MICROSIM - PHASE TRANSFORMATION: AN AUSTENITE TRANSFORMATION MODEL FOR LOW ALLOY STEELS*

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Abstract

The simulation of steel hot rolling processes is gaining more and more importance, since well-fitted models allow accelerating and reducing the costs associated with the development of new products, the optimization of thermomechanical processing and increase of the mechanical homogeneity of the final products, within the rolled product and from product to product. A great deal of work in this direction has been carried out for more than ten years by CEIT, sponsored by CBMM, initially with the development of MicroSim®, which calculates the evolution of the distribution of austenitic grain size during the hot rolling process of structural steels, microalloyed or not. This is a work in progress, towards the calculation of the mechanical properties of the final product, now with the development of MicroSim – Phase Transformation (PhasTranSim®), an intermediate model for calculating austenite transformation and characteristics of the ferritic-pearlitic microstructure of the final product, which will be described in this work.

Keywords: Austenite Transformation; CCT/TTT Diagrams; Microalloyed Steels; Mathematical Model

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1 INTRODUCTION

MicroSim®, a mathematical model for the calculation of austenite microstructural evolution during flat and long hot rolling, developed by Centro de Estudios e Investigaciones Técnicas de Gipuzkoa – CEIT, Spain, under the sponsorship of Companhia Brasileira de Metalurgia e Mineração – CBMM, has been used and improved for several years now [1]. As part of its evolution, it has now been developed an austenite transformation model, which aim is to predict the parameters that are required for the further development of a mechanical property model, as follows: microstructural constituent fractions (ferrite, pearlite, bainite, martensite), ferrite grain size and hardness, as well CCT and TTT diagrams. This model, called PhasTranSim® (MicroSim – Phase Transformation), considers the effect of carbon and alloy elements (Mn, Cr, Ni, Mo and others), including microalloys like soluble Nb, Ti and V, as well the effect of austenite mean grain size and its retained strain (ε_{acc}), that is, its strain hardening. These last two parameters can be previously calculated from TMCP conditions using MicroSim®.

2 MODEL DEVELOPMENT

The approach adopted for the development of the PhasTranSim® model includes a transformation kinetics model closely based on the original algorithm proposed by Kirkaldy [2], but considering the modifications suggested by Li and co-workers [3], and Saunders and co-workers [4]. This model will allow to predict TTT and CCT diagrams, as well as the resulting final microstructure (ferrite grain size and constituent fractions) of the steel after a given cooling path, which not necessarily must be a constant cooling rate.
The general equation for calculation of the TTT diagram is based in the modelling proposed by Zener [5] and Hillert [6], where **ζ** is the time required for the formation of the constituent **X** under temperature **T**:

$$\tau(X,T) = \frac{F(C,Mn,Si,Ni,Cr,Mo\ldots,G)}{\Delta T^{n} \exp(-\frac{Q}{RT})} I(X) \quad (1)$$

and **F** is a function of steel composition, expressed by the amounts of C, Mn, Si, Ni, Cr, and Mo, in weight percent; **G** is the prior austenite grain size (ASTM number); **ΔT** is the undercooling; and **Q** is the activation energy of the diffusional reaction. The exponent of undercooling **n** is an empirical constant determined by the effective diffusion mechanism (being equal to 2 for volume and 3 for boundary diffusion). Finally, **I(X)** is the reaction rate term, which is an approximation to the sigmoidal effect of phase transformations [3].
The **F** equation used here has exponential form and the factors that multiply alloy element amounts were fitted, not only considering the original values of the basic model [3], but also the parameters experimentally got from many other steels characterized in CEIT as well. Its variant corresponding to bainite kinetics also includes the effect of soluble Nb prior to austenite transformation, which can be calculated by MicroSim®. So, CCT diagrams from some dozens of alloys were determined using dilatometry, including transformation start and finish temperatures (**F_s**, **P_s**, **B_s**, **M_s**, **M_f**). The measurements of fractions of constituents, as well ferrite grain size, were also performed at different cooling rates, from dilatometry and

multipass torsion tests. In order to include strain hardening of austenite after hot rolling, the value of its grain size is corrected to an effective grain size $d_{\gamma eff}$, according to the following equation:

$$d_{\gamma eff} = d_{\gamma} \exp(-\varepsilon_{acc}) \quad (2)$$

where d_{γ} is the austenite mean grain size and ε_{acc} is the accumulated strain in austenite, both calculated by MicroSim®.
Critical temperatures for start and finish of constituent formation from austenite were proposed:

$$A_{e3} = 933 - 208\sqrt{C} - 34\,Mn + 59\,Si - 13\,Cr - 21\,Cu + 97\,Ti \quad (3)$$

