Neural Network Model for Isothermal Pearlite Transformation. Part I: Interlamellar Spacing

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The present paper is the first of a two-part paper which deals with a neural network model to describe the isothermal pearlite formation. The isothermal austenite-to-pearlite transformation has been analyzed using a neural network technique within a Bayesian framework. In this framework, the pearlite interlamellar spacing and growth rate of pearlite can be represented as a general empirical function of variables such as Mn, Cr, Ni, Si and Mo alloying contents and temperature which are of great importance for the pearlite growth mechanisms. The method has limitations owing to its empirical character, but it has been demonstrated that it can be used in such way that the predicted trends make metallurgical sense. In this first part paper, the method has been used to examine the relative importance of the alloying elements on pearlite interlamellar spacing.

KEY WORDS: neural network analysis; pearlite; interlamellar spacing; modelling phase transformation; steels.

1. Introduction

Crude steel production by the major steel-producing countries is of the order of 850 millions tones per annum, the vast majority of which is subsequently fabricated into plates, bars, rods, strips, sheets and coils, using large scale deformation processes, in which the cooling rate from austenite phase field is relatively slow. Such products are destined for use in the construction, power generation, shipbuilding and automotive industries (among others), where structural materials of high strength, good toughness, low cost and weldability are required. The microstructure of these steels is usually a mixture of allotriomorphic ferrite and pearlite. The mechanical properties are derived from these microstructural constituents.

Nowadays, there are available quantitative computerized models regarding ferrite and pearlite transformation. Such models would yield information on composition, grain size and distribution of phases and reaction kinetics, and the output of most of these models is the evolution of volume fraction of phases. However, an intermediate stage of calculation is necessary. More precisely, determination of interlamellar spacing is a key factor on the austenite-to-pearlite transformation.

Interlamellar spacing is one of the most fundamental parameters that characterize the pearlite microstructure. The wide range of mechanical properties of pearlitic microstructure, and hence the main reason of why ferritic–pearlitic steels are by far the most consumed structural material in the world, are intrinsically related to the pearlite interlamellar spacing. It is therefore not surprising that it has been reported for decades the influence of alloying elements and cooling conditions on interlamellar spacing of pearlite. On the other hand, it has been recently reported the role of interlamellar spacing on austenite formation during the isothermal and continuous heating austenite formation. Thus, the study of the factors which influence interlamellar spacing of pearlite formation is, at present, an interesting topic.

The purpose of the present work is to investigate whether an artificial neural network can be trained to predict interlamellar spacing of pearlite and pearlite growth rate as a non-linear function of chemical composition and temperature, and whether the patterns that emerge from this model emulate the metallurgical experience.

In normal regression methods, the analysis begins with prior choice of a relationship (usually linear) between the output and input variables. A neural network is capable of performing a greater variety of non-linear relationships of considerable complexity. Data are presented to the network in the form of input and output parameters, and the optimum non-linear relationship is found by minimizing a penalized likelihood. In effect the network tries out many kinds of relationships in its search for an optimum fit. As in regression analysis, the results consist of a function that relates the inputs to the outputs by a series of coefficients called weights. In spite of its apparent sophistication, the method is as blind as regression analysis, and neural networks can be susceptible to overfitting. This paper deals with the analysis of the influence of alloying elements such as Mn, Cr, Ni, Si, and Mo, separately and together, on interlamellar spacing by means of neural networks.
2. Experimental: Build of the Model

2.1. Technique

Neural networks are parameterized non-linear models used for empirical regression and classification modeling. Their flexibility enables them to discover more complex relationships between the data than traditional linear statistical models.

A neural network is ‘trained’ on a set of examples of input and output data. The outcome of the training is a set of coefficients (referred to as weights) and a specification of the functions which in combination with the weights relate the input to the output. The training process involves a search for the optimum non-linear relationship between the input and output data and is computer intensive. Once the network is trained, estimation of the outputs for any given inputs is very rapid.

One of the difficulties with blind data modeling is that of ‘overfitting’, in which spurious details and noise in the training data are overrated by the model. This gives rise to solutions that generalize poorly. MacKay10,11 has developed a Bayesian framework for neural networks in which the appropriate model complexity is inferred from the data.

