

## Thermodynamic Modeling Using Thermo-Calc in the Development of Specialty Welding Consumables

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### **Abstract**

The development of welding consumables for High Strength Steels welding is in increasing importance nowadays. In this research, the thermodynamic modeling tool Thermo-Calc computing package, was utilized to undertake the design of a filler wire for submerge arc welding to weld high strength steels. Important information can be obtained from the analysis of the results, such as the influence of individual chemical elements in the formation of different phases during weldment solidification, the determination of the amount of carbides and nitrides at high temperatures, the temperature at which they form and their behavior during solidification in non-equilibrium conditions. Solidification under equilibrium conditions was also modeled for comparison purposes. It was found that the amount of carbonitrides predicted from equilibrium solidification is 0.13 wt. %; however, in the case of non-equilibrium solidification this amount is 0.03 wt. %. In addition, the chemical elements and their percentages present within the carbonitrides were determined in both the equilibrium and non-equilibrium cases, from which the exact carbides and nitrides can be identified. These data are important because carbides and nitrides are important in the microstructural development of weldments. Oxides are also very important; however, calculations for these compounds are not presented in this document.

### **Introduction**

Computational thermodynamic modeling can be utilized as an important tool in the design of welding consumables because it provides important predictions such as the formation of carbides, and nitrides, and their respective amounts. In addition, the composition of this carbonitrides can be obtained in the cases of equilibrium and non-equilibrium solidification, from which the exact carbide or nitride formed can be identified. The analysis procedure is explained below.

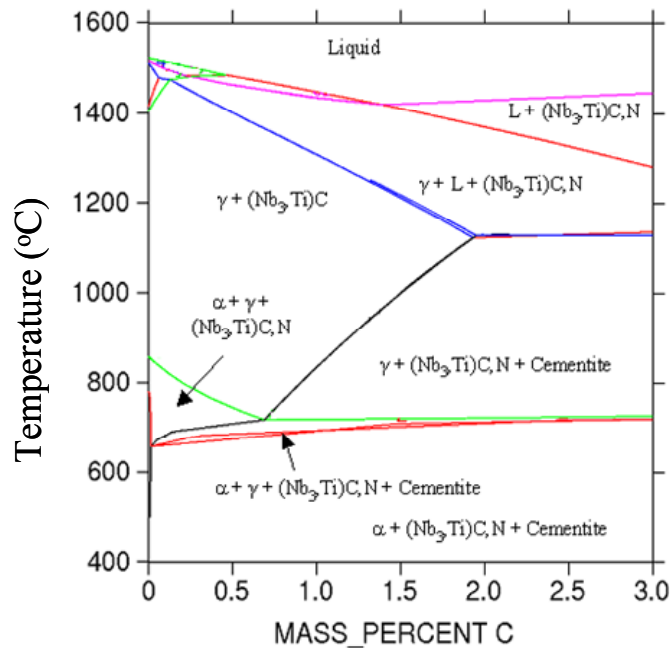
### **Experimental procedure**

A specific high strength steel alloy composition, shown in Table 1, was selected for thermodynamic analysis. The reason for selecting this composition was to simulate the chemical composition of the base metal.

**Table 1.** Chemical composition for thermodynamic modeling to design a welding wire to weld high strength steels.

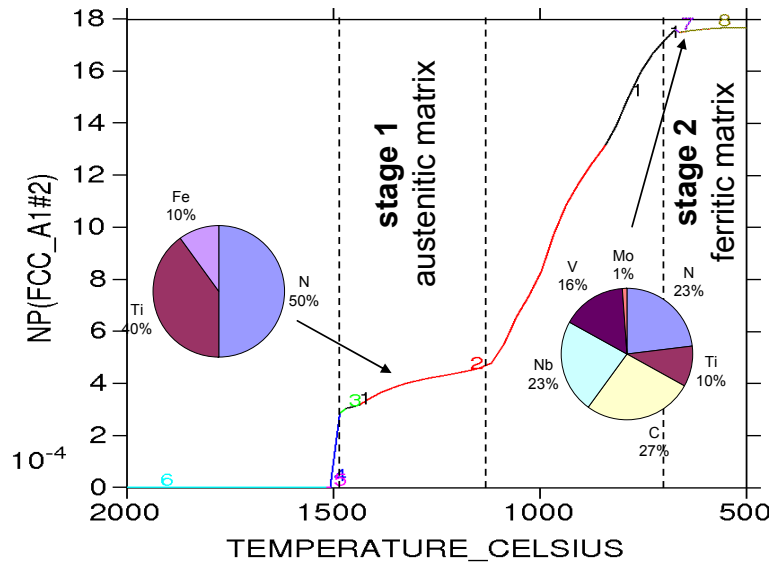
C	Si	Mn	P	S	Al	Nb	V	Cu	Ti	Cr	Mo	N
wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%
0.05	0.2	1.84	0.015	0.002	0.034	0.066	0.027	0.01	0.015	0.13	0.20	0.01