]

$$A_{e1} = 725 - 38Mn + 34\,Si + 25\,Cr - 22\,Mo + 128\,Ti - 21\,Cu + 115\,Al \quad (4)$$

$$B_s = 745 - 110\,C - 59\,Mn - 39\,Ni - 68\,Cr - 106\,Mo + 17MnNi + 6\,Cr^2 + 29\,Mo^2 \quad (5)$$

$$M_s = 530 - 344\,C - 51\,Mn - 40\,Si - 17\,Cr - 47\,Mo \quad (6)$$

$$M_f = 482 - 426\,C - 70\,Mn - 20\,Si - 23\,Cr \quad (7)$$

where A_{e3} and A_{e1} where determined by regression from the data provided by ThermoCalc for the matrix of steels considered here; B_s was proposed in [7] and M_s-M_f were determined fitting experimental data got from dilatometry tests at CEIT.
A model to predict hardness has been also developed, as described below:

$$\%C < 0.6\% \rightarrow HV = f_M * HV_M + f_B * HV_B + (f_F + f_P) * HV_{F+P} \quad (8)$$

$$\%C \geq 0.6\% \rightarrow HV = f_M * HV_M + f_B * HV_B + f_P * HV_P + f_F * HV_F \quad (9)$$

where f_x is the volumetric fraction of the constituent **x** and HV_x its hardness. These equations were developed by the regression of experimental results as a function of composition, austenite mean grain size and cooling rate.
The current range of alloy compositions for application of PhasTranSim® is shown in Table 1.

Table 1: Current composition range for application of the PhasTranSim® model, expressed in weight percent.

Range	C	Si	Mn	P	S	Cr	Ni	Mo	V	Cu	Sn	Ti	Nb	N	Al	B
Min	0.044	0.013	0.33	0.005	0	0	0	0	0	0	0	0	0	0.002	0	0
Max	0.865	0.94	1.67	0.042	0.042	1.02	0.21	0.41	0.14	0.43	0.054	0.072	0.09	0.016	0.047	0.011

3 SOFTWARE FUNCTIONS

The PhasTranSim® software was conceived for the calculation of TTT and CCT diagrams, considering several cooling rates, as well to calculate the resulting microstructure after the application of any cooling path to the original austenite. Its output is graphic, but its numerical results can be exported in the form of Excel spreadsheets. In all cases, it is mandatory to input the chemical composition of the steel, austenite mean grain size and its accumulated strain. It is important to note the required Nb and Ti amounts refer to their soluble content in austenite after hot rolling, which are not necessarily identical to their nominal amounts.
Figure 1 shows the input screen of PhasTranSim®. The TTT diagram can be immediately calculated after the input of the mandatory data, as it does not consider cooling rates. So,

just only press the button **Calculate TTT** and a screen like Figure 2(a) will appear. The option **Copy Chart**, available in both options, copies the corresponding diagram to the clipboard for later use. The option **Save Results** saves the numerical coordinates of the graphical diagram in an Excel spreadsheet, if the user needs this data in tabular form. **Go Back** returns to the input screen.
To draw the CCT diagram it is necessary to set the option **Constant Cooling**. In this case, austenite transformation will be calculated for a number of cooling rates, from 0.1 to 200°C/s, or defined by the user, as can be seen in the table at the left side of Figure 1. After data input, the **Calculate CCT** button must be pressed to generate this diagram, as shown in Figure 2(b). Each curve of cooling rate also includes numerical values of ferrite grain size and hardness. The same buttons already described for the TTT Diagram screen are also available for the CCT Diagram.

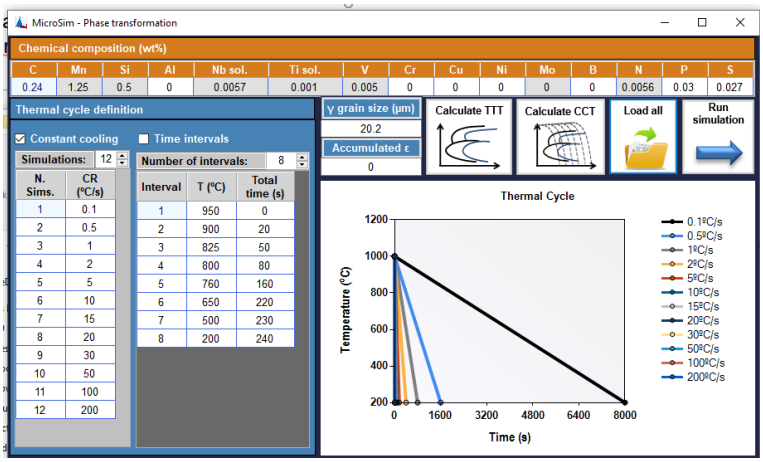

Figure 1: Screen input of PhasTranSim®. The option **Constant Cooling** was chosen in this case.

