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Computational Model of Boride Diffusion Layer on the Low Carbon Steel

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Abastract: In this paper, a computation model was used to analysis the growth kinetic of two boride layers FeB and Fe_2B on the surface of low carbon steel. St41 one of the low carbon steel was used as the basic sample and given the treatment by adding the powder pack boriding in the temperature of 700, 800, and 900^0C for the 8 hours of treatment time. To perform the morphology and dimension of the boride layers used the optical microscope. The calculation model is based on the diffusion equation of Fick's law and is solved under certain assumptions with parabolic growth of iron boride. For this study, a numerical method was created to determine the thickness of the iron boride layer based on process parameters (temperature and time). Using the parabolic growth constant, it is possible to determine the diffusion coefficient for the FeB, Fe_2B phases and the diffusion region. Based on the diffusion coefficient it can be predicted the depth and thickness of borided layer on the surface of St41 low carbon steel. The diffusion coefficient of boron in the FeB phase is D_{FeB} = 5,67x10^{-14}exp(-99,72kJ/RT, while in the Fe2B phase it is D_{Fe2B} =1,03x10^{-13}exp(-58,17kJ/RT), and in the diffusion zone it is D_Z = 1,14x10^{-13}exp(-1,7kJ/RT). This result indicates that the larger the diffusion coefficient, the faster the diffusion process.

Keywords **:** *powder pack boriding, Fick's Law, parabolic growth constant, diffusion coefficient, FeB/Fe_2B layer.*
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INTRODUCTION

Boronizing is a surface hardening process that thermo chemical lasted. In this process occurs the dynamics change of heat [1], which can produce phase transformation on the basic sample [2]. The phase change can be determined by XRD analysis method [3]. Boronizing can be applied to hard the surface of ferrous and non ferrous metals. To determine the phases in the sample, it was observed using an optical microscope metallographic [4]. In general, the process of boronizing performed by heating treatment at a temperature between 700 ° C up to 1000^{O}C for 1 to 12 hours at a metal surface that has been cleaned [5]. In the process of boronizing occurs the contact between the metal surface as a sample base with hardener media in the form of paste, solid powder, liquid, and gas [6]. These contacts are intertition diffusion process, namely the inclusion of boron atoms (B) into the sidelines between the atoms of iron (Fe) [7]. Boronizing results obtained in the form of a layer of iron boride (FeB, Fe2B) with hardness between 1500-2000 HV and the depth of the layer can reach 300 µm from the surface of the sample base [6].

Mechanical properties of the iron boride layer can be determined through testing [8] while the growth process of the formation of iron boride layer on the surface of the sample can be computed using the numerical diffusion equation [9]. Research on the growth mechanism of thermo chemical iron borides have been conducted using a sample of 99.9% pure iron with a temperature of 850 ° C for 15 hours but the results still in qualitative form [10]. The next study for AISI 4140 steel as the samples heated at temperatures varying 1123, 1173, 1223K and treatment time 2, 4, 6 and 8 hours. This boronizing done with molten bath technique consisting of 65% borax, 15% boric acid, and 20% ferro-silicon produce boron growth constant of 3.10^{-9} to 2.10^{-8} cm^{-2}s^{-1} [11]. Growth kinetic of Fe_2B layer with various thickness of boron paste on AISI 1045 steel samples have produced the activation energy from 288.62 kJ for FeB layer and 253.402 kJ for the Fe_2B layer [12]. Growth diffusion model based on Fick's second law for a two layers of iron boride FeB and Fe_2B [13] and also on AISI H13 samples with powder pack boriding technique has been reported by researcher [14].

The next developments use computer simulation through the growth phase of iron boride paste boriding process. This model can be developed for application on another iron sample, because the results of simulations match with the experimental data [15]. Study of layer formed diffusion on the iron-based boride Cr has been done. Samples H13 steel and AISI 304 heated at temperatures of 1073 and 1223 for 3, 5, and 7 hours. This boronizing used bath salt slurry technique consisting of borax, boric acid, ferrosilicon and produce the activation energy of 253.35 and 244.37 kJ mol-1 [16]. The method of fuzzy logic, dimensional analysis and artificial neural network has been applied to measure the growth of boride layers on AISI 1045 steel samples with paste boriding technique. This boriding process is performed at a temperature of 1193 - 1273K for 2, 4, 6 hours and produce a feasible method to apply in industry with automation systems [17, 18, 19]. Besides the method of growth computation on boride layers mentioned above, there are other methods that use mass balance equations assuming a linear concentration profile at the boundary between the layers. The method has been applied to samples of AISI 1045 steel, M2, class 30 gray cast iron (ASTM A48), and gray cast iron. Boronizing process was done using paste boriding technique and powder-pack heated at temperatures of 1173, 1223, and 1273K for 2, 4, 6, 8 hours [20,21,22].