The Bayesian framework for neural networks has two further advantages. First, the significance of the input variables is automatically quantified. Consequently, the significance perceived by the model of each input variable can be compared against metallurgical theory. Second, the network’s predictions are accompanied by error bars which depend on the specific position in input space. These quantify the model’s certainty about its predictions.

2.2. The Experimental Database

Two measured parameters may characterize the interlamellar spacing of pearlite: the average minimum observed spacing taken from several colonies, and the mean intercept spacing. The former parameter is a perpendicular distance across two consecutive lamellae i.e. ferrite and cementite, while the mean intercept spacing is an average distance across two successive lamellae taken from test lines randomly applied to the plane of polish.

Experimental evidence in pearlite produced under isothermal conditions prove that the true spacing is not the minimum spacing observed in metallographically prepared surfaces. The true spacing does not have a constant value, but it is a distribution of spacings about a mean true value. Stereological studies concluded that the mean true spacing of pearlite is half of the mean intercept spacing.12 By contrast, the factor which relates the minimum and the mean true spacing is not constant and may vary from system to system, and with transformation temperature in a given system. It is because of the uncertainty in the relationship between the minimum and the mean true spacing that the former parameter is sometimes reported as the parameter that characterizes the pearlite microstructure. However, it would be in fact more satisfactory to characterize the microstructure in terms of the mean true spacing ($S_o$). In this sense, the interlamellar spacing parameter in the database corresponds to mean true spacings reported in literature for eutectoid steels.

A complete description of the chemical composition and the isothermal transformation temperature is required to ideally model the interlamellar spacing of pearlite in steels. A search of the literature5,7,13–18 allows us to collect 220 individual cases where detailed chemical composition, isothermal temperature, and $S_o$ values were reported. Table 1 shows the list of 6 input variables used for the interlamellar spacing analysis. Because of higher sensitivity of the model to small variations, the $S_o$ values are expressed as logarithm values.

2.3. Neural Network Analysis

The aim is to be able to estimate the pearlite interlamellar spacing as a function of the input variables listed in Table 1. The network consists of 6 input nodes, a number of hidden nodes, and an output node representing the interlamellar spacing of pearlite (Fig. 1). The network was trained using 110 examples randomly chosen from a total of 220 available, the remaining 110 examples being used as ‘new’ experiments to test the trained network.

Chemical composition of each alloy element and temperature ($x_i$) defines the inputs nodes, and the interlamellar spacing, $y$, the output node. Each input is multiplied by a random weight $w_j^{(1)}$, and the sum of all these products, together with a constant $\theta_j^{(1)}$, forms the argument of a hyperbolic tangent (tanh):

$$h = \tanh \left( \sum_j w_j^{(1)} x_j + \theta_j^{(1)} \right)$$

$$y = w^{(2)} h - \theta^{(2)}$$

Table 1. Variables that influence Pearlite Interlamellar Spacing.

<table>
<thead>
<tr>
<th>Minimum</th>
<th>Maximum</th>
<th>Average</th>
<th>SD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn</td>
<td>0.00</td>
<td>1.80</td>
<td>1.77</td>
</tr>
<tr>
<td>Cr</td>
<td>0.00</td>
<td>1.94</td>
<td>2.02</td>
</tr>
<tr>
<td>Ni</td>
<td>0.00</td>
<td>9.00</td>
<td>8.35</td>
</tr>
<tr>
<td>Si</td>
<td>0.00</td>
<td>0.48</td>
<td>0.96</td>
</tr>
<tr>
<td>Mo</td>
<td>0.00</td>
<td>3.00</td>
<td>1.71</td>
</tr>
<tr>
<td>T, °C</td>
<td>567.00</td>
<td>802.00</td>
<td>660.6986 40.9968</td>
</tr>
<tr>
<td>Log$S_o$, μm</td>
<td>-1.4473</td>
<td>-0.0969</td>
<td>-0.9082 0.3082</td>
</tr>
</tbody>
</table>

SD is standard deviation.

