Naima Hadjadj[1,2], Bendaoud Mebarek[3], Yassine El Guerri[4], Mourad Keddam[5]

[1]Département Sciences de la Matière, Faculté des Sciences et Technologie, Université de Tissemsilt, BP 182, 38000 Tissemsilt, Algérie, [2]Laboratoire d'Etudes Physique des Matériaux, Université des Sciences et de Technologies USTO-MB, BP 1505 El M'Naouar, Oran, Algérie, [3]Laboratoire de Recherche en Intelligence Artificielle et Systèmes (LRIAS), University of Tiaret, Algeria, [4]Research laboratory of industrial technologies, University of Tiaret, Algeria, [5]Laboratoire de Technologie des Matériaux, Faculté de Génie Mécanique et Génie des Procédés, USTHB, B.P No. 32, 16111, El-Alia, Bab-Ezzouar, Alger, Algérie

Scientific paper
ISSN 0351-9465, E-ISSN 2466-2585
https://doi.org/10.62638/ZasMat1125

Zastita Materijala 65 (2)
220 - 235 (2024)

Dybkov model for the estimation of boron diffusion in the FeB/Fe_2B bilayer on AISI 316 steel

ABSTRACT

The aim of this work is to apply three models to simulate the boron diffusion in AISI 316 steel, with an approach based on classical mass balance equations, the Dybkov model and the integral method. From the numerical solutions of both models, the predicted values of layers'thicknesseshave been compared to the experimental results. In addition, in order to improve the predictability of the two models, it is necessary to find precise measurements on the diffusion of boron in each phase.The comparison of experimental and theoretical results allows us to confirm the validity of both models. After validation, the root mean square error and the diffusion coefficient were calculated to achieve good performance and better accuracy. The comparison of the results from the two simulation models with confronted with the experimental data to verify the validity of this theoretical study. Finally, the comparison of the derived results gave the values of the root mean square error equal to 1.6μm for Fe_2B and 0.75μm forFeB.

Keywords:*Boriding, diffusion, Iron borides, Dybkov model, Integral method*

1. INTRODUCTION

The purpose of treating materials is to improve or modify the mechanical and physical properties of a part [1-2], electrical conductivity, resistance to wear or friction, etc., to control its performance, resistance to corrosion, solidity, and to improve its external appearance [3]. The treatment of a material increases the life of a product [2].

For this reason, several processes have been developed to give the active surfaces of mechanical parts optimal properties in relation to the conditions of their use in service[1-4]. Among these surface treatments, emphasis may be put into the thermochemical treatments which include (nitriding, carburizing and boriding) [2].

The boriding treatment used to achieve hard layers that withstand wear and corrosion [2]. It can be carried out either in solid, liquid or gaseous phase [4].

The borides that are produced have interesting physico-chemical and mechanical properties for different industrial applications [1,5]. Single-phase or two-phase boride layers can be produced with this technique[6].The thermochemical method of boriding hardening can be applied to many ferrous, non-ferrous and cermet materials[1,2]. The process involves the diffusion of boron atoms into the base metal lattice by forming a hard interstitial boron compound on the surface [7].

The boriding process is based on a two-step reaction; the first step occurs between the boron source and the treated materiel [2,3]. Depending on time and temperature, the second step generates a boride layer at the substrate surface [8] by thermal diffusion.

The boride layer can be either mono-phased or bi-phased [9]. Themorphology of the layers can be tooth shaped or planar depending on the alloying elements present in the steel [1,10]. For carbon steel, the diffusion of boron atoms into the substrate gives rise to the formation of a (boride layers/substrate) interface with saw-tooth morphology [2]. For the high alloy steels, the generated (boride layer/substrate) interface tend to flatten [1-3].

Corresponding author: Naima Hadjadj
E-mail:naima.hadjadj@univ-tissemsilt.dz
Paper received: 27. 09. 2023.
Paper accepted: 15. 11. 2023.
Paper is available on the website: www.idk.org.rs/journal

Like all thermochemical surface treatments, boriding can be carried out by various processes and techniques in a solid medium in powders or with pastesor in a gaseous medium [11].

Powder boriding is realized in a temperature range between 1100-1300 K and a boriding time ranging from 2 to 24 hours [12]. In powder boriding, parts are placed in cases filled with powder and inserted into muffle furnaces. The advantages of such a process are, is the ability of changing the composition of the mixture powder [1,13].

Boriding provides a hardness gradient decreasing from the surface to the material core [14]. The hardness is much higher than that achieved through any other surface hardening process[15]. The combination of high hardness and low coefficient of friction improves the properties of resistance to fatigue, abrasion and wear [1,15]. Other benefits associated with boriding are retainingof hardness at elevated temperature, corrosion resistance in an acidic environment, and reduction in the use of lubricants [2,16].

The thickness of the resulting layer varies from 50 to 350 µm. This treatment makes it possible to obtain a very high surface hardness: from 1800 to 2000 HV for non-alloy steels, and up to 4000 HV for certain titanium alloys [1,2,17].

The thickness and proportion of each of the two borides depend on the chemical composition of the boriding medium, the temperature and the holding time[13,18].

Boron coatings are often developed on steels or iron to give them better resistance to corrosion and erosion[1,19]. Very hard layers of iron borides (FeB, Fe_2B) are formed on the surface of these materials [1,2]. FeB is harder than Fe_2B, but it is more brittle and more easily fractured duringimpact[1,2,20]. The structures of FeB and Fe_2B were known to be interstitial, FeB is orthorhombic and Fe_2Bphase crystallizes ina body-centered tetragonal structure[21].

Several researchers have carried out the modeling of boridingkinetics among them, Keddam et al [22, 23] whopresenteda simple model and the integral methodto simulate the boridingkineticsin powders. With the integral diffusion model, one can determinethe diffusion coefficients of boron in the FeB and Fe_2B layersandpredict their thicknesses. Twodifferentmodels have beenproposed by Campos et al [24], theirfirstmodel was based on artificial intelligence with the use of an artificial neural network and the second one used the least square approach. The alternative method called pulsed direct current powder boriding (PDCPB) process was also presented in [25].To study the boridingkinetics, Mebarek et al. [26] used fuzzy logic (FL) approach to model the diffusion of boron in steel, which is mainly based on a number of assumptions to estimate the kinetics ofboridelayer. To determine the effect of different parameters (temperature, boriding time, boron concentration) on this process, an LS-SVM method was employed[27], in another study, Dybkov et al.[28] have proposed and developed a kinetic approach. Theirmathematical model consisting in studying the growth of the bilayer (FeB/Fe_2B) on binary alloys.Through this approach, the parabolic growth law for boride layers was assumed and the kinetics can alternatively be described by a system of two nonlinear differential equations.For the calculation of the diffusion coefficient, many modelsexist and being used to estimate the value of this parameter [29,30]. In another work,ElGuerri et al [31] studied the impact of the diffusion coefficient calculation on predicting the boride layer thickness.

In this work, we were interested in studying the growth kinetics of FeB and Fe_2B layers using the three diffusion models based on Fick's second law. Subsequent calculations performed using these models aim to predict theboride layer thickness and boron concentration profiles in each phase, Generally the boron coefficient diffusion is calculated by an expression based on the experimental data. In this work we used three different models to calculate the boron diffusion coefficients in the boride layers produced on an AISI 316 steel by the powder technique andwe have studied the impact of the boron diffusivity on the kinetic simulation. In addition, the mass gains relative to the formation of FeB and Fe_2B layers were also evaluated. Finally, the three models were experimentally validated in the considered temperature range.

2. MATHEMATICAL MODEL OF DIFFUSION

The formation of iron borides layers is a phenomenon which is controlled by the diffusion process of boron atoms into the steel surface.The boron concentration profile is described by the solution of second Fick's diffusion equation for a semi-infinite medium given by Equation (1):

$$\frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i(x,t)}{\partial x^2} \quad (1)$$

The partial differential Equation (1) is of a parabolic type. It has analytical solution for the specific initial conditions detailed below.Where $C_i(x,t)$is the concentration of boron at depth x after diffusiontime (t), andD_i is the diffusion coefficient.

The growth process of FeB and Fe_2B layers will continue at the considered interface under the twopartial chemical reactions at the further stage, over prolonged time duration:

B + Fe_2B = 2 FeB and FeB + Fe = Fe_2B

Figure 1 illustrates the boron concentration distribution along the depth of surface-hardened layerfor a given temperature and under a boron potential that allows the formation of a two-phase layer (FeB/Fe_2B) on the substrate:

$C_{up}^{Fe_2B}$and$C_{low}^{Fe_2B}$ represent the values of the upper and lower boron levels in the Fe_2B layer,

$C_{ads}$is given as the amount of boron adsorbed on the surface of the material.