RESEARCH METHODS

A computation model to determine the diffusion coefficient derived from a scenario involving a solvent saturated with solute B. The chemical potential B of surrounding conditions are such that they are capable of forming one or more phases on the surface of steel samples St41. At the stage of equilibrium components A and B form FeB phase, Fe_2B and diffusion zones.

The concentration profile exhibits the growth of two or more phases with a linear progression, and it is presumed that the boron concentration remains constant throughout the process of layer growth.. Thermodynamic equilibrium is achieved at all times during the boriding process. Therefore, according the concentration profile for the three phases below (figure 1), it can be used the following computation model [20] :

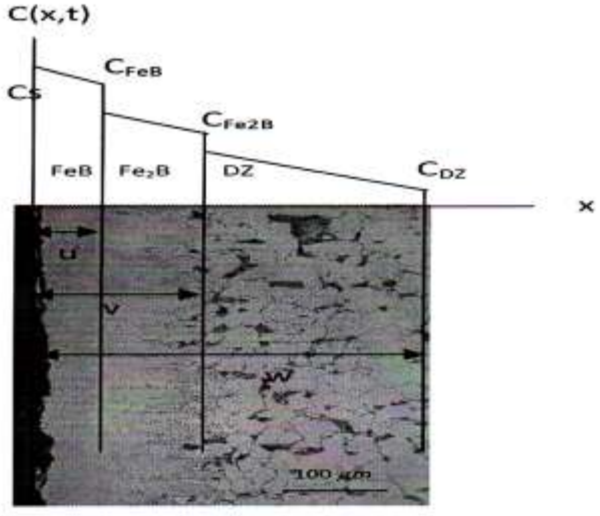


Figure 1. Boron concentration profile for three phases FeB, Fe_2B, and diffusion zone.

for :

$$0 \leq x \leq u \quad ; \qquad C_1(x,t) = \frac{C_{FeB} - C_s}{u} x + C_s \tag{1}$$

$$u \leq x \leq v \quad ; \qquad C_2(x,t) = \frac{C_{Fe_2B} - C_{Fe_B}}{v-u} (x-u) + C_{FeB} \tag{2}$$

$$v \leq x \leq w \quad ; \qquad C_3(x,t) = \frac{C_{DZ} - C_{Fe2_B}}{w-v} (x-v) + C_{Fe2B} \tag{3}$$

$$\text{where :} \qquad u = k_1 \sqrt{t}\,; \quad v = k_2 \sqrt{t}\,; \quad w = k_3 \sqrt{t} \tag{4}$$

C(x, t) represents the concentration with respect to both x and t. C_1 (x, t) signifies the boron concentration within the range from the surface to the initial interface, while C_2 (x, t) denotes the boron concentration between the first and second interfaces. C_3 (x, t) represents the boron concentration in the diffusion region, and C_{DZ} stands for the concentration within the diffusion zone. C_{FeB} indicates the concentration at the FeB interface, C_{Fe2B} represents the concentration at the Fe_2B interface, and Cs denotes the concentration above the surface.

Furthermore, the variable t represents the duration of heating, with k1 being the parabolic growth constant for the FeB interface, k2 for the Fe_2B interface, and k3 for the diffusion region. The parabolic growth functions u, v, and w correspond to the FeB interface, Fe_2B interface, and the diffusion region, respectively. The distance x denotes the distance to the steel surface.