![Scheme of the Neural Network model used in this study.](image-url)
where \( w^{(2)} \) is a weight and \( \theta^{(2)} \) another constant. Therefore, the output \( y \) is a non-linear function of \( x_j \). The function is usually chosen to be the hyperbolic tangent because of its flexibility.\(^{19,20}\) The exact shape of the hyperbolic tangent can be varied by altering the weights \( w_j \). The specification of the network structure together with the set of weights is a complete description of the formula relating the inputs and the output. The weights are systematically changed until a best-fit description of the output is obtained as a function of the inputs. This operation is known as training the network. The training involves a minimization of the regularized sum of squared errors.

Further degrees of non-linearity can be introduced by combining several of the hyperbolic tangents, permitting the neural network method to capture almost arbitrarily non-linear relationships. The number of ‘tanh’ functions is the number of hidden units. The function for a network of \( i \) hidden units is given by,

\[
y = \sum_i w_i^{(2)} h_i + \theta^{(2)} \quad \text{(2)}
\]

where

\[
h_i = \tanh \left( \sum_j w_j^{(1)} + \theta^{(1)} \right) \quad \text{(3)}
\]

Notice that the complexity of the function is related to the number of hidden units but one hidden-unit model may not be sufficiently flexible. The availability of a sufficiently complex and flexible function means that the analysis is not as restricted as in linear regression where the form of the equation has to be specified before the analysis. Figure 2(a) shows that as expected the inferred noise level of data \( (\sigma_i^{(1)})^{10} \) decreases monotonically as the number of hidden units increases. However, a high degree of complexity owing to a large number of hidden units may not be justified, and in an extreme case, the model may meaninglessly attempt to fit the noise in the experimental data. MacKay\(^{11}\) has made a detailed study of this problem and has defined a quantity (the ‘evidence’) which comments on the probability of a model.\(^{11}\) In circumstances where two models give similar results over the known data set, the more probable model would be predicted to be the simplest one; this simple model would have a higher value of evidence. The evidence framework was used to control the regularization constants and \( \sigma_{\nu}^{(1)} \) Mackay has developed a particular useful treatment of neural networks in a Bayesian framework,\(^{21}\) which allows the calculation of error bars representing the uncertainty in the fitting parameters. The method recognizes that there are many functions which can be fitted or extrapolated into uncertain regions of the input space, without unduly compromising the fit in adjacent regions which are rich in accurate data. Instead of calculating a unique set of weights, a probability distribution of sets of weights is use to define the fitting uncertainty. The error bars therefore become large when data are sparse or locally noisy.

To find out the optimum number of hidden units of the model the following procedure was used. The experimental data were partitioned equally and randomly into a test dataset and a training dataset. Only the latter was used to train the model, whose ability to generalize was examined by checking its performance on the unseen test data. The test error \( (T_{en})^{10} \) is a reflection of the ability of the model to predict the output value in the test data:

\[
T_{en} = 0.5 \sum_n (y_n - t_n)^2 \quad \text{(4)}
\]

where \( y_n \) is the set of predictions made by the model and \( t_n \) is the set of target (experimental) values. In Fig. 2(b), it can be seen that the calculated test error for this pearlite interlamellar spacing model goes through a minimum at nine hidden unit. Therefore, the optimum model is that which considers only nine hidden units. The level of agreement for the training and the test data is shown in Figs. 3(a) and 3(b); good predictions occur in both instances.

### 2.4. Significance of Input Variables

Figure 4 illustrates the significance of each of the input variables \( (\sigma_{\nu}) \), as perceived by the neural network, in influencing the interlamellar spacing of pearlite.\(^{10}\) The temperature clearly has a large intrinsic effect, which is consistent with experimental evidences reported in the literature for decades. The content in chromium and nickel in the steel also have a significant effect on pearlite interlamellar spacing, as it was well established in literature,\(^{13}\) meanwhile the influence of manganese is moderate. By contrast, silicon has only a small effect.
3. Results and Discussion

3.1. Use of the Model: Fe–C Steels

A neural network model was used to obtain, in a first step, an empirical expression for the pearlite interlamellar spacing as a function of temperature in plain carbon steels. In this sense, Fig. 5 shows the evolution of interlamellar spacing with undercooling for Fe–C steels. It is clear that a linear dependence between $\log S_0$ and $\log \left( \frac{T_E - T}{T_E} \right)$, where $T_E$ is the eutectoid temperature, is obtained. Therefore, the evolution of interlamellar spacing with temperature could be expressed by,

$$
\log S_0 = -2.114 - 0.958 \log \left( \frac{T_E - T}{T_E} \right)
$$

(5)