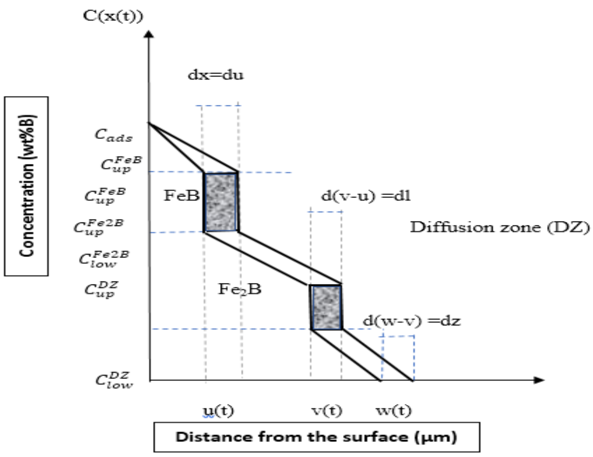

Figure 1.Schematic profile of boron concentration along the FeB and Fe_2B layers

Slika 1. Šematski profil koncentracije bora duž slojeva FeB i Fe_2B

C_0 is the limit of boron solubility in the substrate for which we subscribe a value of 35×10^{-4} % in weight of Boron, *u* and *v* are respectively the thicknesses of the FeB and (FeB+ Fe_2B) layers, which vary with the processing time according to the following equations:

$$u = k_1 t^{1/2} \quad (2)$$

$$v = k_2 t^{1/2} \quad (3)$$

where k_1 and $k_2$the parabolic growth rate constantsat the first and second interfaces.

The development of the models which we aim at proposing will be based on a set of conditions that will facilitate the calculations and render simpler mathematical formulae without prejudicing the integrity of the models when compared to experimental results. Thus,we firstly we consider only a flux of boron atoms perpendicular to the material surface, the temperature of the sample is set to be constant during the process, we also assume that the concentration of boron on the surface does not change with time and temperature. Iron boride is considered to grow parabolically over time, the boride layer is assumed to be sufficiently thin relative to the thickness of the sample, and finally the diffusion of Fe may be disregarded. Furthermore, the solution of the equation (1) can be obtained using the following boundary conditions set as follows:

$C_i\{x(t>0)=0\}=0,$

$C_{FeB}\{x(t=0)\} = C_{up}^{FeB}$=$C_B^{S/FeB}$

if C_{ads} >16.23% in boron weight (wt.% B),

$C_{FeB}\{x(t=0)\} = C_{low}^{FeB}ifC_{ads}$<16.23%

in wt.% B and with the FeB phase,

$C_{Fe_2B}\{x(t=0)\} = C_{up}^{Fe_2B}$if 8,83 in mass

B <C_{ads}<16.23% B weight and without the FeB phase,

$C_{Fe_2B}\{x(t=0)\} = C_{low}^{Fe_2B}ifC_{ads}$<8.83% B weight and without the FeB phase,

$C_{FeB}\{x(t=t)=u\} = C_{low}^{FeB},$

$C_{Fe_2B}\{x(t=t)=u\} = C_{up}^{Fe_2B},$

$C_{Fe_2B}(x(t=t)=v) = C_{low}^{Fe_2B},$

$C_{Fe}(x(t=t)=v) = C_0.$

The models which we aim at developing are designed to predict the thickness of bilayer based on the following parameters: (boron surface concentration, time and temperature).This model is used to predict the thickness of the boride layers based on the followingparameters: (boron surface concentration, time and temperature).

A simple model of the boride layer growth (FeB/Fe_2B)

For the phase (Fe_2B or FeB), as proposed by Kirkcaldy [32], the general solution of the equation (01) is given by the following equation:

$$C_i(x,t) = A_i + B_i erf\left(\frac{x}{2\sqrt{D_i t}}\right) \quad (4)$$

Where erf the Gauss errorfunction;A_i and B_i are constants to be determined according to the boundary conditions. The interfaces (FeB/Fe_2B) and (Fe_2B/Fe), shift by an infinitely small distance *dx,* which results from the flows in and out of the surface concerned, and is expressed by the following formulae:

$$W_{FeB}\frac{du}{dt} = \left(J_{FeB} - J_{Fe_2B}\right)_{x=u} \quad (5)$$

$$W_{Fe_2B}\frac{dv}{dt} + \sigma\frac{du}{dt} = \left(J_{Fe_2B} - J_{Fe}\right)_{x=v} \quad (6)$$

The models which we aim at developing are designed to predict the thickness of bilayer based on the following parameters: (boron surface concentration, time and temperature).This model is used to predict the thickness of the boride layers based on the followingparameters: (boron surface concentration, time and temperature).

A simple model of the boride layer growth (FeB/Fe_2B)

For the phase (Fe_2B or FeB), as proposed by Kirkcaldy [32], the general solution of the equation (01) is given by the following equation:

$$C_i(x,t) = A_i + B_i erf\left(\frac{x}{2\sqrt{D_i t}}\right) \quad (4)$$

where erf the Gauss errorfunction; A_i and B_i are constants to be determined according to the boundary conditions. The interfaces(FeB/Fe_2B) and (Fe_2B/Fe), shift by an infinitely small distance *dx,* which results from the flows in and out of the surface concerned, and is expressed by the following formulae:

$$W_{FeB}\frac{du}{dt} = \left(J_{FeB} - J_{Fe_2B}\right)_{x=u} \quad (5)$$

$$W_{Fe_2B}\frac{dv}{dt} + \sigma\frac{du}{dt} = \left(J_{Fe_2B} - J_{Fe}\right)_{x=v} \quad (6)$$

with

$$W_{FeB} = \frac{1}{2}\left(C_B^{\frac{S}{FeB}} - C_B^{\frac{FeB}{Fe_2B}}\right) + $$
$$+\left(C_B^{Fe_2B/FeB} - C_B^{FeB/Fe_2B}\right) \quad (7)$$

$$W_{Fe_2B} = \frac{1}{2}\left(C_B^{\frac{FeB}{Fe_2B}} - C_B^{\frac{Fe}{Fe_2B}}\right) + $$
$$+\left(C_B^{Fe/Fe_2B} - C_B^{Fe_2B/Fe}\right) \quad (8)$$

$$\sigma = \frac{1}{2}\left(C_B^{FeB/Fe_2B} - C_B^{Fe/Fe_2B}\right) \quad (9)$$

$$J_i = -D_i\frac{\partial C_i(x,t)}{\partial x} \quad (10)$$

with

$i = (FeB, Fe_2B, Fe)$.

The kinetics of the evolution of the thickness of the Fe_2B layer is a process limited by the diffusion of boron atoms in the Fe_2B layer. The evolution of this layer follows a parabolic law as a function of time.Where:J_i is the flows of boron atoms in phase i at depth x, and it is related to the gradient of the concentration. $k_1$andk_2 can be obtainedby solvingthe non-linear equations (04) and (05).And by simplifyingequations (4) and (5) we get:

$$W_1\frac{k_1}{2} = (-B_1D_1\frac{2}{\sqrt{\pi}}\frac{1}{2\sqrt{D_1t}}e^{-\frac{x^2}{4D_1t}} - A_2D_2\frac{2}{\sqrt{\pi}}\frac{1}{2\sqrt{D_2t}}e^{-\frac{x^2}{4D_2t}}) \quad (11)$$

$$W_1\frac{k_1}{2} = (-B_1D_1\frac{2}{\sqrt{\pi}}\frac{1}{2\sqrt{D_1t}}e^{-\frac{x^2}{4D_1t}} - A_2D_2\frac{2}{\sqrt{\pi}}\frac{1}{2\sqrt{D_2t}}e^{-\frac{x^2}{4D_2t}}) \quad (12)$$

where

$$A_1 = C_{FeB}^{up},\ B_1 = \frac{C_{FeB}^{low} - C_{FeB}^{up}}{erf(\frac{u}{2\sqrt{D_1t}})},\ A_2 = \frac{C_{Fe_2B}^{up}}{erfc(\frac{v}{2\sqrt{D_2t}})},\ B_2 = -A_2,\ A_3 = \frac{C_{Fe_2B}^{low}}{erfc(\frac{v}{2\sqrt{D_3t}})},\ B_3 = -A_2$$

After solving these two equations, the solution ($k_1$andk_2) is used to calculate the thickness of the boride layers(u andv), and also to determine the boron concentration with respect to the depth.

A diffusionmodel based on the integral method

This model considers [23] the growth of the Fe_2B and FeB layers in steel, the distribution of boron concentration along the two layers is described by a parabolic relationship.

In the integral method,the variation ofboron concentration with respect to time and the depth (distance) of diffusion in each boride layer is not linear and satisfies the second Fick law given by Equation (1).