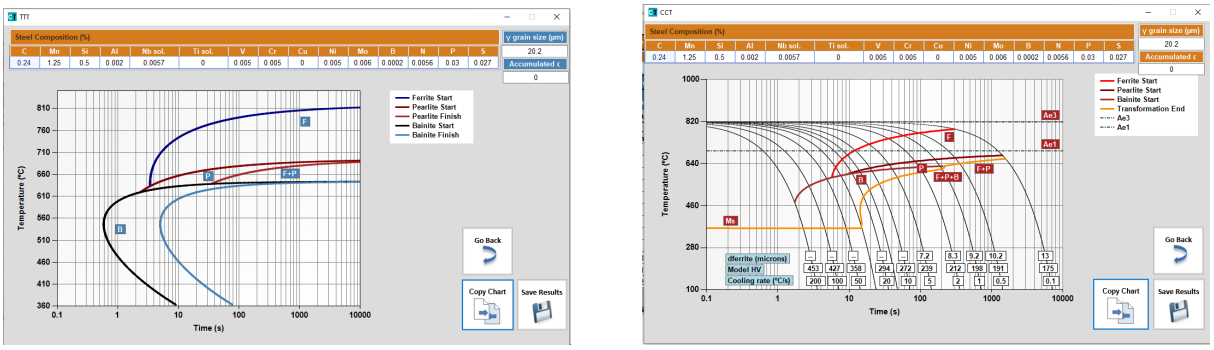

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Figure 2: TTT (a) and CCT (b) diagrams calculated by PhasTranSim®.

Results for the same number of cooling rates, but in numerical form, can also be calculated pressing the button **Run Simulation**. In this case, no diagram will be generated, but rather the output seen in Figure 3, with critical temperatures, constituent fractions, ferrite grain size and hardness of microstructure. This screen also includes two graphics, one showing the thermal cycles that were input, and the other the respective fractions of constituents, in the form of stacked bars. A table output in an Excel spreadsheet can also be generated using the button **Save Results**.
If the option **Time Intervals** is set in the input screen (Figure 4), then a more complex single cooling path, expressed as pairs of total elapsed time and temperature, which will be used to calculate austenite transformation, must be input

in the table at right. The number of intervals can be very high, at the discretion of the user – in this example, 205 intervals were input. The temperature evolution proposed by the user can be seen in the graphic at the right side of the input screen. In this case, after pressing the button **Run Simulation**, it is generated the screen seen in Figure 5. The metallurgical parameters shown in this screen are the same seen in Figure 3, but they are limited to the single cooling path proposed by the user. The graphic at the left side of Figure 5 shows two cooling paths: that in blue color is the cooling path proposed by the user, while the yellow is a more realistic cooling path, as it considers heat generated by austenite transformation, which is relevant for steels with higher carbon amount. The bar graphic at the right side shows the forecast constituents fractions in the microstructure. As already seen in the other options, a numeric output as an Excel spreadsheet can also be generated using the button **Save Results**.

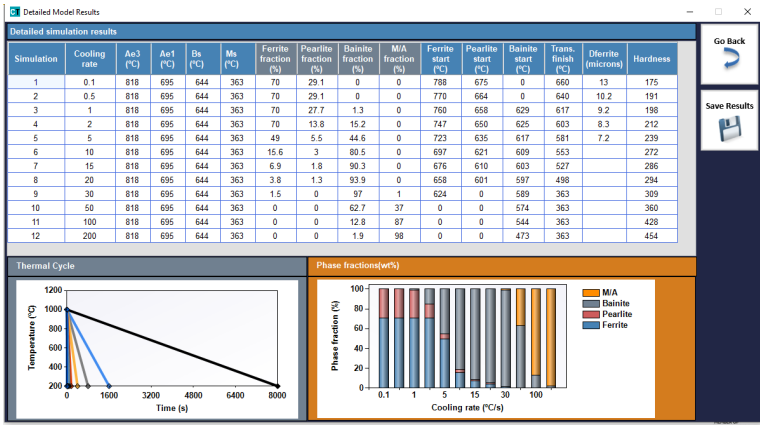

Figure 3: Detailed metallurgical results of austenite transformation, calculated by PhasTranSim®, in function the constant cooling rates input by the user.