Theories on pearlite growth assume that the reaction product grows into the parent austenite phase at a constant velocity, $G$, and maintains a constant interlamellar spacing, $S_0$. During pearlite growth distribution of solute may occur ahead of the transformation front by volume diffusion through the austenite, and/or by diffusion along the austenite–pearlite interface. Zener predicted that the system stabilizes at a spacing for which the growth rate is a maximum and this criterion leads to,$^{7,22)}$

$$
S_0 = 2S_C = \frac{4\sigma_w T_E}{\Delta H \Delta T}
$$

(6)

with $S_C$ as the critical spacing,$^7$ $\sigma_w$ as the surface energy of ferrite/cementite interface ($\sigma_w$); $\Delta H$ as change in enthalpy between the parent and product phases; $T_E$ as the eutectoid temperature; and $\Delta T = T_E - T$ as the undercooling below the eutectoid temperature.

On the other hand, the maximum rate of entropy production criterion proposed by Kirkaldy,$^{23}$ which has its theoretical basis in irreversible thermodynamics, and is supported by perturbation tests leads to,

$$
\sigma_w = \frac{\Delta H}{\Delta S}
$$

(7)

In principle, it should be possible to use the experimental value of $S_0\Delta T$ to identify the optimization criterion. In this sense, Eq. (5) could be rewritten as $S_0\Delta T = 6.22$ assuming an approximated eutectoid temperature, $T_E$, of 728°C. Combining this value with Eqs. (6) and (7), and considering the enthalpy data of Kramer et al.$^{24}$ $\Delta H = 6.09 \times 10^4$ J m$^{-3}$, the maximum growth criterion (Eq. (6)) gives a value of interfacial surface energy of $\sigma_w = 0.94$ J m$^{-2}$, while the maximum rate of entropy production criterion predicts $\sigma_w = 0.63$ J m$^{-2}$. Between these two values the latter would seem the more realistic since the boundary involved must be at least semi-coherent. However, both values fall within the range $0.7 \pm 0.3$ J m$^{-2}$ obtained by Kramer et al.$^{24}$

An alternative method to validate the optimization criterion consists in plotting the evolution of $S_0/3$ and $S_0/2$ values as a function of undercooling, and comparing those val-
ues with the calculated critical spacing $S_c$ considering a surface energy of 0.7 J m$^{-2}$. Figure 6 shows a comparison between the $S_i/3$ and $S_i/2$ values obtained from the neural network model with the calculated $S_c$. It is clear from this figure that the results predicted by the maximum rate of entropy production criterion ($S_i/3$) are in reasonable good agreement with those predicted from neural networks analysis except at very low undercooling.

3.2. Use of the Model: Fe–C–X Steels

Equation (5) is only valid for plain carbon steel but in the case of a Fe–C–X alloy the independent parameter is function of the chemical composition of the steel. In such case, the above equations could be expressed as,

$$\log S_o = c + \sum_i b_i [X_i] - \log \left( \frac{T_E - T}{T_E} \right)$$

where $[X_i]$ is the alloy content in weight%, and $c$ and $b_i$ are constants. The corresponding eutectoid temperatures ($T_E$) have been calculated from the equation compiled by Andrews and by means of the thermodynamic MTDATA software.

Figure 7 shows the evolution of the factor $\log S_o + \log ((T_E-T)/T_E)$ with different contents of Mn, Cr, Ni, Si and Mo.

The fitting of the data presented in Fig. 7 to a straight line leads to an equation for the pearlite interlamellar spacing which represents the dependence of such parameter with the chemical composition of the steel:

$$\log S_o = -2.212 + 0.0514 \times [\text{Mn}] - 0.0396 \times [\text{Cr}] + 0.0967 \times [\text{Ni}] - 0.002 \times [\text{Si}] - 0.4812 \times [\text{Mo}]$$

where $S_o$ is measured in $\mu$m, and [Mn], [Cr], [Ni], [Si], and [Mo] are the different alloy contents in wt%. The behavior of Cr is probably so troublesome (at high Cr levels Fig 7(b)) due to alloy carbides ($M_2C_3$, $M_2C_6$) replacing $M_3C$, and also due to changes in morphology (spiky pearlite). Likewise, it is worth mentioning that the left hand side of Eq. (9) becomes $-2.212$ for plain carbon steels which is very close to the previously obtained value of $-2.114$ (Eq. (5)). It is noted that the addition of Mo and Cr decreases the pearlite interlamellar spacing, whereas additions of Mn and Ni causes an increase in this parameter. Silicon, however,
has a slight influence on interlamellar spacing, although the tendency indicates a decrease with increasing silicon content.