The mathematical expressions of boron concentrations in each phase are essential to apply this approach, where they are considered to have a parabolic form as suggested by the Goodman method[33].Therefore, boron concentrations along the FeB$(0 \le x \le u)$ and $Fe_2B(u \le x \le v)$ layers are given respectively by the equations (14) and (15) as follows:

$$C_{FeB}(x,t) = C_{low}^{FeB} + a_1(t)(u(t) - x) + b_1(t)(u(t) - x)^2 \quad (13)$$

$$C_{Fe_2B}(x,t) = C_{low}^{Fe_2B} + a_2(t)(v(t) - x) + b_2(t)(v(t) - x)^2 \quad (14)$$

The parameters $a_1(t), b_1(t), a_2(t), b_2(t), u(t), v(t)$must meet boundary conditions. Thus, when applying these conditions at the surface and at the (FeB/ Fe_2B) we get respectively, equation (16 and 17):

$$a_1(t)u(t) + b_1(t)u^2(t) = \left(C_{up}^{FeB} - C_{low}^{FeB}\right) \quad (15)$$

$$a_2(t)[v(t) - u(t)] + b_1(t)[v(t) - u(t)]^2 = \left(C_{up}^{Fe_2B} - C_{low}^{Fe_2B}\right) \quad (16)$$

By integrating Fick second law between 0 and $u(t)$ for the FeB phase, and between $u(t)$ and $v(t)$ for the Fe_2B phase, and then by applying the Leibniz rule, we arrive at the following ordinary differential equations:

$$\frac{d}{dt}\left[\frac{u^2(t)}{2}a_1(t) + \frac{u^3(t)}{3}b_1(t) = 2D_1\ b_1(t)u(t)\right] \quad (17)$$

$$2\ w_{12}\frac{dv(t)}{dt} + \frac{[v(t)-u(t)]^2}{2}\frac{da_2(t)}{dt} + \frac{[v(t)-u(t)]^3}{3}\frac{db_2(t)}{dt} = 2D_2\ b_2(t)[v(t) - u(t)] \quad (18)$$

The two algebraic constraints applied on this diffusion problem can be derived Equations (17 and 18) from the continuity equation at the (Fe_2B/Substrate) interface as follows:

$$2\ w_1 b_1(t)D_1 \ = D_1\ a_1^2(t) - D_2\ a_1(t)(a_2(t) + 2b_2(t)[v(t) - u(t)]) \quad (19)$$

with $w_1 = [\frac{(C_{up}^{FeB}+C_{low}^{FeB})}{2} - C_{up}^{Fe_2B})]$:

$$2\ w_{12}b_1(t)D_1\ a_2(t) + 2\ w_2 b_2(t)D_2\ a_1(t) = D_2\ a_2^2(t)a_1(t) \quad (20)$$

with $w_2 = [\frac{(C_{up}^{Fe_2B}+C_{low}^{Fe_2B})}{2} - C_0]$ and $w_{12} = \frac{(C_{up}^{Fe_2B}-C_{low}^{Fe_2B})}{2}$.

Equations 16 and 21 form a Differential-algebraic system of equations (DAE) whose unknowns are $a_1(t), b_1(t), a_2(t), b_2(t), u(t), v(t)$, which satisfy the given algebraic constraints. This system (DAE) can therefore be solved analytically using the equation for the variation in the boride layer thickness in each phase.

To determine the coefficients of boron diffusion in each phase (FeB and Fe_2B), the following variable changes are made:

$$a_1(t) = \frac{\alpha_1}{u(t)},\ b_1(t) = \frac{\beta_1}{u(t)^2},\ a_2(t) = \frac{\alpha_2}{[v(t)-u(t)]},\quad b_2(t) = \frac{\beta_2}{[v(t)-u(t)]^2} \quad (21)$$

In which, the constants $\alpha_1, \beta_1, \alpha_2$ and β_2 should satisfy the boundary conditions. Thus, the expression of boron diffusion coefficients in the FeB and Fe_2B phases are calculated as follows:

$$D_1 \ = {k_1}^2\left[\frac{(C_{up}^{FeB}-C_{low}^{FeB})}{8\beta_1} - \frac{1}{24}\right],\quad for\ \beta_1 < \ 3\left(C_{up}^{FeB} - C_{low}^{FeB}\right) \quad (22)$$

$$D_2 \ = \frac{k_2(k_2-k_1)\left(C_{up}^{Fe_2B}-C_{low}^{Fe_2B}\right)}{4\beta_2} - (k_2 - k_1)^2\left[\frac{\left(C_{up}^{Fe_2B}-C_{low}^{Fe_2B}\right)}{8\beta_1} - \frac{1}{24}\right] \quad (23)$$

The relationships between constants α_1 and β_1, and between α_2 and β_2 are given respectively by:

$$\alpha_1 + \beta_1 = \left(C_{up}^{Fe_2B} - C_{low}^{FeB}\right) \quad (24)$$

$$\alpha_2 + \beta_2 = \left(C_{up}^{Fe_2B} - C_{low}^{Fe_2B}\right) \quad (25)$$

To determine the value of boron diffusion in each phase, it is important to calculate the value of β_2 from the β_1 using the following equation:

$$(\alpha_1^2 - 2\ W_1\beta_1)(\alpha_2^2 - 2\ W_2\beta_2) = 2\,W_{12}\beta_1\alpha_2(2\ W_{12} + \beta_2) \quad (26)$$

Dybkov Model

The further growth of boride layers is controlled by the diffusion step at the expense of boron element [34,35].The growth kinetics of boride layers at the diffusion stage of their formation is described by a system of two differential equations in dependence of treatment time at a given boriding temperature:

$$\frac{du(t)}{dt} = \frac{D_1}{u(t)} - \frac{rg}{p}\frac{D_2}{l(t)} \quad (27)$$

$$\frac{dv(t)}{dt} = \left(1 - \frac{q}{sg}\right)\frac{D_1}{u(t)} + (1 - \frac{rg}{p})\frac{D_2}{(v(t)-u(t))} \quad (28)$$

With *u(t)* and *l(t)* the thicknesses of FeB and Fe_2Blayers.The constant g depends on the molar volume of FeB and Fe_2B phases withg=0.60.As obtained from the stoichiometriccoefficients for phases FeBandFe_2B the constants were the following: p = 1, q = 1, r = 1 and s = 2.

3. CALCULATION OF THE BORON COEFFICIENT DIFFUSION

By the Dybkov Model (DM)

Based on this approach, [34,35]we can calculate the values of boron diffusion coefficients in FeB and $Fe_2B$by the twofollowing equations:

$$D_1 = \frac{0.5\ k_1}{(p - \frac{rq}{s})}[(p - rg)k_1 + rgk_2]$$

$$D_2 = \frac{0.5\ (k_2 - k_1)}{(1 - \frac{rq}{sp})}\left[k_2 + \left(\frac{q}{sg} - 1\right)k_1\right]$$

Therefore, the determination of these two parameters D_1 and D_2,requires the fitting of experimental results with Equations (2) and (3) to obtain the $k_1$andk_2 values.

By Arrhenius expression (AE)

The diffusion coefficient can be related to the processing time and thickness of the boride layer by Arrhenius expression. To estimate the boron activation energy, we must have a minimum of three processing temperatures with three durations for each temperature to obtain the corresponding layers' thicknesses. Based on the experimental data, we can estimate the activation energy of boron diffusion in the treatedsteel using the following Equation (30):

$$u^2 = D_1 t = D_0^1 \quad t.exp\left(-\frac{Q_1}{RT}\right) \quad (29)$$

$$v^2 = D_2 t = D_0^2\ t.exp\left(-\frac{Q_2}{RT}\right) \quad (30)$$

The variable u represents the thickness of FeBlayer and v that of (FeB+ Fe_2B) layer given in (μm), D_0^i is the boron diffusion coefficient ($\mu m^2/s$), t is the boriding time, $Q_i$is the value of the activation energy measured in Joule/mol, R is the gas constant and T is the temperature in Kelvin.It is easy to estimate the value of the activation energy Q_i using Arrhenius's Law in a linear form given by equation (29), where Q_i can be easily deduced from the slope of the straight line expressed in (kJ/mol).

$$ln(D_i\ ) = ln(D_0^i) - \frac{Q_i}{RT} i=1,2 \quad (31)$$

By the Integral method (IM)

Using the following equations provided for the Integral method,[23] we can calculate the boron coefficient diffusion in each phaseusing Equation (32 and 32):

$$D_1 \ = {k_1}^2[\frac{(C_{up}^{FeB} - C_{low}^{FeB})}{8\beta_1} - \frac{1}{24}] \quad (32)$$

$$D_2 \ = \frac{k_2(k_2 - k_1)\left(C_{up}^{Fe_2B} - C_{low}^{Fe_2B}\right)}{4\beta_2} -$$

$$-(k_2 - k_1)^2\left[\frac{\left(C_{up}^{Fe_2B} - C_{low}^{Fe_2B}\right)}{8\beta_1} - \frac{1}{24}\right] \quad (33)$$

4. EXPERIMENTAL PROCEDURE

We use the experimental of reference work [36], the process of boriding of AISI 316 steel was carried out with the powder technique using B_4C Durborid. This treatment was done atdifferent temperatures 1123, 1173, 1223 and 1273 K with processing duration between 2 and 10h.The chemical composition of the AISI316steel is given in Table 1.

Table 1. The chemical composition of AISI 316 steel (in % mass) [36]

Tabela 1. Hemijski sastav čelika AISI 316 (u % mase)[36]

Elements	C	Mn	Si	Ni	Mo	Cr	P	S
(wt %)	0.07	1.99	1.0	12.5	2.2	17.3	0.04	0.02

According to reference [36] and just before processing, all samples underwent a surface pre-treatment (preparation) with abrasive elements to eliminate any contamination that may interfere with boron diffusion. The thickness of the resulting boride layer (FeB and Fe_2B) was measured by optical microscopy. To ensure the accuracy of the layer thickness measurements, an average of ten measurements were taken on different locations of the cross-sections of the borided samples.

