensed state with B\textsubscript{2}O\textsubscript{3} liquid phase formation.

![Phase equilibria in the Fe-B-C system](image)

**Figure 2.** Phase equilibria in the Fe-B-C system in the temperature range from 773 to 1173 \text{ K} under a pressure of 10^{-3} \text{ Pa}.

4. **Self-propagating high-temperature synthesis (SHS) of iron borides**

Fe\textsubscript{2}B and FeB layers have been synthesized from a reaction mixture containing boron carbide B\textsubscript{4}C, Fe\textsubscript{2}O\textsubscript{3} oxide, C carbon and the organic binder. During the experiment we used the electron beam installation of special design which is equipped with a powerful electron beam projector (gun) on thermal cathodes [9].
Figure 3. The isotherms in the system Fe-B-C at the pressure of 10⁻³ Pa.

Figure 3 shows the isotherms in Fe-B-C systems at pressure of 10⁻³ Pa which indicate significant release of the energy, that initiates SHS interaction process of Fe with B₄C resulting in the formation of iron carbide as a secondary phase with respect to the metal base. This may occur in the structure of the boride layer obtained by electron beam boriding. Hence, such studies of the boride layer structure support this assumption.

5. Experimental technique

During this experiment we used metal samples (St 3) in the form of cylinders of 15 mm diameter and 7 mm in height. The surface of a sample was coated by various stoichiometric compositions such as Fe₂O₃:3B:3C, Fe₂O₃:2B:3C. Then this coated surface was exposed to highly concentrated steams of energy which initiated the SHS process accompanied by the high heat release (exothermic reaction). Electron beam treatment was carried out in vacuum not higher than 2×10⁻³ Pa with electron beam power of 2.5×10⁶ W·cm⁻² for 1–3 minutes. Finally, we obtain solid combustion products, particularly iron borides [8].

At the pressure is 10⁻³ Pa, the temperature for generating iron borides is ~ 900 K which allows forming the layer without melting the steel surface but during the beam exposure accompanied by a large amount of energy due to SHS, the thin melt layer (5–7 µm) appears on a metal surface. This melted layer is embedded by boride particles which are evenly distributed throughout the whole surface. After the beam exposure the crystallization process results in the formation of a dendroid layer. Dendrites grow along the heat transfer perpendicular to thermal fields (figure 4a).

Figure 4. The structure of the boride layer Fe₂B + B₂O₃.
The study of layers structure confirmed this method of coating on the base of iron borides. Microstructure shows the principles of crystallization of the boride layer. Photos made by METAM PB-22 metallographic microscope with NEXSYS Image Expert provide a clear image of the visible boundary between the layer and the base as well as the zone of thermal exposure by the electron beam. The thickness of the whole layer runs up to 250 µm.

The study of layers’ microhardness obtained by this technique proves that the hardest borides are FeB of 1200–1500 MPa. The microhardness of Fe2B was 1100–1300 MPa. Separate particles located on the surface of a layer are the hardest with its microhardness of 3000–3500 MPa (figure 4b). The thickness of this microlayer is about 10 µm. Microhardness was measured using PMT-3 microhardness tester according to Vickers method (figure 4c).

6. Conclusion
This paper presents a thermophysical model of the formation of iron borides using a scanning electron beam. Thermodynamic study and analysis of thermal processes were performed and the phase equilibria of these structures were considered. It also provides investigations of strength properties of obtained iron boride layers that prove the significant increase of microhardness and wear resistance of studied materials.

Acknowledgments
The work was performed within the framework of the project for basic research programs of the Siberian Branch of the Russian Academy of Sciences (No. 0336-2016-0005).

References
[1] Pobol I L 1990 Metal Science and Heat Treatment 32 520
[2] Rykalin N N, Uglov A A and Zuev I V 1985 Laser and electron beam treatment of materials (Moscow: Mashinostroyeniye) p 217 [in Russian]
[3] Knyazeva A G, Kryukova O N, Bukrina N V and Sorokova S N 2010 Izvestiya Tomskogo politekhnicheskogo universiteta. Matematika i mehanika. Fizika 316 93 [in Russian]
[4] Knyazeva A G (2009) Vestnik PGTU. Mathematical modeling of systems and processes 17 66
[5] Knyazeva A G, Pobol I I, Gordienko A I, Demidov V N, Kryukova O N and Oleschuk I G 2007 Physical Mesomechanics 10 105
[6] Rykalin N N 1951 Calculations of thermal processes during welding (Moscow: Mashgiz) 296 p
[7] Polukonova A E, Smirnyagina N N and Dasheev D E 2015 Proceedings of the 4th international scientific-practical conference p 118
[8] Dasheev D E and Smirnyagina N N 2017 J. Phys.: Conf. Series 830 012070
[9] Dasheev D E, Smirnyagina N N, Khaltanova V M and Semenov A P 2015 J. Phys.: Conf. Series 652 012002