$$(-C_s + C_{FeB})\frac{du}{dt} = D_{FeB}\frac{dC_1}{dx} - D_{Fe2B}\frac{dC_2}{dx} \tag{5}$$

$$(-C_{FeB} + C_{Fe2B})\frac{dv}{dt} = D_{Fe2B}\frac{dC_2}{dx} - D_{DZ}\frac{dC_3}{dx} \tag{6}$$

$$(-C_{DZ} + C_{Fe2B})\frac{dw}{dt} = D_{DZ}\frac{dC_2}{dx} \tag{7}$$

Here, D represents the diffusion coefficient of the solvent on the surface, Do is the pre-exponential factor ($m^2\ sec^{-1}$), D_{Dz} is the boron diffusion coefficient in the diffusion region, D_{FeB} is the diffusion coefficient of boron at the FeB interface, and DFe2B is the diffusion coefficient of boron at the Fe_2B interface. Assuming that the interface conditions adhere to the parabolic growth law and employing a concentration function as described in equations (5), (6), and (7), the following system of simultaneous equations can be derived:

$$\frac{1}{2}(C_{FeB} - C_S)k_1 = D_{FeB}\frac{(C_{FeB}-C_S}{k_1} - D_{Fe2B}\frac{(C_{Fe2B}-C_{FeB})}{k_2-k_1} \tag{8}$$

$$\frac{1}{2}(C_{Fe2B} - C_{FeB})k_2 = D_{Fe2B}\frac{(C_{Fe2B}-C_{FeB})}{k_2-k_1} - D_{DZ}\frac{(C_{DZ}-C_{Fe2B})}{k_3-k_2} \tag{9}$$

$$\frac{1}{2}(C_{DZ} - C_{Fe2B})k_3 = D_{DZ}\frac{(C_{DZ}-C_{Fe2B})}{k_3-k_2} \tag{10}$$

This system of equations can be solved to determine the mobility of boron in the layer FeB, Fe_2B and diffusion zones with Newton-Raphson numerical method (20). Mobility is indicated by the boron diffusion coefficient value for each layer that is D_{FeB} , D_{Fe2B} , and D_{DZ}.

Samples used in this study is cylindrical shape of St41 low carbon steel with a diameter of 3 cm and 1 cm high. The chemical composition of the sample is as shown in table 1.

Table 1. The chemical composition of sample

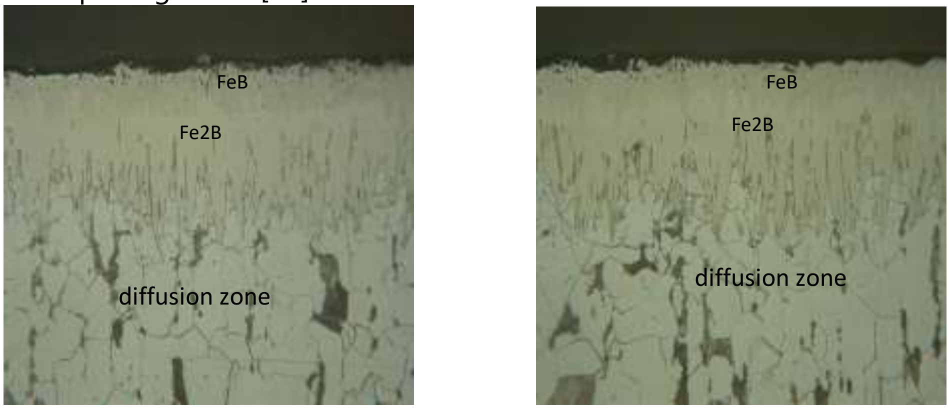
Element	**C**	**Si**	**Mn**	**P**	**S**	**N**	**Cu**	**Nb**	**Ti**	**Al**	**Cr**	**Mo**	**Ni**	**Vi**
Wt%	0.2	0.8-1.4	0.03	0.025	0.015	0.012	0.3	0.02	0.03	0.02	0.3	0.08	0.3	Bal

The specimens were immersed in a boriding agent powder pack comprising 5wt% B_4C, 5wt% KBF4, and 90wt% SiC. Afterwards, the samples were heated in the furnace with temperature of 700°C, 800°C, 900°C and 8 hours treatment time. After heated sample was cooled to room temperature.

To show the morphology of iron boride, layer thickness, and diffusion zones, the sample was done a cross-sectional cutting and observed using optical microscopy. To determine the layer thickness, minimum 15 measurements were done on boride layers and diffusion zone at different points on the sample. To ensure the phases of iron borides in boride layer on the surface of samples used XRD analysis with Cu and Mo radiation and wave length between 0.6 and l.9 A°.