A pseudo binary Fe-Fe<sub>3</sub>C phase diagram was obtained in Figure 1, in which the phases during solidification and the carbides and nitrides are displayed. This phase diagram is important because clearly indicates that at high carbon content the formation of (Nb<sub>3</sub>, Ti)C, N occurs before any other phase is formed. These (Nb<sub>3</sub>, Ti)N, C compounds are also present at low carbon contents, such is this case.



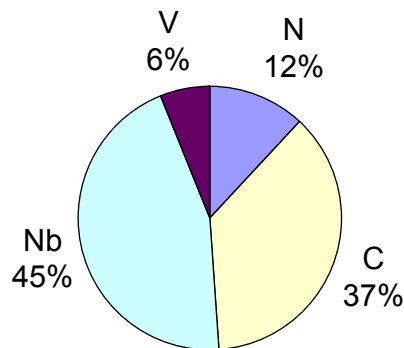
**Figure 1.** Pseudo binary Fe-Fe<sub>3</sub>C equilibrium phase diagram using the chemistry in Table 1.

The amount of phases present in equilibrium solidification can be obtained by plotting the individual phase fraction as a function of temperature. As an example, Figure 2 displays the amount of carbonitrides as a function of temperature. It can be observed that as the temperature decreases the amount of carbonitrides increases according to the line with steps in the Figure 2. Not only that but the percentages of the chemical elements present in the two plateaus can be determined, from which the exact carbide or nitride compositions can be obtained.



**Figure 2.** Evolution of carbonitrides composition as a function of temperature.

In the case of non-equilibrium solidification, the amount of carbonitrides was determined by using Scheil solidification modeling, plotting the mass fraction of carbonitrides as a function of the mass fraction of all solid phases. The final composition of the carbonitride phase is composed of Nb, V, N and C, as illustrated in Figure 3.



**Figure 3.** Final composition of carbonitrides generated during non-equilibrium solidification.

### Results and discussion

Calculations using the Thermo-Calc computer package indicate that the amounts and compositions of the carbonitrides can be obtained for equilibrium and non-equilibrium solidification conditions. Figure 2 shows that the alloy will solidify as ferrite matrix with the precipitation of carbonitrides. It can be seen how carbonitrides start growing approximately at 1500°C and how they grow as temperature decreases. These precipitates grow faster at temperatures above 1500°C and between 1100°C and 727°C; however, in the high austenitic region they grow slowly indicated by the plateau, and in the ferritic region their amount is

almost constant. The amount of carbonitrides expected from equilibrium cooling is (0.13 wt%).

In the case of non-equilibrium solidification, the determination of the amount of carbonitrides is done using Scheil solidification calculations. Here, solidification takes place over a much higher temperature range from 1520 to 1160° C. However, even though the solidification range is large, the precipitation of carbonitrides occurs constantly from approximately 1360°C to 1160°C. The total amount of carbonitrides expected from non-equilibrium cooling is (0.03 wt%), and the chemical elements and their amounts identified within them are 45% Nb, 6% V, 12% N, and 37% C.

### Conclusions

Thermo-Calc calculations show to be a useful tool in the design of welding consumables. The temperature at which different carbides and nitrides form and their respective amounts were determined for a specific chemical composition, in both cases, equilibrium and non-equilibrium solidification. In addition, from the final chemical compositions of the carbonitrides, the specific carbides or nitrates formed can be determined. These data is useful for the design of welding consumables, specifically in the prediction of the amount of the chemical elements of the carbonitride formers that need to be present in the welding consumable.

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