The measurement of the thickness of the boride layer adopts the following method, that consists in measuring with an optical microscope the lengths of the two deepest needles and those of the two shallowest needles and taking the average length of these four needles as the value of the thickness of the boride layer at the selected location.

Table 2. Experimental data of k_1 and k_2 [36]

Tabela 2. Eksperimentalni podaci za k_1 i k_2 [36]

	Growth rate constant (μm/s$^{0.5}$)	
Temperature	k_1	k_2
1123	0.068	0.145
1173	0.118	0.254
1223	0.157	0.337
1273	0.241	0.542

The experimental data facilitates the computation of growth rate constants; Table 2 illustrates the experimental growth rate constants for the two phases, where k_1 and k_2 represent the growth rate constants in the FeB and Fe2B phases, respectively.

5. SIMULATION RESULT AND DISCUSSION

The data concerning the boron diffusivity and the different concentrations are collected in Tab.3, these data were used in our simulation code.

Table 3. Data used in the simulation

Tabela 3. Podaci korišćeni u simulaciji

$C_{up}^{FeB} = 16.40\ wt.\%$ and $C_{low}^{FeB} = 16.23\%$	The maximum and minimum boron contents in FeB
$C_{up}^{Fe2B} = 9\%$ and $C_{low}^{Fe2B} = 8.83\%$	Stand for the maximum and minimum boron contents in Fe_2B
C_{ads}	The adsorbed concentration of boron
$C_0 = 35\times 10^{-4}\%$	Stands for the solubility limit of boron within the matrix

Calculation of diffusion coefficients in FeB and Fe_2B

Figure 2 representsthe calculated diffusion coefficients of boron in the FeB layer which varies exponentially as a function of temperature based on the three approaches (the integral model, Dybkov model and the Arrhenius expression). It is observed that the coefficient of the Arrhenius expression increases faster compared to the coefficients of other models which increase slowly with the temperature rise,for the calculation of the boron diffusion coefficienta good agreement between the three models at the temperature 1123 K and a good agreement between the integral model and the Dybkov model at the temperature 1273 K.

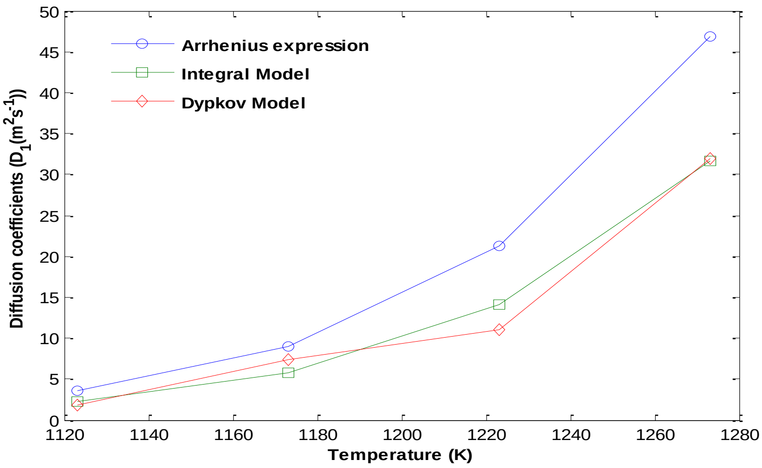

Figure 2. Calculation of boron diffusion coefficients in the FeB layers using the three models

Slika 2. Proračun koeficijenata difuzije bora u slojevima FeB koristeći tri modela

Figure 3 shows the calculated diffusion coefficients of boron in Fe_2B which vary exponen-tially versus the processing temperature with theintegral model, Dybkov model and the Arrhenius relationship.It is noticed that the coefficient estimated from the Arrhenius relationship increases speedily compared to the values determined from the integral method and Dybkov model.

Table 4 representsthe estimated values of boron diffusion coefficients in Fe_2B and FeB at temperatures between 1173 K and 1273 K for Arrhenius expression, integral model and Dybkov model. From theresults of Table 4, we determined the corresponding values of $D_0$and Q in FeB and Fe_2B layers with different models (see Table 5).

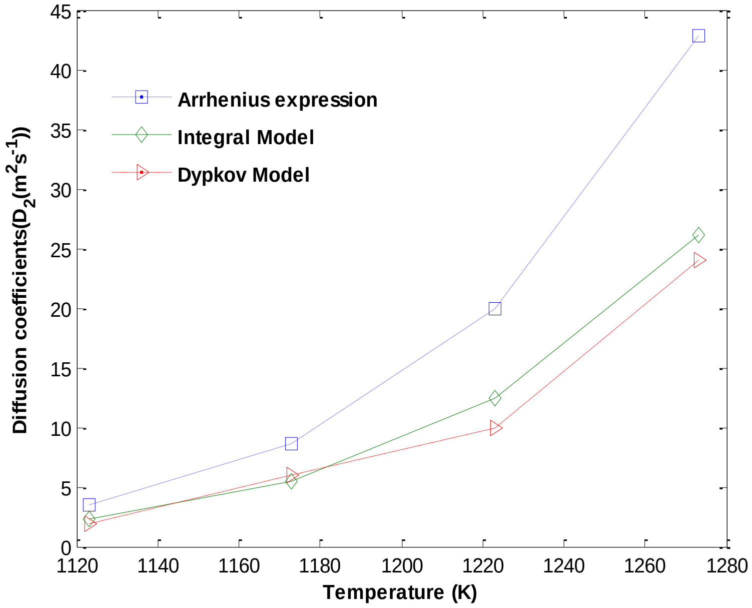

Figure 3. Calculation of boron diffusion coefficients in the Fe_2B layers using the three models

Slika 3. Proračun koeficijenata difuzije bora u slojevima Fe_2B korišćenjem tri modela

Table 4 representsthe estimated values of boron diffusion coefficients in Fe_2B and FeB at temperatures between 1173 K and 1273 K for Arrhenius expression, integral model and Dybkov model. From theresults of Table 4, we determined the corresponding values of $D_0$and Q in FeB and Fe_2B layers with different models (see Table 5).

Table 4. Calculated values of boron diffusion coefficients in the Fe_2B layers usingdifferent models

Tabela 4. Izračunate vrednosti koeficijenata difuzije bora u slojevima Fe_2B korišćenjem različitih modela

	Calculatedboron diffusion coefficient (m^2/s)					
Temperature (K)	***D_1***			***D_2***		
	Arrhenius expression	Integral Model	Dybkov Model	Arrhenius expression	Integral Model	Dybkov Model
1123	3.56×10^{-13}	2.23×10^{-13}	1.80×10^{-13}	3.51×10^{-13}	2.28×10^{-13}	1.90×10^{-13}
1173	9.05×10^{-13}	5.83×10^{-13}	7.38×10^{-13}	8.67×10^{-13}	5.52×10^{-13}	5.95×10^{-13}
1223	2.13×10^{-12}	1.41×10^{-12}	1.11×10^{-12}	1.99×10^{-12}	1.24×10^{-12}	10^{-12}
1273	4.68×10^{-12}	3.16×10^{-12}	3.20×10^{-12}	4.28×10^{-12}	2.61×10^{-12}	2.40×10^{-12}

Table 5. Calculated values of D_0 and Q in FeB and Fe_2B employing different models

Tabela 5. Izračunate vrednosti D_0 i Q u FeB i Fe_2B primenom različitih modela

	Boron diffusion coefficients (m^2/s)					
Temperature (K)	***D_1***			***D_2***		
	Arrhenius Expression +(AE)	Integral Model +(AE)	Dybkov Model +(AE)	Arrhenius expression +(AE)	Integral Model +(AE)	Dybkov Model +(AE)
D_0 $(\times10^{-4})$	11	14	22	5.5308	2.2487	2.0347
Q (kj/mol)	207.85	207.85	216.164	199.536	191.222	191.222

Table 6 provides a comparison between the activation energies of boron in various steels, as reported in previous research [37-42], and the values obtained in our study. An initial evaluation indicates variations in the activation energies. These variations can be related to a multitude of influential factors: the selection of the boronizing method, the temperature range applied, the methodology employed for the determination of boron activation energies,aand the chemical composition of the substrate.

Table 6. Values of bor on activation energies obtained in the case of borided steels using different methods

Tabela 6. Vrednosti bora na energijama aktivacije dobijene u slučaju boriranih čelika različitim metodama

Material	Boriding Method	Q (kj.mol^{-1})		Ref
		FeB	Fe_2B	
AISI 316	Powder technique	204	198	Campos et al [37]
AISIM2	Powder	220.2	213	NaitAbdellah et al.[38]
AISID2	Powder	a/ 207.84	197.04	Keddam et al [39] a:Dybkov model b:Integral model
		b/208.04	197.46	
AISI316	Plasma paste	118.12 (FeB+Fe_2B)		Keddam et al [40]
Royalloy steel	Powder	242.79	223	Orihel et al [41]
AISIM2	Paste	283	239.4	Campos et al [42]
AISI 316	Powder technique	a/207.85	199.536	This work a: Arrhenius expression b: Integral model c: Dybkov model
		b/207.85	191.222	
		c/216.164	191.222	

Layers' thicknesses of FeB and Fe_2B by the proposed models

In order to run numerical simulationsof the phenomena using the proposed model, the parameters needed are the temperature, boriding time and diffusivity of boron in each phase, as well as the concentration of boron. Whereas the kinetic data and boron activation energies for iron boriding were taken from the reference [6].

