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Modeling Effects of Ti and Nb on Phase Transformation of Low Carbon Steel

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Abstract

General steels are conventionally used in automobiles and as structural components for over two centuries. However, environmental legislations and restrictions open up a new window for light-metallic alloys. In this scenario, steel needs to show its exceptional potential by providing extra-ordinary strength and resistance to corrosion. In this current work, effects of micro-alloying by adding different amounts of titanium (Ti) and niobium (Nb) in a low carbon containing plain carbon steel was observed. The work was carried out in thermodynamic modeling method—CALPHAD. Using of modeling allows observation of properties over a broad range in a reasonable quick time. It was predicted that addition of Ti and Nb behaves differently in mechanical properties. If these elements were added at the same time, phase composition of the alloy changes significantly. TTT and CCT curves for the alloys showed different patterns for nose-shifting. The changes of yield strength and hardness values were also vividly co-related with phase fractions and trends of CCT curves. In conclusion, the models were validated with the theoretical attributes of iron and carbon with other alloying elements.

Keywords: CALPHAD, Micro-Alloying, Mechanical Properties

1. Introduction

An abundance of research work has been done to explore the effects of various alloying elements on steel. Among various elements, effects of Nb, Ti and V addition have been observed most thoroughly. Phase transformation behaviors from austenite to ferrite in Nb containing low carbon steels have been predicted using modeling technique[1]. This model claims that Nb retards austenite to ferrite transformation kinetics by forming NbC and also controls grain size. Also, effect of Nb on the hardenability of ultra-thin cast strip (UCS) steels produced via rapid solidification using the CASTRIP© process was investigated. Results show that, higher Nb additions suppressed the formation of ferrite to even lower cooling rates, increasingly lowered the transformation start and finish temperatures and promoted the transformation of bainite instead of acicular ferrite[2]. In another study, effects of additions of Ti on micro alloyed Nb TRIP steel have been investigated [3]. Here, amount of Ti was limited to 0.005% and 0.028%. Results show that, Ti did not have a significant effect on the stability of retained austenite in the Nb microalloyed steel. However, a different work showed that, Ti additions in the range of 0 to 0.031% with constant Nb content decreased the ferrite start transformation temperature and increased the austenite grain size [4]. In this current work, a modeling technique has been adopted using CALPHAD to predict the changes in phase transformation for adding Ti ranging from 0-0.2wt% in Nb microalloyed low carbon steel.

2. Experimental procedure

The CALPHAD (Calculation of Phase Diagram) method is a dominant method to model phase equilibria of an alloy system. Using mathematical expressions for thermodynamic properties of the phases, this approach can accurately predict phases in complex systems under varying conditions. It is based on the Gibbs free energy concept. Gibbs free energy is minimized to obtain an equilibrium state for a given set of conditions, such as pressure, temperature and compositions. This energy for pure element and stoichiometric compound phases (e.g., Al_2Cu) can be expressed as

$$G_{m[T]} - H_m^{SER} = a + bT + cT\ln(T) + \sum_{2}^{n} d_n T^n$$

where left hand side represents the Gibbs free energy relative to a standard element reference state (SER), H_m is the enthalpy of the element under SER at 298.15 K, a, b, c and d_n are experimentally determined coefficients, n is a set of integers with value 2, 3 & -1 and T is the absolute temperature.

Gibbs free energy is elaborately expressed in terms of pressure, temperature and composition. For a phase φ

$$G^{\varphi} = G_T^{\varphi}(T, x) + G_P^{\varphi}(p, T, x) + G_m^{\varphi}(T_C \beta_0, T, x)$$

where the 1st term shows the dependency on temperature (T) and composition (x), the 2nd term shows pressure dependency and the 3rd term is the magnetic contribution.

Compensation for interactions in multi-component systems can be introduced if deviation from the experimental values is obtained.

3. Results and Discussion

Phase transformations of the steel under equilibrium conditions

CALPHAD software was used to analyze the phase transformations of the low carbon steel under equilibrium conditions. The evolutions of the phases as a function of temperature are represented in Figures 1—3. Here, changes of microstructure during a very slow cooling which corresponds to thermodynamic equilibrium conditions is represented. With the help of this plot, it is possible to identify temperatures of specific phase transitions and to determine a volume fraction of the particular phases at certain temperatures. With addition of Ti, the liquidus and solidus temperature do not vary too much and the area of stable austenite phase increases. During the austenization at 860◦C, the calculated amount of austenite is almost 100%. MnS and cementite disappear with increment of Ti, while M(C,N)-type carbides and $Ti_4C_2S_2$ increase.