On the other hand, Eq. (8) could be rewritten as,

\[ S_o \Delta T = T_e \left( 10^{-2.21 + 2A(X_i)} \right) \] ........................(10)

where \([X_i]\) represents the concentrations of alloying elements, and \(b_i\) is a constant. This equation leads to a value of \(S_o \Delta T=6.22\) for plain carbon steels, which is in excellent agreement with that proposed by Ridley et al.\(^{27}\) (\(S_o \Delta T=6.19\)). Figure 8 presents the evolution of the \(S_o \Delta T\) factor as a function of alloy composition for those elements which stabilize austenite such as Mn and Ni, and those which are very strong carbide formers such as Cr and Mo.

In general, it is clear from Fig. 8 that strong carbide formers such as Cr and Mo tend to decrease the \(S_o \Delta T\) factor, and therefore induce lower values of the pearlite interlamellar spacing. On the other hand, austenite stabilizer elements such as Mn and Ni tend to increase the \(S_o \Delta T\) factor, and thus induce higher values of spacing.

Figure 9 shows the variation of the reciprocal of interlamellar spacing with transformation temperature for Fe–C–X steels with different grades of Mn, Cr, Ni, Si and Mo. These results are plotted together with previous data for Fe–C steels.

Results presented in Figs. 8 and 9 suggest that Mn in-

![Fig. 8. Evolution of \(S_o \Delta T\) factor as content of (a) Mn, Ni and Si increases, and (b) Cr and Mo increases.](image)

![Fig. 9. Reciprocal pearlite interlamellar spacing versus temperature for different grades of (a) Mn, (b) Cr, (c) Ni, (d) Si, and (e) Mo.](image)
creases the spacing for a given reaction temperature. This observation is consistent with earlier measurements on commercially based manganese steels reviewed by Cahn and Hagel. Likewise, it can be seen from these figures that nickel additions, like manganese, increase pearlite spacing for a given reaction temperature, although the reciprocal spacing plot is steeper than for the Fe–C steels.

On the other hand, it can also be seen from Fig. 9 that chromium additions progressively reduce the interlamellar spacing of pearlite for a given reaction temperature the higher the chromium content. Reciprocal spacing data for chromium alloys in Fig. 9 lie on a straight line with lower slope than that for Fe–C.

Likewise, it could be concluded from Figs. 8 and 9 that Mo strongly affects the interlamellar spacing. The higher the molybdenum content, the finer spacing is. Reciprocal spacing data for molybdenum lie on a straight line whose slope changes with alloy content. This behavior may reflect the variation of pearlite morphology with transformation temperature. As it has been reported in the literature for steels with a 0.3 wt% Mo content,29) pearlite has a typical lamellar structure at high temperature. However, at an intermediate range of temperatures the pearlite is markedly degenerated. Finally, silicon has a slight effect on interlamellar spacing as shown in Figs. 8 and 9. Regarding the effect of silicon, the reciprocal spacing values versus temperature lie on a straight line with a slope close to that of Fe–C.

Extrapolation of each of the graphs of reciprocal interlamellar spacing vs. temperature (Fig. 9) to infinite interlamellar spacing gave the value for the eutectoid temperature for the different composition analyzed. In this sense, Fig. 10(a) shows the evolution of the extrapolated $A_{e1}$ temperature with increasing alloy content, which is consistent with the well established effect of alloying elements on eutectoid temperature. This concentration has been considered as $X^*$, which is the ratio between the X-element concentration ([X]) of the Fe–C–X steels and, the maximum concentration considered in at% ([X]$_{max}$, see Table 1), i.e. $X^* = [X]/[X]_{max}$. Therefore, it is clear that silicon together with the strong carbide formers elements such as Cr and Mo increase the eutectoid temperature, meanwhile elements such as Mn and Ni decrease this temperature. Likewise, the extrapolated $A_{e1}$ temperatures have been compared with those calculated according to Andrews and MTDATA software. Figure 10(b) shows a reasonable agreement between extrapolated and calculated $A_{e1}$ temperatures.