For the first model, the values of boron diffusion coefficients in the α-Fe and γ-Fe phases were found in references [6].The boron diffusion coefficients in iron borides (m^2/s) are given in the previous section. For the simple model, we used the values of $k_1$and k_2 to calculate the thickness of the boride layer (*u*and*v*).

For the diffusion integral method, to solve the system of algebraic-differential equations [23]a numerical method is employed, moreover, the thickness of the borided layer (Fe_2B) can be calculated using the following equation:

$$k_1 = \sqrt{\frac{D_1}{\frac{C_{up}^{FeB}-C_{low}^{FeB}}{8\beta_1}-\frac{1}{24}}} \quad (34)$$

$$D_2 = \frac{k_2(k_2-k_{*1})\left(C_{up}^{Fe_2B}-C_{low}^{Fe_2B}\right)}{4\beta_2} - -(k_2-k_1)^2\left[\frac{\left(C_{up}^{Fe_2B}-C_{low}^{Fe_2B}\right)}{8\beta_1}-\frac{1}{24}\right] \quad (35)$$

From the values of $\alpha_1/\beta_1/\alpha_2/\beta_2$ we! Calculate the parameter a_1, a_2, b_1, b_2, the estimation of this value allow to simulate the layer thickness FeB and Fe_2B.

The calculation of these thicknesses was done with Equations (36) and (37):

$$u(t) = \frac{\alpha_1}{a_1(t)} \quad (36)$$

$$v(t) = \frac{\alpha_2}{a_2(t)} + u(t) \quad (37)$$

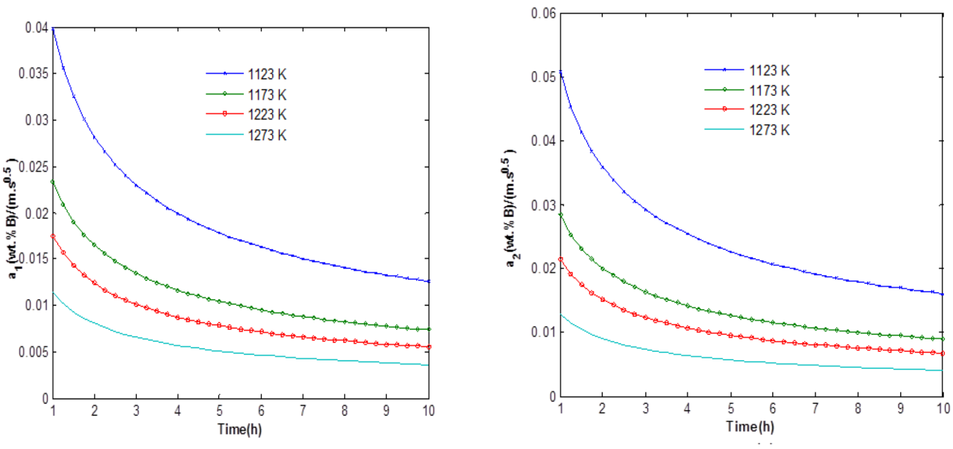

Figure 4. Values of a_1, a_2 parameters as function of time

Slika 4. Vrednosti parametara a_1, a_2 u funkciji vremena

Table 5 shows increase in the temperature-related growth rate constants for the two phases FeB and Fe_2B, there is a good agreement between the simulation resultsand experimental data.

The growth rate constants are noticed to change exponentially, and we obtained a good match between the simulation resultsand the experimental data.A comparison was made between the calculated values of growth rate constants and those determined empirically [36] and the results are displayed in Table 7.

Table 7. Comparing the calculated growth rate constants with the experimental ones

Tabela 7. Poređenje izračunatih konstanti brzine rasta sa eksperimentalnim

	Growth rate Constants (μm/s$^{0.5}$)							
	FeB				Fe_2B			
Temperature (K)	Exp [36]	Simulation			Exp [36]	Simulation		
		Simple Model	Integral Model	Dybkov Model		Simple Model	Integral Model	Dybkov Model
1123	0.069	0.07156	0.05712	0.0581	0.145	0.1522	0.1527	0.1561
1173	0.118	0.10970	0.09099	0.1110	0.254	0.2326	0.2399	0.2520
1223	0.157	0.16560	0.13950	0.1421	0.337	0.3592	0.3633	0.3600
1273	0.241	0.23830	0.20690	0.2201	0.542	0.5332	0.5325	0.5542

After determining the diffusivity of boron in each phase, the layers' thickness $u(t)$ and $v(t)$ can be estimated for a given time and temperature.

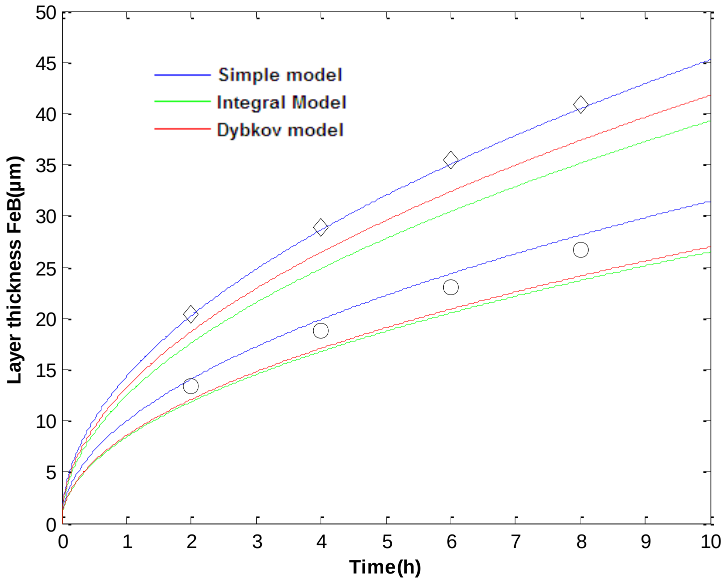

Figure 5. Comparison of calculated layers' thicknesses of FeB with the experimental data [36], using three models at 1223K and 1273K

Slika 5. Poređenje izračunatih debljina slojeva FeB sa eksperimentalnim podacima [36], korišćenjem tri modela na 1223K i 1273K

Figure 5 and 6 give the time evolution of estimated thicknesses of FeB and Fe_2Blayersatthe two temperatures 1223K and 1273K, using three models. We note that when the temperature increases, the diffusion process becomes very fast.

Table 7 shows that the threemodels have consistent results with the experimental data, which confirms their validity.With the proposed models we can calculate the thickness of each boride layer.

We can calculate the instantaneous velocities of the (FeB/Fe_2B) and (Fe_2B/diffusion zone) interfaces as follows:

$$v_{FeB} = \frac{du}{dt} = \frac{k_1}{2\sqrt{t}}\ v_{Fe_2B} = \frac{dv}{dt} = \frac{k_2}{2\sqrt{t}}. \qquad (38)$$

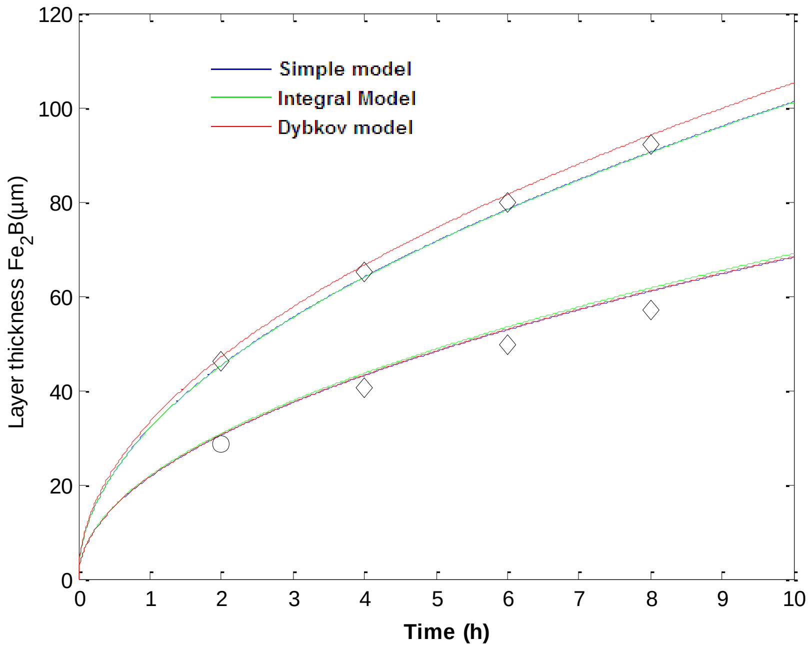

Figure 6. Comparison of calculated layers' thicknesses of FeB with the experimental data [36], using three models at 1223K and 1273K

Slika 6. Poređenje izračunatih debljina slojeva FeB sa eksperimentalnim podacima [36], korišćenjem tri modela na 1223K i 1273K

Figure 7 and 8 describe the time dependencies of the instantaneous velocities at the two growing interfaces using the three approaches: the simple model, the integral method and Dybkov model.