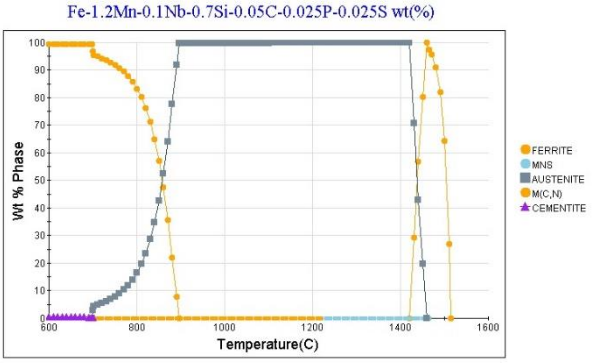

Fig. 1. Thermodynamic evolution of the phases of Ti free low carbon steel

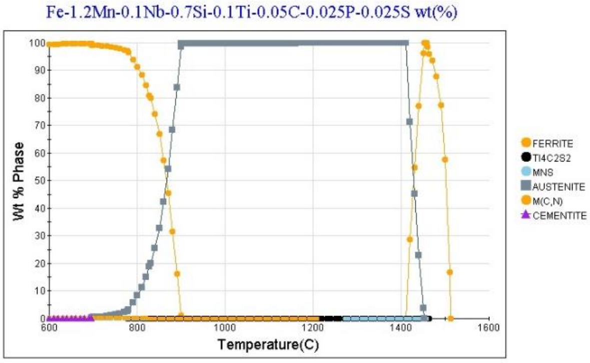

Fig. 2. Thermodynamic evolution of the phases of 0.1% Ti low carbon steel

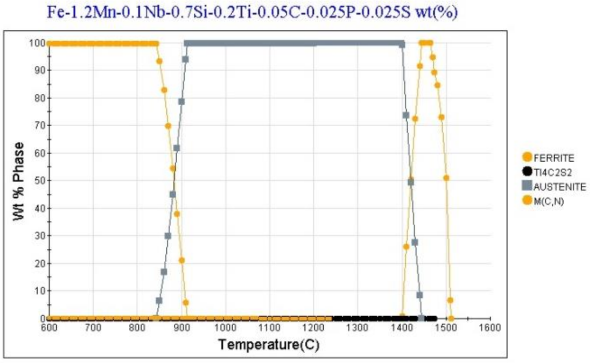

Fig. 3. Thermodynamic evolution of the phases of 0.2% Ti low carbon steel

Table 1 shows the variation of solidus and liquidus temperatures with the addition of Ti. With this minor addition of Ti, these temperatures were not largely affected. Nonetheless, austenite formation and complete transformation temperatures were significantly modified due to the presence of Ti.

Table 1. Data of important temperatures in equilibrium phase diagram

% Ti	Liquidus(˚C)	Solidus(˚C)	Austenite appears(˚C)	Austenite disappears(˚C)	A_1(˚C)
0	1513.99	1460	1459.9	697.49	694.3
0.1	1512.501	1457.382	1452.159	695.9906	685.85
0.2	1511.006	1460	1444.813	842.4325	663.94

Continuous cooling transformation (CCT) diagram

To produce continuous cooling transformation (CCT) diagram of the low carbon steel, CALPHAD software was used. For equilibrium conditions, increment of Ti addition increases the ferritic transformation starting temperature (F_s), as can be seen in Figures 4—6. As cooling rate, which was kept constant for the whole temperature range increases, formation of ferrite decreases. However, this reduction of ferrite formation lowers the cooling rate required to prevent pearlitic transformation (c.r.$_p$) reduces with increase of %Ti. Figure 7 shows the summary trend against Ti. F_s effects are separately shown in Table 2.

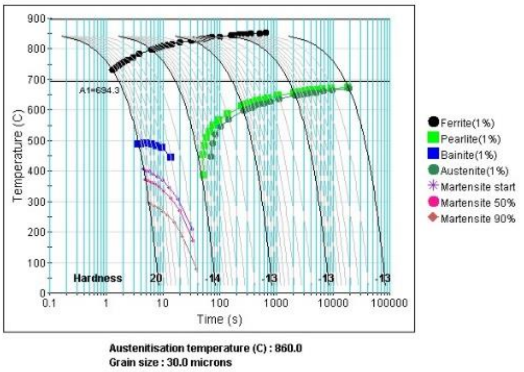

Fig. 4. Continuous cooling transformation (CCT) diagram of Ti free low carbon steel