### 3.3. Validation of the Model

The main advantage of the proposed neural network model as compared with other empirical or semi-empirical models reported in the literature is the ability of predicting the evolution of interlamellar spacing as several alloying elements vary simultaneously. In this sense, it has been studied the evolution of interlamellar spacing in the two steels listed in Table 2. A hypo eutectoid steel, marked as Steel A, has been experimentally analyzed for this work, meanwhile the result for the eutectoid steel, marked as Steel B, has been reported in the literature by Brown and Ridley.30)

Figure 11 shows scanning electron micrographs of pearlite obtained after full decomposition of austenite (30 min) at 670, 660, 640 and 600°C in steel A. The $S_0$ value at these temperatures has been measured from micrographs in Fig. 11. Figure 12 represents the variation of the pearlite interlamellar spacing as a function of the temperature formation. Likewise, superimposed to the measured values, the calculated trends by means of the neural network model are also presented. The dashed lines in this figure represent the uncertainty in calculations, i.e. the error bounds of the neural network model. It is clear form this figure the good agreement between measured and calculated values.

Table 2. Steels composition (in wt%).

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.37</td>
<td>0.56</td>
<td>1.45</td>
<td>0.04</td>
<td>0.024</td>
<td>0.025</td>
</tr>
<tr>
<td>B</td>
<td>0.61</td>
<td>0.11</td>
<td>0.28</td>
<td>2.28</td>
<td>2.02</td>
<td>0.48</td>
</tr>
</tbody>
</table>

Furthermore, a comparison between interlamellar spacing data obtained by Brown and Ridley30) in Steel B for different transformation temperatures has been carried out, and the results are presented in Fig. 13. It might be concluded from this figure that there is an excellent agreement between the neural network values and the steels reported data. The agreement is not only with experimental values, but also with the shape of the reciprocal spacing versus temperature curve. The data clearly show a change of slope at about 670°C. It was argued by Brown and Ridley that the apparent change in slope at 670°C was due to the change in pearlite growth mechanism. At temperatures above 670°C, partitioning of alloying elements are the rate controlling
mechanism, since at temperatures below partitioning ceases to play any significant part.

4. Conclusions

(1) The modeling of the interlamellar spacing of pearlite during isothermal decomposition of austenite in a Fe–C–X alloy is carried out in this paper. An artificial neural network method based on a Bayesian framework has been used to rationalize the published experimental data on interlamellar spacing of pearlite in steels. The analysis is empirical but after appropriate training, it is found to reliably reproduce known metallurgical experience. The method is useful because the optimized network summarizes knowledge in a quantitative manner and can be retrained as new data became available. This model is different to those empirical and semi-empirical models created by fitting equations to experimental data.

(2) It is now possible, therefore, to estimate the role of elements such as Mn, Cr, Ni, Si and Mo which are traditionally used as alloying elements in steel industry. It might be concluded from the results presented that increases of Mn and Ni coarsen the interlamellar spacing of pearlite, but an increase in Cr produces finer pearlite spacing. Special attention to the influence of Mo has been paid, and it is concluded that Mo dramatically decreases the interlamellar spacing. Finally, Si has a slight influence on pearlite spacing.

(3) The neural network model presented in this work has been used to identify the pearlite growth optimization criterion in a Fe–C steel. Comparison between the $S_o$ determined through the neural network model predictions and $S_C$ calculated under the assumption of maximum growth rate criterion and maximum rate of entropy production criterion,
clearly shows that the results predicted by the latter are in better agreement with those predicted from neural networks analysis.

(4) Finally, it has been studied the evolution of pearlite interlamellar spacing in two different steels to illustrate the ability of the neural network model proposed to predict the evolution of interlamellar spacing as several alloying elements vary simultaneously. It could be concluded that the results predicted by the model not only fit those experimentally determined but also follows the same tendency.

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