Microstructure Modelling of Effects of Phosphorus on Phase Transformation of Plain Carbon Steel

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Abstract

Plain carbon steels are used profoundly for structural purposes and also in automobiles for approximately over a century. Phosphorus (P) is found in minor quantity in general steels. It is considered as the impurity in steels. In Bangladesh, steels are commonly used as structural materials as rebar. In rebar, P is typically expected to be present in less than 0.025 weight per cent. However, due to improper manufacturing processes, sometimes P is found in considerably higher amounts. This work focuses con microstructural modelling of different amounts of P in plain carbon steels. P was added is different quantities as modelling work was carried out to predict phase formation at different temperatures. Also, the amount of retained austenite and martensite were calculated. The relationship of martensite and phosphorus content is crucial since most local rebars are produced in controlled cooling method, known as TMT process, where the transformation of austenite to martensite is the role maker for imparting strength in the rebar. In this context, the shifting of nose of TTT diagrams and response to corresponding CCT curves clearly explained the increased amount of retained austenite with the higher quantity of P. Strengths at room temperatures were also modelled to clarify the obtained data from modelling.

Keywords: CALPHAD, Phosphorus in Steel, Retained Austenite

Introduction

Steel is an alloy of Iron (Fe) and Carbon (C) in which the percentage of C can range from 0.03% to 2% depending on grade. Steel preserves it's metallic properties while gaining specific attributes due to inclusion of various alloying elements such as Manganese (Mn), Chromium (Cr), Vanadium (V), Phosphorous (P) etc. Different combinations of alloying elements introduce unique properties making steel one of the most versatile and widely-used material to date [1,]. Plain carbon steel attains most of its properties from C. However, it contains other elements like Mn, Silicon (Si), Sulphur (S) and P due to production processes, not for property modification purposes [2].

P can have both beneficial and harmful effects on the properties of steel depending on amount. It is one of the best solid strengthening elements for ferrite. Just 0.17% increase in phosphorous can raise the tensile strength by 62 MPa [3]. Conversely, P can cause different types of embrittlement in steel—consequently toughness deteriorates [4]. Effects of P was recently observed on hot deformation behaviour using neural network [5].

This work is focused on microstructural modeling of plain carbon steels with varying amounts of P. Observations were made on phase distributions along a range of temperatures with steel having different amounts of P in the composition. Observations were made on steels with 0.002 (1st alloy), 0.02 (2nd alloy), 0.2 (3rd alloy) and 0.4 (4th alloy) wt. % P. These results were obtained by the means of microstructural modeling. The amount of retained austenite and martensite were also observed.

Methodology

The CALPHAD (Calculation of Phase Diagram) method is currently the dominant approach used to model phase equilibria of a system [6]. It is possible to use multi-component thermodynamic database for material property data and use those data to incorporate C sub-routines to extrapolate properties to predict final materials properties and behavior under different conditions [7]. CALPHAD method employs Gibbs free energy method to envisage mechanical and physical properties of engineering materials [8]. Steel of a common composition, C 0.2%, Mn 1.0%, Si 0.25%, P 0.002 and S 0.002% (wt.% basis) was chosen and data prediction was based on this composition. P content was increased for the same composition, and its effect on different properties were thoroughly investigated.

Result and Discussion

As can be seen from the curves, P has a significant effect on the solidus and liquidus line. On the base alloy, where with wt% of P is 0.002, the gap between the solidus and liquidus line is very short. The solidus and liquidus



Fig. 1. Equilibrium phases at different temperatures for carbon steel with 0.002(top left), 0.02(top right), 0.2(bottom left), 0.4(bottom right) wt% P

temperature here is around 1480° C and 1500° C respectively. Not much difference can be noticed on the steel with 0.02% P. However, significant changes can be observed at 0.2 and 0.4 wt% P steels. For 0.2 wt% P, the steel's solidus-liquidus gap seems to have grown much wider ranging from 1500° C to 1400° C bringing the solidus temperature down to 1400° C. Finally, the steel with 0.4% P shows the widest solidus-liquidus gap among all the alloys. The solidus temperature here is approximately 1320° C. It should be noted that the liquidus temperature remains consistent across the different percentages of P at 1500° C. It can thus be concluded that the liquidus line is unaffected by the addition of P.

The trend seems that the solidus temperature continuously decreases with increasing amount of P. Other observations can be made from these curves such as increasing P stabilizes ferrite phase at higher temperatures. On the base alloy (0.002% P), all the ferrite is transformed to austenite at 800° C. Ferrite to austenite transformation temperature for the steels with 0.2 and 0.4 wt% P are approximately 880° C and 970° C respectively.



Fig. 2. Effect of P on Solidus(left) and Liquidus(right) temperature



Fig. 3. TTT diagram for steels with 0.002(top left), 0.02(top right), 0.2(bottom left), 0.4(bottom right) wt% P

Here, it is observed that the nose for bainite formation shifts significantly at the P wt% 0.4 while the other alloys show a nearly consistent result. For the 1st, 2nd and 3rd alloy, the nose is approximately at 0.3s and 500^oC. For thye 4th alloy, however, it's at approximately 450^oC and 3s.

Alloy	Temperature	Time
1 st Alloy	520°C	0.31s
2 nd Alloy	520°C	0.28s
3 rd Alloy	530°C	0.3s
4 th Alloy	450°C	3s

 Table 1. Position of nose for different alloys



Fig. 4. CCT diagram for steels with 0.002(top left), 0.02(top right), 0.2(bottom left), 0.4(bottom right) wt% P

It is noteworthy that with the same cooling rate, higher hardness values were predicted for the alloy with high P content. For the 1^{st} and 2^{nd} alloys, hardness values were 35 and 38 for a specific cooling rate. However, for the 3^{rd} and 4^{th} alloys, hardness values were 41 and 62 respectively for the same cooling rate. This is attributed to the higher amount of martensite formed. It can thus be concluded that increasing P shifts the critical cooling rate to the right and helps the formation of martensite.

Conclusion

Phosphorus content abruptly affects solidus and liquidus temperatures of the alloy. Such changes are crucial to determine the range of solidification. At the same time, bainite formation is also altered by the addition of P. More P shifts the nose of the TTT curve, and this can delay the transformation of bainite. Since bainite imparts strength in the material, bainite formation temperature adversely modify materials tensile properties. On the other hand, CCT curves are shifted to the right by the addition of P. This is significantly helpful for martensite formation. Therefore, to obtain good mechanical properties, P can be beneficial depending on its amount and the composition of the steel.

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