Design of the Directly Air-cooled Pearlite-free Multiphase Steel from CCT Diagrams Developed Using ANN and Dilatometric Methods

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Present study aims to predict the effect of Ti, B, Cu and Ni on continuous cooling transformation diagrams of low carbon (0.04–0.05 wt%) steels by artificial neural network model. The predicted results are validated with dilatometric studies. Comparison of the phase fields in different continuous cooling transformation diagrams demonstrated that in Ni containing 1.5 wt% Cu-added Ti–B microalloyed steel it is possible to achieve dual phase (ferrite–martensite) microstructure in directly air-cooled condition (i.e., at cooling rate close to 1°C/s) by suppressing pearlite formation. Addition of Cu has remarkably improved the hardness of the dilatometric samples.

KEY WORDS: CCT diagram; microalloyed steels; ANN model; dilatometric method.

1. Introduction

Microstructure formation in low carbon multiphase steels like dual phase steels is essentially governed by the thermomechanical schedule adopted for forming the alloy. Steps like intercritical annealing and/or isothermal holding at particular temperature between hot rolling and cooling necessitate additional installation and control. Any attempt towards simplification of such schedules by judicious modification of composition requires understanding in respect of the continuous cooling transformation (CCT) behavior of the probable compositions. Experimental determination of a CCT diagram necessitates rigorous dilatometric experiments in combination with microstructural studies. However, experimental determinations of CCT diagrams are time consuming and often fail to reveal the narrow temperature regimes of the intermediate transformation of austenite. It is therefore advantageous to predict the different features of CCT diagram of the wide range of probable compositions. Such attempts help in the first-cut understanding of the continuous cooling transformation behavior for a larger population of compositions thereby reduce the required number of experimental trials and improve the accuracy of experiment. Artificial neural network (ANN) has been established as a potential method for predicting austenite transformation using the chemical composition, the austenitization temperature and cooling rate as input.1–5) The attempts successfully predicted the transformation temperature range, but with uncertainties particularly for the bainite reaction.

In the present attempt, ANN models are developed with an aim to predict the phase fields in the CCT diagram of Ti–B microalloyed steel. Subsequently, the effect of Cu and Ni on the phase formation in Ti–B steel has been assessed by predicting the CCT diagrams of Ti–B steels containing varying amount of Ni and Cu. In such diagrams possibility of retarding pearlite formation under favourable cooling conditions, like air cooling, has been examined. The results of the aforesaid ANN exercise allowed to ascertain the formation of ferrite–martensite dual phase microstructure in Ni (0.8 wt%) and Cu (1.5 wt%) containing microalloyed steel under air cooling condition. A brief description of ANN exercise, incorporating the most relevant results, is presented here with an aim to hint upon the role of ANN in envisaging the continuous cooling behaviour of the alloys. Subsequently, the selected alloys are subjected to dilatometric study to verify the results predicted by ANN.

2. Modeling and Experimental Techniques

The artificial neural network used in the present case is a supervised multilayered feed forward network trained with standard gradient descent back propagation algorithms. Ten compositional and six process variables are defined as input nodes and the three property variables are described as output nodes. The inputs and outputs are connected through hidden units. The inputs \((X_i)\) are multiplied by weights \((W_{ji})\) for a hidden node \((h_j)\). Summation of all the \(W_{ji}X_i\) is then added to a bias value \((\theta_j)\) and finally operated by a suitable transfer function \((f)\). The operation may be written as:
Similar operations are repeated for varying number of hidden layers in order to obtain the suitable network architecture. Hidden layers contribute to the output nodes through a linear operation. The output \( Y \) is expressed as:

\[
h_j = f\left(\sum W_j X_i + \theta_i\right) \quad \text{(1)}
\]

where \( W_j \) and \( \theta_i \) are new sets of weights and bias values. In the process of learning, the difference between the predicted and actual output is back propagated to adjust all the weight and bias values.