RESULTS AND DISCUSSION

Morphology and development of the boride layer on St41 low carbon steel with a treatment time of 8 hours and temperature of 700^{O}C, 800^{O}C, and 900^{O}C are shown in figure 2. The thickness of the layer was determined as the mean length of the elongated boride protrusions [20]. On the St41 low carbon steel for all temperature treatment was formed two boride layers FeB and Fe_2B. It can be seen on the pattern of XRD data (see figure 3). The growth change of iron boride is determined by the thickness of the boron powder package. It controls the surface concentration of the specimen and attains the crucial concentration threshold for the development of boride phases [20]. The variation in boron potential energy under constant time and temperature leads to the formation of denser and more uninterrupted layers as the thickness of the boron powder package rises [20].



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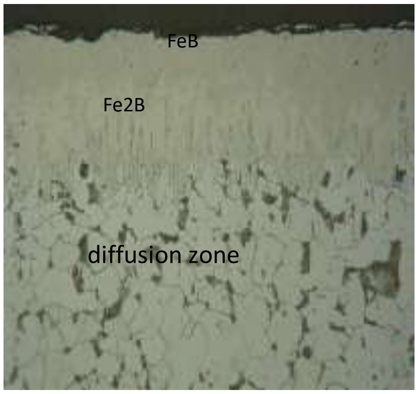

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Figure 2. View of borided cross-sections (St41 steel) treated at (a)700^{O}C, (b) 800^{O}C, and (c) 900^{O}C for 8 hours with powder pack boriding thickness.

On the same condition, the increment of present phases growth kinetic showed the dependence of time and temperature. Elevating the duration, temperature, and boron potential results in substantial precipitation of Fe_2B iron boride beneath the layers, influenced by the chemical composition of low carbon steel St41. The figure 4 illustrates the progression of boride layers and the diffusion zone concerning the process time. Values of the slopes presented in figure 4 shows the growth of boride layers and diffusion zone. The parabolic growth constants listed in Table 1 are contingent on the equilibrium between boron concentration and the surface of the reference sample.

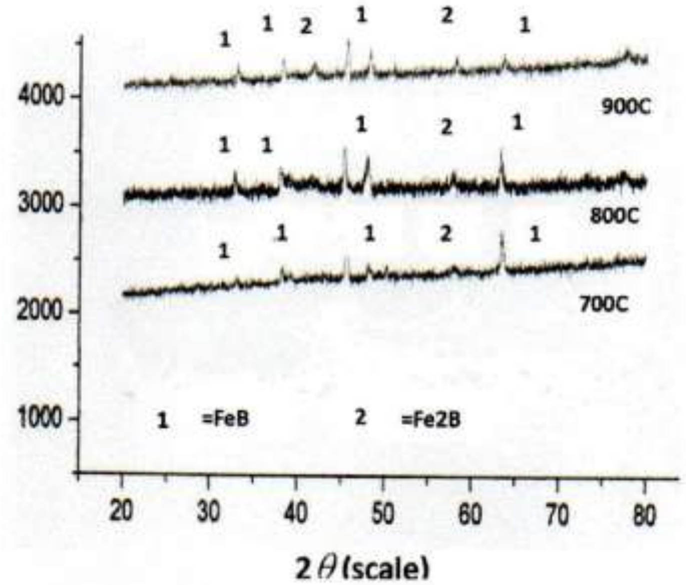
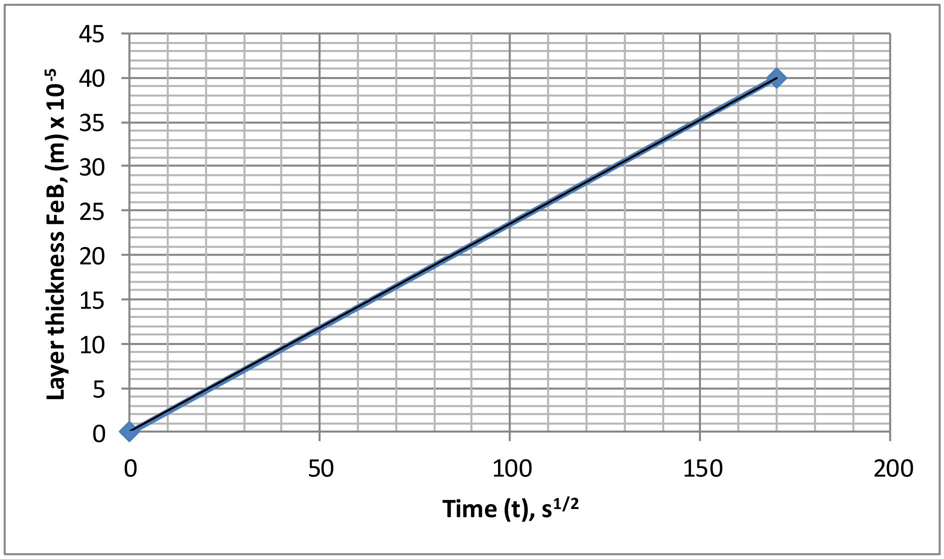


Fig. 3. Pattern of XRD data for St41steel borided at 700, 800, and 900 Celcius with 8 hours of treatment.