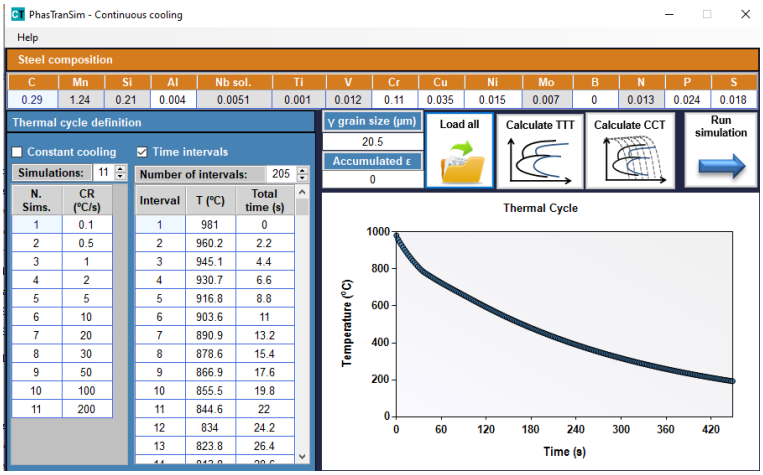

Figure 4: Screen input of PhasTranSim®. The option **Number of Intervals** was chosen in this case.

4 MODEL VALIDATION

In order to validate the PhasTranSim® model, it was applied predict austenite transformation for some steel compositions not included in the data set used for its development. CCT diagrams and hardness evolution for several cooling rates predicted by this model for three steels, namely, Medium CMnVNb, SAE 1045 and

Low CMnCrCuNiVNb were very good, as shown in Figures 6 to 8. The mean quadratic error for hardness predictions was, respectively, 22, 42 and 49 HV.

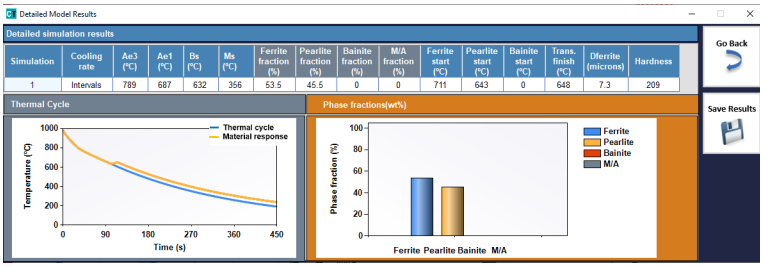

Figure 5: Detailed metallurgical results of austenite transformation, calculated by PhasTranSim®, in function the cooling path input by the user.

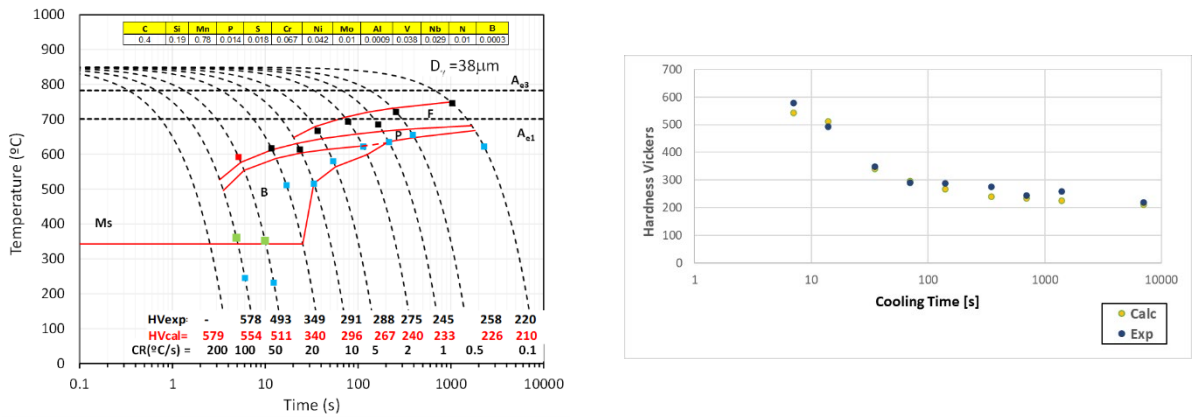

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Figure 6: Validation of PhasTranSim® using a Medium CMnVNb steel as example: (a) CCT diagram; (b) comparison of experimental and calculated hardness evolutions with cooling time.