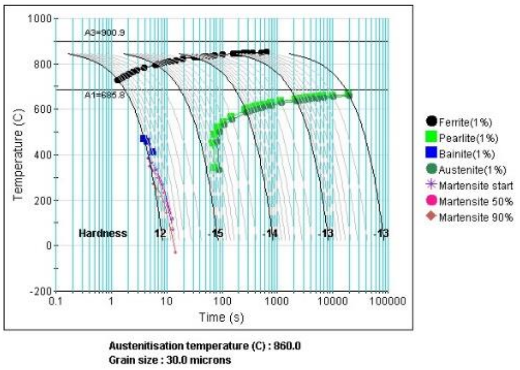

Fig. 5. Continuous cooling transformation (CCT) diagram of 0.1% Ti low carbon steel

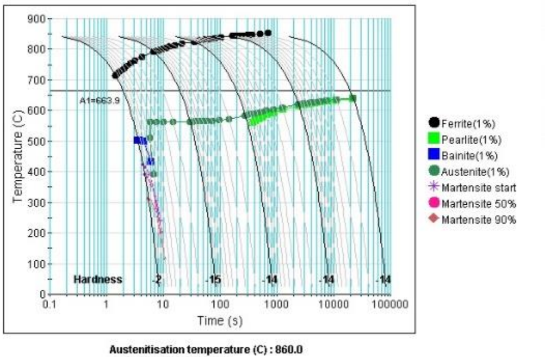

Fig. 6. Continuous cooling transformation (CCT) diagram of 0.2% Ti low carbon steel

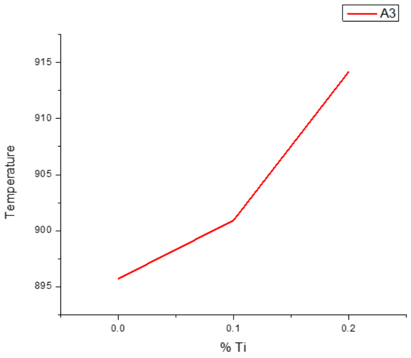

Fig. 7. Upper transformation temperature vs %Ti

From Figure 7, it can be seen that with increase of % Ti, the upper transformation temperature increases. It can be attributed to Ti's transformation kinetics retardation effect. Ti is a strong carbide former. It forms both TiC and $Ti_4C_2S_2$. Solubility of Ti decreases by increasing temperature. The solubility of Ti at 770℃ equal zero that means that any Ti content must form TiC [5]. The small TiC particles precipitate in the austenite grain boundary. This hinders dislocation movement and reduces carbon diffusion rate. As a result, austenite stabilizes. Therefore, with increase of %Ti, the ferrite transformation temperature rises.

Table 2. Data of transformation temperature and critical cooling rate

% Ti	F_s (˚C)	c.r.$_p$ (˚C/s)
0	860	50
0.1	900.9	50
0.2	914.2	30

Time–temperature–transformation (TTT) diagram

In Figures 8—10, the calculation of the time–temperature–transformation (TTT) diagram is presented. With addition of Ti, both the pearlite and bainite formation curve shifts toward right. As a result, time required to complete formation of bainite increases. Figure 11 shows the completion time to bainite formation. Ti is predicted to significantly contribute the complete transformation of bainite. Bainite is an important phase in steel to impart strength. Therefore, such prediction of changes of completion time of bainite transformation has important effect on alloy design.

Figures 8—10 also shows that pearlite transformation curve moves toward right or longer times—in each case. This happens due to the fact that as austenite is stabilized, more Ti content ensures more carbide formation. Nevertheless, in austenite, a lack of carbon occurs, which inhibits cementite formation. For this reason, austenite is stabilized at a higher amount and pearlite transformation is lowered too. A slight shift of bainite curve towards right is also observed for all compositions. At low temperatures, all Ti and C remains solution in austenite. Few fine precipitates of TiC form which is determined by the carbon content of the steel. Ti reduces the diffusion rate of carbon. Hence, bainite formation slows down.