To determine the diffusion coefficients of boron on the boride layers and diffusion zone used the concentration value at interfaces and the parabolic growth constans from mass balance equation (8), (9), and (10).

The parabolic growth constants for St41 low carbon steel exhibit their peak values on the FeB, Fe_2B phases, and diffusion zone at a temperature of 900°C during an 8-hour heat treatment (Table 1).

The average diffusion coefficients are presumed to follow Arrhenius behavior. This pattern assesses these coefficients in relation to temperature, with Q/R denoting the slope depicted in Figure 5. The activation energy, Q, is construed as the boron diffusion along the favored crystallographic direction [0 0 1] [20]. Specifically, the activation energy for the FeB phase surpasses that of the Fe_2B phase, and similarly, the activation energy for Fe_2B exceeds that of the diffusion zone.



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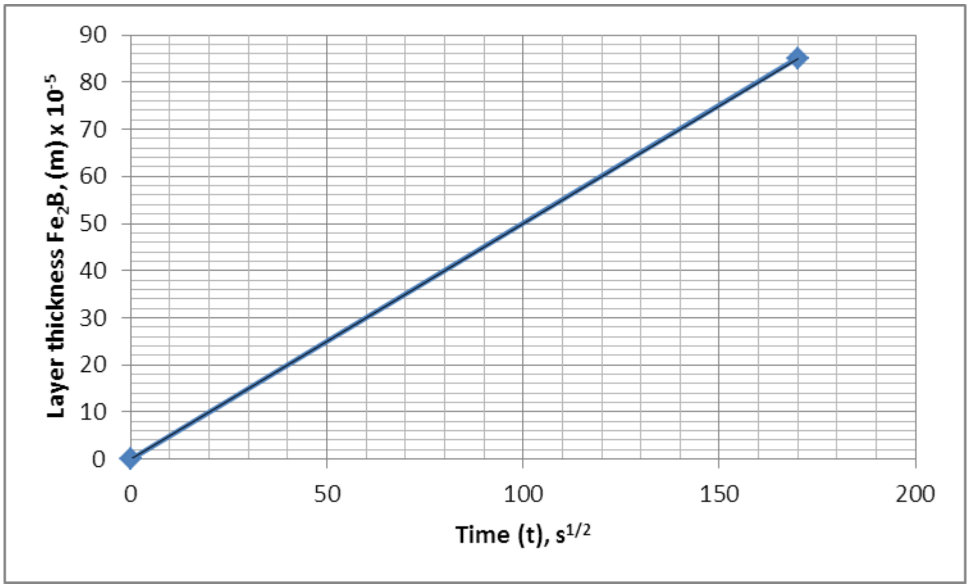

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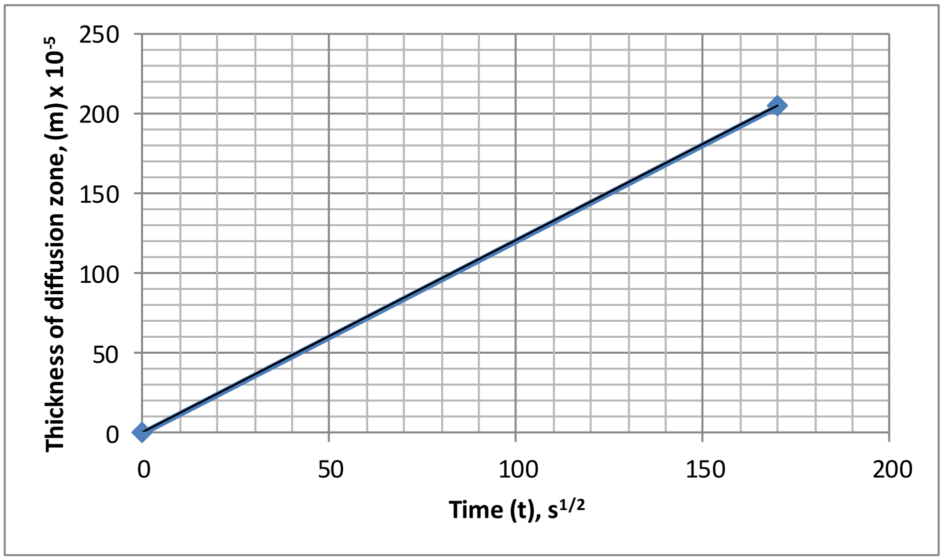