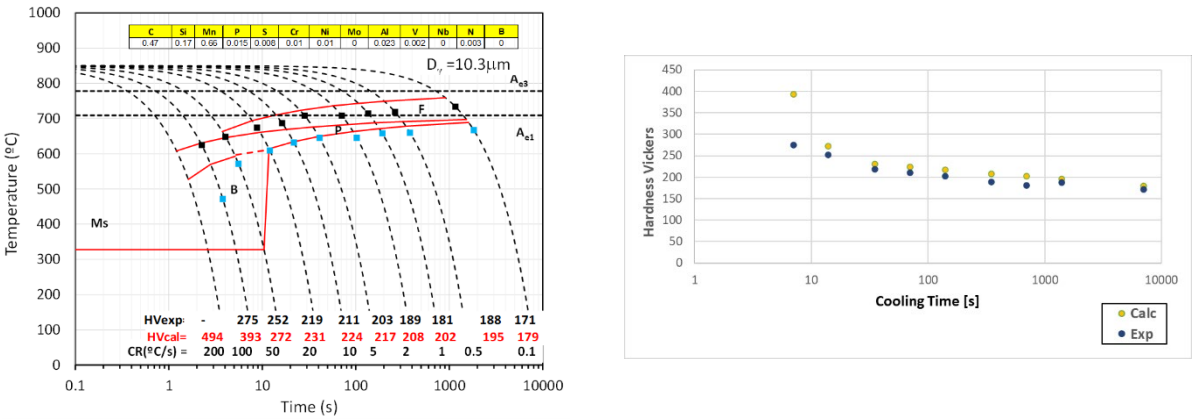

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Figure 7: Validation of PhasTranSim® using a SAE 1045 steel as example: (a) CCT diagram; (b) comparison of experimental and calculated hardness evolutions with cooling time.

Regarding hardness, the overall fitting degree of PhasTranSim® was very good for the Medium CMnVNb. The prediction for the SAE 1045 steel was also very good, except for the case for the maximum cooling rate. The forecast hardness results for the Low CMnCrCuNiVNb steel were not so bad, except for two high cooling rates,

namely 50 and 100°C/s. It must be considered that the model is being continuously improved, with the development of new fitting equations as new steels are being studied and included in the data matrix available for the model, so its precision will be higher in the near future.

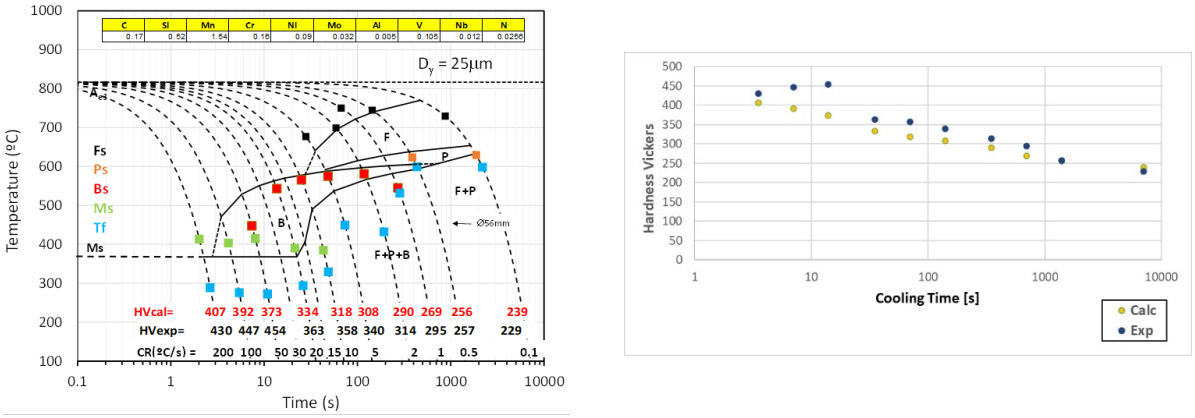

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Figure 8: Validation of PhasTranSim® using a Low CMnCrCuNiVNb steel as example: (a) CCT diagram; (b) comparison of experimental and calculated hardness evolutions with cooling time.

4 CONCLUSIONS

The MicroSim - Phase Transformation (PhasTranSim®) model, recently developed by CEIT under the sponsorship of CBMM, represents another forward step in the development of a global model for simulation of the thermomechanical treatment of steels, aiming to reach the final objective of predicting the mechanical properties of the final product. It uses classical metallurgical models available in the literature to predict austenite transformation, in the form of CCT/TTT diagrams, as well characterization of the final ferritic-pearlitic microstructure. Their algorithms are continuously being fitted according to the results got from structural steels that have been continuously studied by CEIT within its activities of scientific support to CBMM and other customers. It has been demonstrated here that PhasTranSim® predictions already exhibit a very high level of accuracy, which will improve further as it is used and validated under the further characterizations of additional industrial steels.

Acknowledgments

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