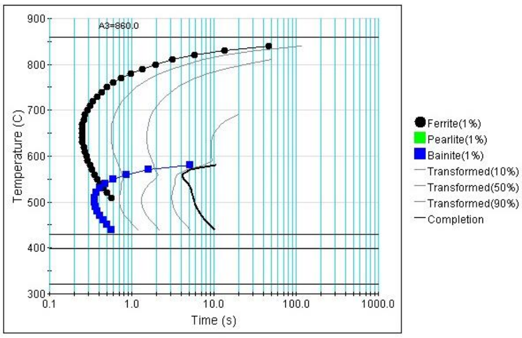

Fig. 8. Time–temperature–transformation (TTT) diagram of Ti free low carbon steel

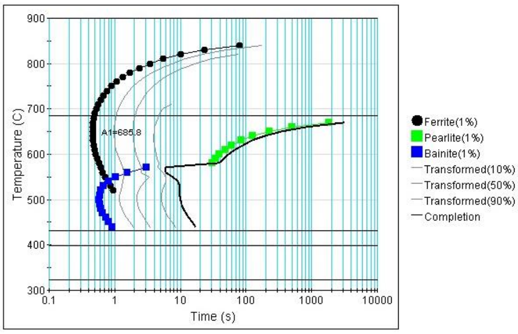

Fig. 9. Time–temperature–transformation (TTT) diagram of 0.1%Ti low carbon steel

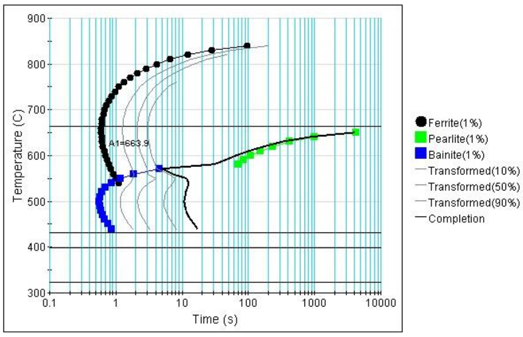

Fig. 10. Time–temperature–transformation (TTT) diagram of 0.2%Ti low carbon steel

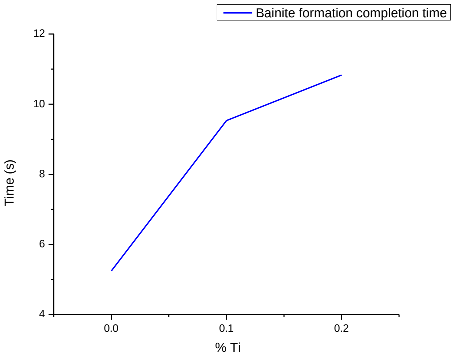

Fig. 11. Time to complete bainite formation vs. %Ti

Hardness and tensile strength

Earlier cooling rate effects on phase transformation was shown. Now, such impact can be partly minimized by Ti addition. It is clear from Figure 12 that without the presence of Ti cooling rate plays a dominating role in hardening of steels. However, such effect can be delayed with the addition of Ti at least up to a certain degree of cooling. This is due to the relevant phase transformation of austenite with the presence of Ti. From Figure

13, it is observed that tensile strength of the steel increases as the cooling rate is increasing for a specific composition. This trend is predicted to be in match with the hardness data.

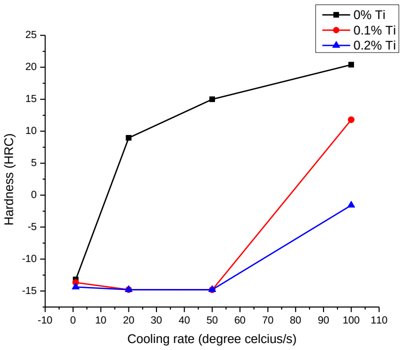

Fig. 12. Hardness vs cooling rate

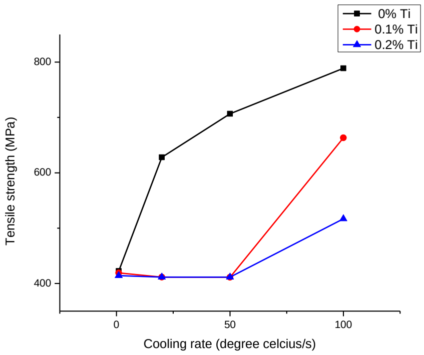

Fig. 13. Tensile strength vs cooling rate

As the amount of Ti increases, a reduction in both hardness and tensile strength can be observed. As, Ti favors ferrite formation and in Figures 4—6, the cooling rate required to form bainite or martensite is very high and their amount is also low, both the hardness and tensile strength lowers. In addition, sulfide in Ti free condition increases brittleness or hardness of the alloy. However, Ti controls their morphology [6] and reduces the hardness.

5. Conclusion

Ti addition stabilizes austenite and retards the transformation of ferrite by forming carbides. These carbides also reduce available C in austenite and both pearlite and bainite formation is slowed down. So, the TTT curves of bainite and pearlite move to the right. And in continuous cooling, Ti favors more ferrite formation and suppresses martensite and bainite formation.

6. Acknowledgements

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6. References

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