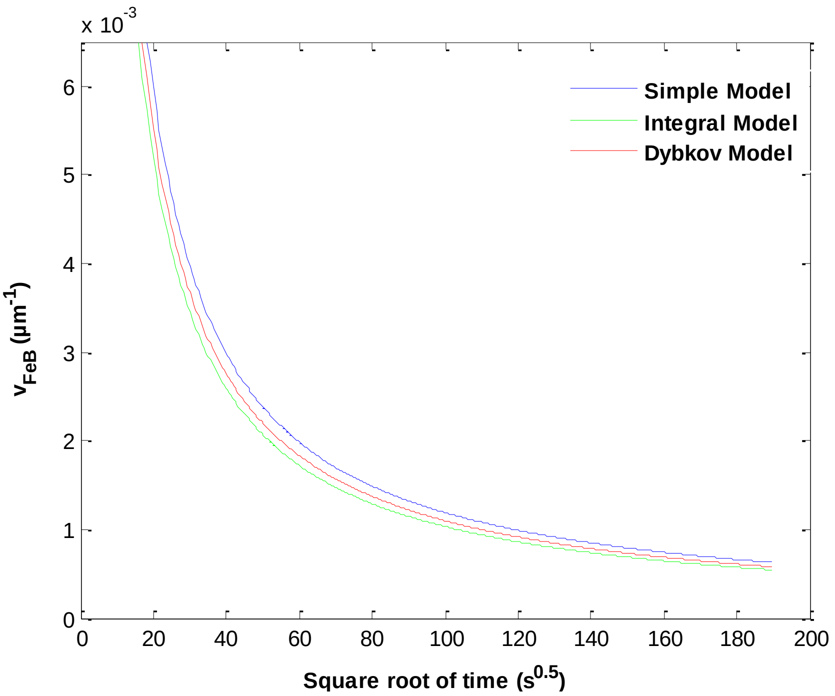

Figure 7. Calculated velocityat the first interface as a function of square root of time at 1273K

Slika 7. Izračunata brzina na prvom interfejsu kao funkcija kvadratnog korena vremena na 1273K

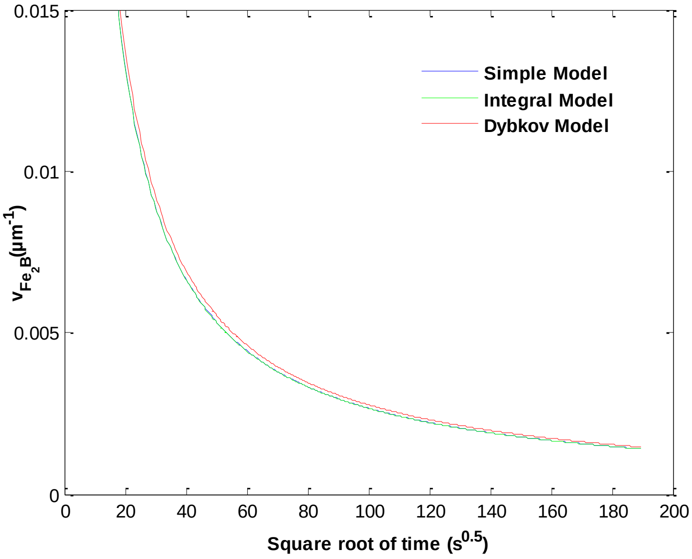

Figure 8. Calculated velocity at the second interface as a function of square root of timeat 1273K

Slika 8. Izračunata brzina na drugom interfejsu kao funkcija kvadratnog korena vremena na 1273K

6. MASS GAIN DETERMINATION

The mass gain for FeB and Fe_2B phases per unit surface [44] can be calculated using the following equations given by Equations (39) and (40):

$$G_{FeB} = \rho_{Fe_2B} w_2 t \frac{du}{dt} \qquad (39)$$

$$G_{Fe_2B} = \rho_{Fe} t((w_2 + w')\frac{du}{dt} + w_2 \frac{dl}{dt}) \qquad (40)$$

With $\rho_{Fe_2B} = 7.336\ g/cm^3$ and $\rho_{Fe} = 7.86\ g/cm^3$ is the density of Fe_2Blayer and the density of iron.

$$\omega_1 = \frac{(C_{up}^{FeB} + C_{low}^{FeB})}{2} - C_{up}^{Fe_2B}$$

$$\omega_2 = \frac{(C_{up}^{Fe_2B} + C_{low}^{Fe_2B})}{2} - C_0$$

$$\omega_{12} = \frac{(C_{up}^{Fe_2B} + C_{low}^{Fe_2B})}{2}$$

With the assumption that the Fe_2B and FeB layers form instantly.$G_{Fe\ \ B}(t)$ and$G_{Fe_2B}(t)$ are the values of mass gain per unit surface (g/cm^2).

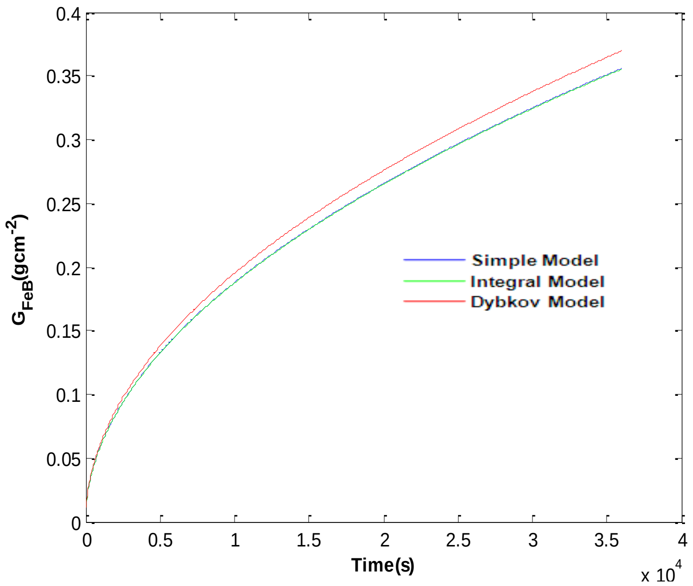

Figure 9. Calculated mass gain of the FeB layer versus the time duration at 1273 K

Slika 9. Izračunato povećanje mase sloja FeB u odnosu na vremensko trajanje na 1273 K

Figure 9 and 10 give the time dependences of calculated mass gain at a temperature of 1273 K using the three models. It is seen that that the values of mass gain determined for both phases increase with the treatment time. It is also worth noting that the mass gain relative to the FeB phase is greater than that of the Fe_2B phase.

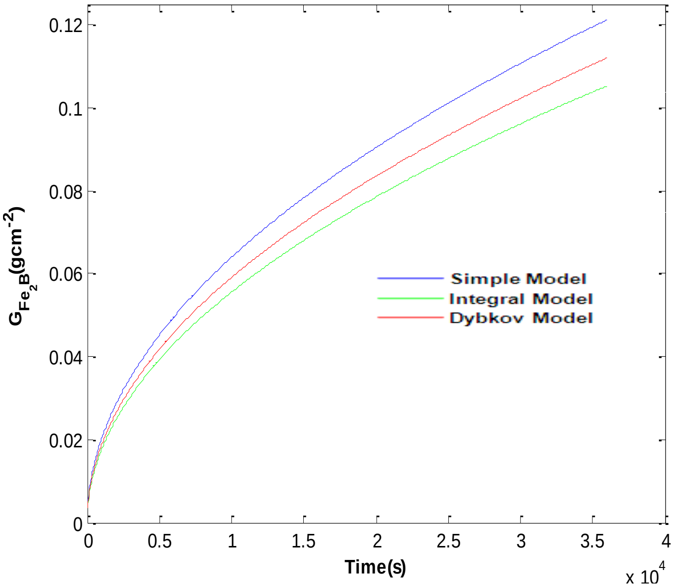

Figure 10. Calculated mass gain of the Fe_2B layer versus the time duration at 1273 K

Slika 10. Izračunato povećanje mase sloja Fe_2B u odnosu na vremensko trajanje na 1273 K

Figure 11 illustrates the calculated ratio (FeB to Fe_2B) in terms of thickness for different temperatures. It is noticed that the results from the integral and Dybkov models are very comparable except for 1173K. However the calculation results given by the simple model are higher than the values provided by Dybkov model and integral method.

Figure 12 displays the comparative ratios in terms of thickness for different processing temperatures by considering FeB and Fe_2 Blayers. Wecan notice that the simple method yield results close to the experimental values compared to the integral method and Dybkov model.

Figure 13 gives the estimated values of absolute error in terms of layers' thicknesses when comparing the three approaches. It is observed that the simple model yields minimum value of absolute error in comparison to the two other models. However, for the Fe_2B layer, the value of error absolute isminimum when applying the Dybkov model.