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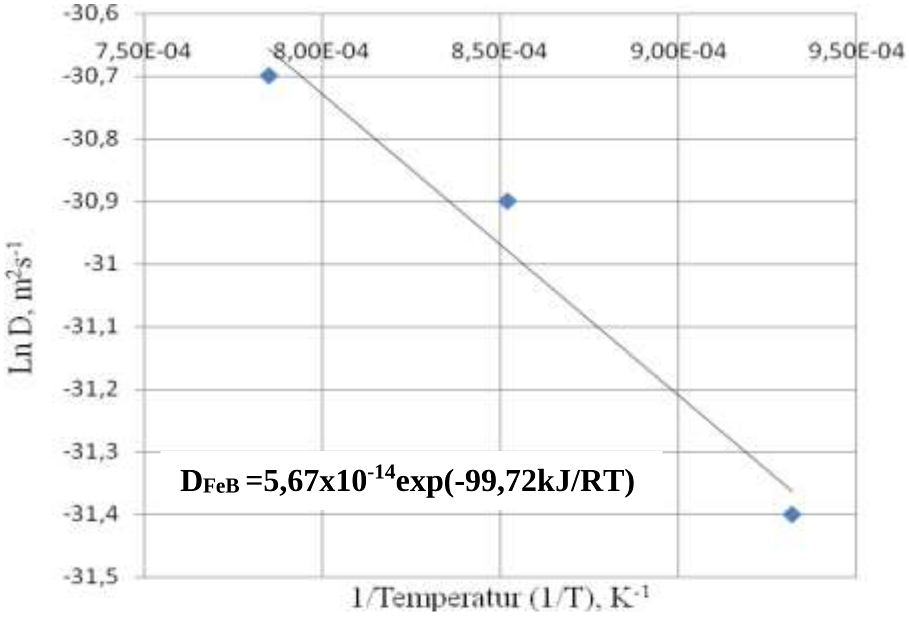
Figure 4. Growth kinetics of iron boride layers and diffusion zone for St41 low carbon steel: (a) FeB, (b) Fe_2B and (c) diffusion zone.

Figure 5 illustrates that the activation energy for boron within the FeB layer surpasses that of the Fe_2B layer. Furthermore, the activation energy for boron in the Fe_2B layer exceeds that of the diffusion zone for St41 low carbon steel.

Table 1. Parabolic growth constants for the St41 low carbon steel at temperature of 700, 800, and 900^{O} C with 8 hours of treatment time.

Layer	Parabolic growth constant (k)		
	T = 700^{0}C	T = 800^{0}C	T = 900^{0}C
Surface	0	0	0
FeB	0.147	0.166	0.220
Fe_2B	0.250	0.282	0.457
Diffusion Zone	0.590	0.610	0.610

Therefore, the Arrhenius relationship gives the diffusion coefficient of boron above FeB, Fe_2B phases, and diffusion zone on the St41 low carbon steel at the temperature range of 700^{O}C $\leq$ T $\leq$ 900^{O}C can be written as:



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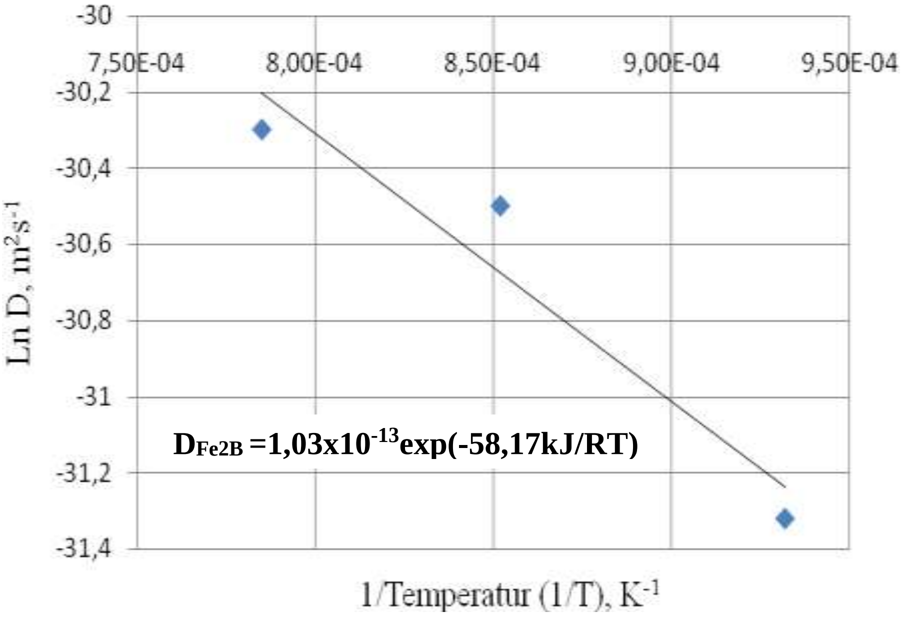

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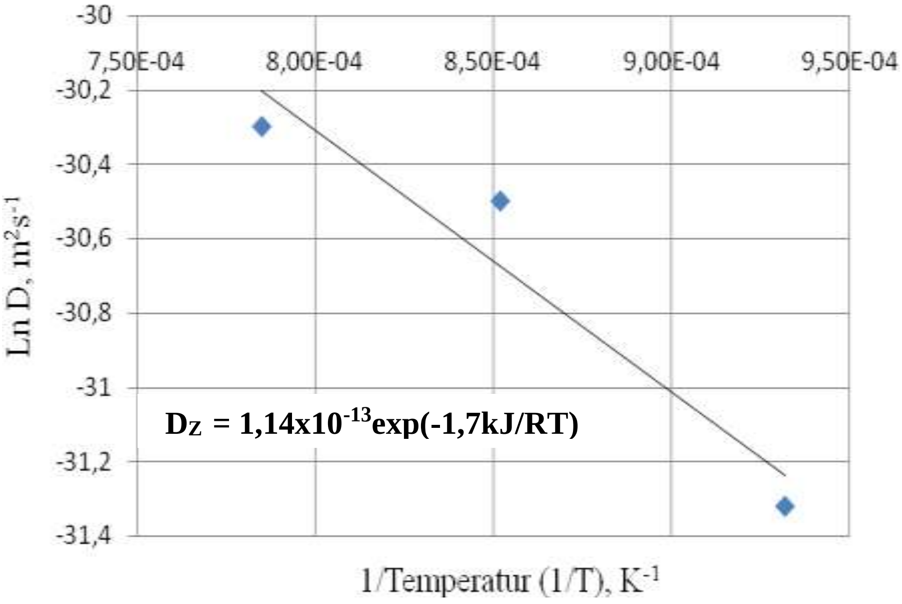

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Figure 5. Arrhenius relationships for boron diffusion coefficients as a function of treatment temperature on the a).FeB, b).Fe_2B and diffusion zone for St41 low carbon steel.

CONCLUSIONS

In this study the growth kinetics of the boride layers and diffusion zones on St41steels has been analysed. The influence of alloy elements creates the formation of FeB/ Fe_2B on the surface of St41 steel, as shown XRD characterization results. The morphology of the iron boride layers present on the St41 steel is saw-toothed after heating at the temperature of 700, 800, and 900^{O}C. The increase in treatment time and temperature is manifested in the growth kinetics of the iron boride layers and diffusion zones. It results in the formation of denser, uninterrupted layers, and larger precipitates of Fe2B beneath those layers. The activation energy for the iron boride layers and diffusion zones is determined by utilizing the boron diffusion coefficients in the Arrhenius relationship, where temperature plays a crucial role. In the St41 steel, the The activation energy for the FeB phase exceeds that of the Fe_2B phase., and also the activation energy of the Fe_2B phase is greater than diffusion zone. The diffusion coefficient of boron in the FeB phase is D_{FeB} = 5,67x10^{-14}exp(-99,72kJ/RT, while in the Fe_2B phase it is D_{Fe2B} =1,03x10^{-13}exp(-58,17kJ/RT), and in the diffusion zone it is D_Z = 1,14x10^{-13}exp(-1,7kJ/RT). This result indicates that the larger the diffusion coefficient, the faster the diffusion process.

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