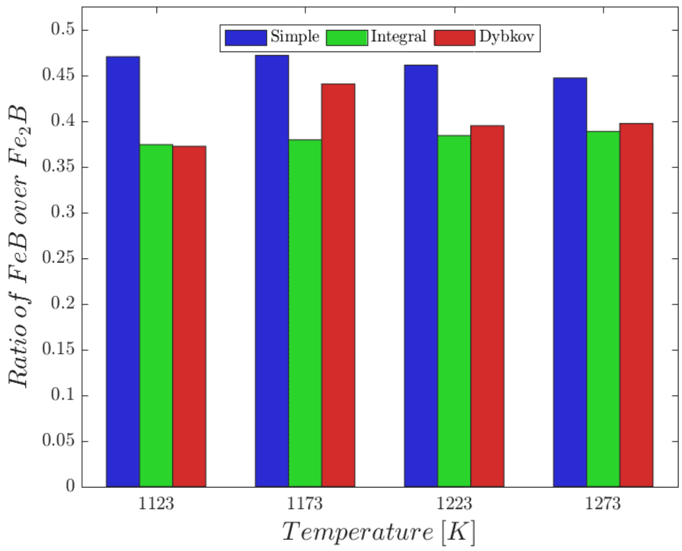

Figure 11. Calculated thickness ratio (FeB to Fe_2B) at increasing temperatures using three models

Slika 11. Izračunati odnos debljine (FeB prema Fe_2B) pri rastućim temperaturama korišćenjem tri modela

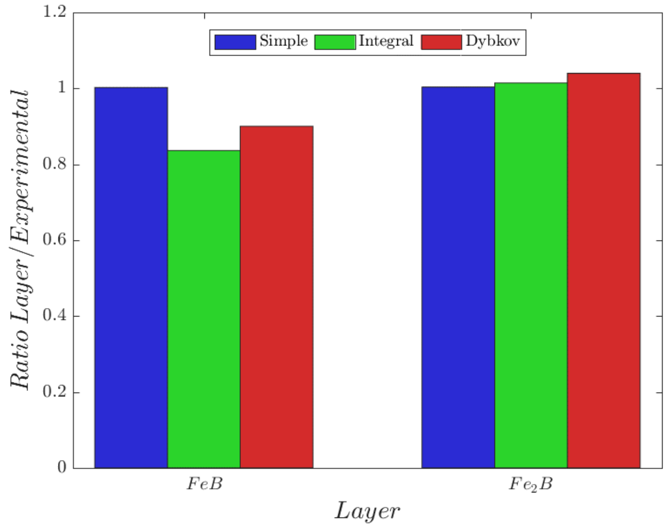

Figure 12. Ratio Simulation/Experimental vs layer

Slika 12. Odnos simulacije/eksperimentalnog prema sloju

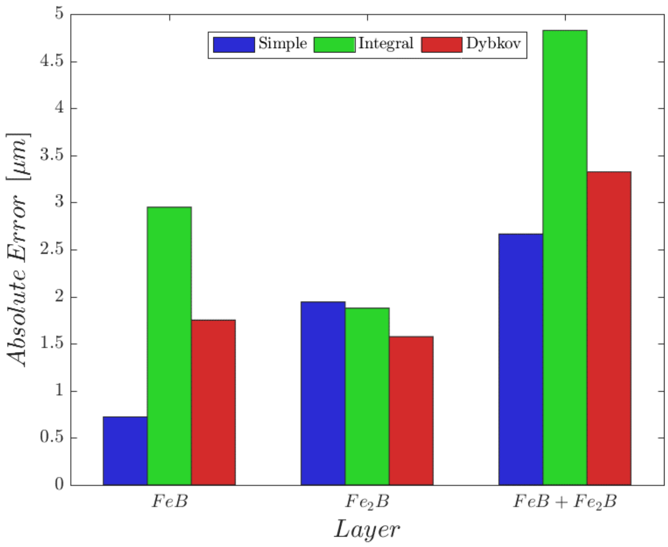

Figure 13. Estimation of absolute errorsin terms of layers' thicknesses

Slika 13. Procena apsolutnih grešaka u smislu debljina slojeva

7. CONCLUSION

In the present work, three different approaches were applied to estimate the boron diffusion coefficients in the FeB and Fe_2B layers formed on AISI 316 steel. The first kinetic approach used a simple model based on the Fick's laws while the second model employed the integral model. The third approach called the Dybkov model was also adopted by considering the experimental fitting parameters as the values of boron diffusion coefficients in FeB and Fe_2B.

These three models have been validated empirically by contrasting the simulated results with the experimental data found in the literature. A comparative study between the three models was achieved by calculating the absolute errors. In addition, the mass gain resulting from the formation of FeB and Fe_2B layers was estimated versus the time duration at 1273 K. The instantaneous velocities for the two growing interfaces were also evaluated. It is concluded that the estimated mass gain within the FeB layer was significant in comparison with that of Fe_2B layer.

8. REFERENCES

[1] M.Kulka (2019) Current Trends in Boriding. Techniques, Engineering Materials book series, *Springer International Publishing*. https://doi.org/10.1007/978-3-030-06782-3

[2] A.G.Matuschka (1980) Boronizing, Hayden and Son Inc, Philadelphia.

[3] A.K.Sinha, N.Boronizing (1991) ASM Int. handbook, The Materials International Society, *Materials Park*, OH, USA, 4 ,437-447.

[4] O.Allaoui, N.Bouaouadja, G.Saindernan (2006) Characterization of boronized layers on a XC38 steel*, Surf. Coat. Tech*. 201, 3475-3483. https://doi.org/10. 1016/ j.surfcoat.2006.07.238

[5] S.A.Bouaziz, N.Boudaoud, A.Zanoun (2009) Boruration thermochimique d'un acier C38 dans un bain de sels borax-SiC, *Matériaux et Techniques,* 97, 253-261. https://doi.org/10.1051/mattech/2009036

[6] M Keddam, SM Chentouf (2005) A diffusion model for describing the bilayer growth (FeB/Fe_2B) during the ironpowder-packboriding ;*Applied Surface Science*, 252(2),393-399. https://doi.org/10.1016/j.apsusc.2005.01.016

[7] B.Mebarek, D.Madouri, A.Zanoun, A.Belaidi (2015) Simulation model of monolayer growth kinetics of Fe2B phase, Matériaux et Techniques, 103, 703 . https://doi.org/10.1051/mattech/2015058

[8] B.Mebarek, A.Benguelloula, A.Zanoun (2018) Efect of Boride Incubation Time During the Formation of Fe_2B Phase, *Materials Research*, 21(1), 23-32. http://dx.doi.org/10.1590/1980-5373-MR-2017-0647.

[9] L.G.Yu, X.J.Chen, K.A.Khor, G.Sundararajan (2005) FeB/Fe_2B phase transformation during SPSpack-boronizing:Boride layer growth kinetics, *Acta Materialia* 53, 2361-2368. https://doi.org/10.1016/j.actamat.2005.01.043

[10] B.Mebarek, M.Keddam, M.Kulka (2021) Simulation of the incubation time for the formation of (FeB/Fe2B) bilayer on pure iron , KOM – Corrosion and Material Protection Journal, 65(2)49-56. https://doi.org/10.2478/kom-2021-0006

[11] B.Mebarek, S.A.Bouaziz, A.Zanoun (2012) Modèle de simulation pour l'étude de la boruration thermochimique de l'acier inoxydable «AISI 316» (X5CrNiMo17-12-2),*Matériaux & Techniques***,**100, 167-175, https://doi.org/10.1051/mattech/2012009

[12] S.Şahin (2009) Effects of boronizing process on the surface roughness and dimensions of AISI 1020, AISI 1040 and AISI 2714, *Journal of Materials Processing Technology*, 209(4),1736-1741, https://doi.org/10.1016/j.jmatprotec.2008.04.040

[13] B.Mebarek (2012) thèse de doctorat, Ecole Nationale Polytechnique d'Oran Maurice Audin.

[14] O.Delai, C.Xia, L.Shiqiang (2021) Growth kinetics of the FeB/Fe_2B boride layer on the surface of 4Cr5MoSiV1 steel: experiments and modelling, *Journal of Materials Research and Technology*, 11, 1272-1280, https://doi.org/10.1016/j.jmrt. 2021. 01.109

[15] M.X.Wei, S.Q.Wang, L.Wang, X.H.Cui, K.M.Chen (2011) Effect of tempering conditions on wear resistance in various wear mechanisms of H13 steel, *Tribol Int*, 44(7), 898-905, https://doi.org/ 10.1016/j.triboint.2011.03.005

[16] A.Günen et al (2019) Properties and Corrosion Resistance of AISI H13 Hot-Work Tool Steel with Borided B_4C Powders. *Metals and Materials International*. 26(9), 329-1340. doi.org/10.1007/ s12540-019-00421-0

[17] I.E.Campos-Silva, G.A.Rodriguez-Castro (2015) Boriding to improve the mechanical properties and corrosion resistance of steels, in Thermochemical surface engineering of steels Elsevier. 651-702. https://doi.org/10.1533/9780857096524.5.651

[18] B.Mebarek, M.Keddam (2019) Prediction model for studying the growth kinetics of Fe2B boride layers during boronizing. *Ingénierie des Systèmes d'Information*, 24(2), 201-205. https://doi.org/ 10.18280/isi.240212

[19] S.Sahin, C.Meric (2002) Investigation of the effect of boronizing on cast irons, *Materials Research Bulletin*, 37(5), 971-979, https://doi.org/10. 1016/S0025-5408(02)00697-9.

[20] B.Mebarek, M.Keddam, H.Boussebha (2020) Simulation model of the Growth Kinetics of Fe_2B Layers with Consideration of the Boride Incubation Time Effect, *Surface Review and Letters*, 27(04), 1950127 https://doi.org/10.1142/S0218625X19501270

[21] Ch.Kapfenberger, A.Barbara, P.Rainer, H.Hubert (2006) Structure refinements of iron borides Fe_2B and FeB; ZeitschriftfürKristallographie - Crystalline Materials, 221(5-7), 477-481. https://doi.org/10. 1524/ zkri.2006.221.5-7.477

[22] M.Keddam (2004) A kinetic model for the borided layers by the paste-boronizing process, *Applied Surface Science*, 236, 451-455. https://doi.org/ 10.1016/j.apsusc.2004.05.141

[23] M.Keddam, M.Kulka (2018) Simulation of the growth kinetics of FeB and Fe_2B layers on AISI D2 steel by the integral method. *Physics of Metals and Metallography,* 119(9), 842-851. doi.org/10.1134/S0031918X18090065

[24] I.Campos, M.Islas, G.Ramírez, C. Villa Velázquez, C.Mota (2007) Growth kinetics of borided layers: Artificial neural network and least square approaches, *Applied Surface Science*, 253(14), 6226-6231, https://doi.org/10.1016/j.apsusc.2007.01.070

[25] I.Campos-Silva, E.J.Hernández-Ramirez, A. Contreras-Hernández, J.L.Rosales-Lopez, E. Valdez-Zayas, I.Mejía-Caballero, J.Martínez-Trinidad (2021) Pulsed-DC powder-pack boriding: Growth kinetics of boride layers on an AISI 316 L stainless steel and Inconel 718 superalloy,*Surface and Coatings Technology*, 421, 127-404, https://doi.org/10.1016/j.surfcoat.2021.127404

[26] B.Mebarek, M.Keddam (2018) A fuzzy neural network approach for modeling the growth kinetics of FeB and Fe_2B layers during the boronizing process, *Matériaux et Techniques*, 06, 603-609. https://doi.org/10.1051/mattech/2019002

[27] B.Mebarek, M.Keddam, H.Aboshighiba (2018) LS-SVM approach for modeling the growth kinetics of FeB and Fe_2B layers formed on Armco iron, *Revue des Sciences et Technologie de l'information*, 23 (5), 29-41. https://doi.org/10.3166/ISI.23.5.29-41

[28] V.I.Dybkov, L.V.Goncharuk, V.G.Khoruzha, K.A. Meleshevich, A.V.Samelyuk, V.R.Sidorko (2008) Diffusional growth kinetics of boride layers on iron-chromium alloys. *SolidState Phenomena.* 138, 181-188.https://doi.org/10.4028/www.scientific.net/SSP.138 .181

[29] M. Keddam, B. Bouarour, Z.Nait Abdellah, R. Chegroune (2013) The effective diffusion coefficient of boron in the Fe_2B layers formed on the iron substrate, *MATEC Web of Conferences* 3, 01012, doi.org/ 10.1051/matecconf/20130301012

[30] S.Taktak (2006) A study on the diffusion kinetics of borides on boronized Cr-basedteels, *J. Mater. Sci.*, 41, 7590–7596. https://doi.org/10.1007/s10853-006-0847-4

[31] Y.ElGuerri, B.Mebarek, M.Keddam (2022) Impact of the diffusion coefficient calculation on predicting Fe_2B boride layer thickness, *KOM – Corrosion and Material Protection Journal*, 66(1), 25-35. https://doi.org/10.2478/kom-2022-0005

[32] J.S.Kirkaldy (1958) diffusion in multicomponent metallic systems: iii. The motion of planar phase interfaces, *Can. J. Phys*. 36 , 917-926.

[33] T.R.Goodman (1964) Application of integral methods to transient nonlinear heat transfer. *Adv. Heat Transfer*, 1,51-122. https://doi.org/10.1016/ S0065-2717(08)70097-2

[34] V.I.Dybkov (2010) Reaction Diffusion and Solid-State Chemical, Kinetics, 2nd ed., Trans Tech Publications, Zuerich.ISBN, 3038134457

[35] V.I.Dybkov (2013) Chemical Kinetics, IPMS Publications, Kyiv, Free online version http://www.dybkov.kiev.ua

[36] I.Campos-Silva, M.Ortiz-Domínguez, O.Bravo Bárcenas, M.A.Doñu-Ruiz, D.Bravo-Bárcenas, C. Tapia-Quintero, M.Y. Jiménez-Reyes (2010) Formation and kinetics of FeB/Fe_2B layers and diffusion zone at the surface of AISI 316 borided steels, *Surf. Coat.Technol*. 205, 403-214. https://doi. org/10.1016/j.surfcoat.2010.06.068

[37] I.Campos-Silva, M.Ortiz-Domínguez, C.Tapia-Quintero et al (2012) Kinetics and Boron Diffusion in the FeB/Fe2B Layers Formed at the Surface of Borided High-Alloy Steel. *J. of MateriEng and Perform*, 21, 1714–1723. https://doi.org/10.1007/ s11665-011-0088-9

[38] Z.NaitAbellah, M.Keddam (2014) Estimation of the boron diffusion coefficients in the FeB and Fe_2B layers during the pack-boriding of a high-alloy steel. Mater. Tehnol., 48, 237–242. http://mit.imt.si/ Revija/izvodi/mit142/abdellah.pdf

[39] M.Keddam, M.Kulka (2020) Simulation of Boriding kinetics of AISID2 steel by using two different approaches, *Met,Sci,Heat Treat*; 61,756–763. https://doi.org/10.1007/s11041-020-00496-2

[40] M.Keddam, R.Chegroune, M.Kulka, N.Makuch, D.Panfil, P.Siwak, S.Taktak (2018) Characterization tribological and mechanical properties of plasma paste boridedAISI 316 steel. *Trans. Indian Inst. Met*. 71, 79–90. doi:10.1007/s12666-017-1142-6

[41] P.Orihel, M.Drienovský, Z.Gabalcová, P.Jurči, M.Keddam (2023) Characterization and Boron Diffusion Kinetics on the Surface-Hardened Layers of Royalloy Steel, *Coatings*, 13,113-122. https://doi.org/10.3390/coatings13010113

[42] I.Campos, R.Torres, O.Bautista, G.Ramírez, L. Zúñiga (2006) Effect of boron paste thickness on the growth kinetics of polyphase boride coatings during the boriding process. *Appl. Surf,Sci*. 252, 2396–2403. http://dx.doi.org/10.1016/j.apsusc.2005. 04.022

[43] T.B.Massalski, H.Okamoto, P.R.Subramanian, L. Kacprzak (1990) Binary Alloy Phase Diagrams, Eds. ASM,480. ISBN: 978-0-87170-403-0

[44] M.Keddam (2011) Simulation of the growth kinetics of the (FeB/Fe_2B) bilayer obtained on a borided stainless steel,*Applied Surface Science*, 257(6), 2004-2010, https://doi.org/10.1016/j.apsusc. 2010. 09.043

IZVOD

DIBKOV MODEL ZA PROCENU DIFUZIJE BORA U DVOSLOJU FeB/Fe_2B NA ČELIKU AISI 316

Cilj ovog rada je primena tri modela za simulaciju difuzije bora u čeliku AISI 316, sa pristupom zasnovanim na klasičnim jednačinama bilansa mase, Dibkovljevom modelu i integralnoj metodi. Iz numeričkih rešenja oba modela, upoređene su predviđene vrednosti debljine slojeva sa eksperimentalnim rezultatima. Pored toga, da bi se poboljšala predvidljivost ova dva modela, neophodno je pronaći precizna merenja difuzije bora u svakoj fazi. Poređenje eksperimentalnih i teorijskih rezultata nam omogućava da potvrdimo validnost oba modela. Nakon validacije, izračunati su srednja kvadratna greška i koeficijent difuzije da bi se postigle dobre performanse i bolja tačnost. Poređenjem rezultata iz dva simulaciona modela suočena su sa eksperimentalnim podacima da bi se potvrdila validnost ove teorijske studije. Konačno, poređenje izvedenih rezultata dalo je vrednosti srednje kvadratne greške jednake 1,6 mm za Fe_2B i 0,75 mm za FeB.

***Ključne reči**: Boriranje, difuzija, boridi gvožđa, Dibkov model, Integralna metoda*

Naučni rad
Rad primljen: 27.09.2023.
Rad prihvaćen: 15.11.2023.
Rad je dostupan na sajtu: www.idk.org.rs/casopis