**Table 1** presents the compositions of the alloys obtained after spectroscopic analysis using an Optical Emission Spectrometer (SPECTROLAB-M8).

A detailed dilatometric study of the alloys was carried out using Gleeble 1500 thermomechanical simulator. Hollow samples of dumbbell and cylindrical shape having wall thickness of \( \sim 1 \) mm, were used for the determination of critical temperatures. After soaking at 1 000°C for 15 min the samples were cooled under constant rates of 0.1, 0.5, 1.0, 5.0, 10.0, 20.0, 30.0, 50.0 and 100.0°C/s. The experiments were carried out under argon atmosphere. Austenite transformation start and finish temperatures were determined from the dilatation curves and the same were used for construction of the CCT diagrams of the steels.

Microstructure of the samples after etching with Vilella’s reagent\(^6\) were examined under the scanning electron microscope (SEM) (Model: JEOL, JSM-5510) operated at 20 kV.

Hardness measurement was carried out with a Brinell cum Vickers hardness tester under 1 kg load of the dilatometric samples. The average of six indentations with an error of approximately \( \pm 3\% \) was reported.

### 3. The Neural Network Model

#### 3.1. Data Selection and Processing

In the present work, the input data were collected from the CCT diagrams of low carbon steels (0.15–0.3 wt% C) reported in literature.\(^7,^8\) The input data set comprises chemical compositions (C, Mn, Si, Cu, B, Ti, V, Cr, Ni, and Mo in wt%), cooling rate and the austenitising temperatures. Austenitising temperature was used as a qualitative representation of grain size in respect of the transformation kinetics.\(^9\) Transformation initiation and completion temperatures for ferrite, pearlite and bainite are used as output parameters as described by the previous workers.\(^1–^3,^10\)

Graphical form of CCT diagram was converted to numerical format as a necessity for using the particular type of neural network. The number of intercepts obtained by superimposition of the Newtonian curves on each CCT diagram were artificially fixed at six, depicting the start and finish temperatures of ferrite, pearlite and bainite transformations respectively, following the earlier approach.\(^1\) For a given cooling rate, in the absence of formation of a particular phase, the start and finish temperature of the concerned transformation are assigned the values same as those of the following transformation.

About 450 sets of data were collected from CCT diagrams of about 60 different steels in numerical format from which 230 data sets were used for training and 115 data sets were used for testing the net. The rest were used for in-process validation of the network. The classifications of different sets were prepared by randomly selecting the data records in order to maintain the uniformity in the training, testing and validation data set.

Representative statistical information of the total data set describing the domain of applicability of the model is listed in **Table 2**. For back propagation neural network the inputs and output are normalized within the range of 0 to 1 by the following conversion operation:

\[
x_N = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} \quad \text{(3)}
\]

where \( x_N \) is the normalized value of a variable \( x \), \( x_{\text{max}} \) and \( x_{\text{min}} \) are the maximum and minimum values of the raw data, respectively.

**Table 1.** Chemical composition of the investigated steels (wt%).

<table>
<thead>
<tr>
<th>Steel Identification</th>
<th>% C</th>
<th>% Mn</th>
<th>% Si</th>
<th>% S</th>
<th>% P</th>
<th>% Ti</th>
<th>% B</th>
<th>% Cu</th>
<th>% Ni</th>
<th>% N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti</td>
<td>0.04</td>
<td>1.57</td>
<td>0.46</td>
<td>0.02</td>
<td>0.014</td>
<td>0.032</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>0.03</td>
<td>1.64</td>
<td>0.49</td>
<td>0.02</td>
<td>0.008</td>
<td>0.0013</td>
<td>0.0061</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ti - B</td>
<td>0.04</td>
<td>1.60</td>
<td>0.49</td>
<td>0.02</td>
<td>0.013</td>
<td>0.028</td>
<td>0.0009</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5Cu - Ti - B</td>
<td>0.04</td>
<td>1.60</td>
<td>0.48</td>
<td>0.02</td>
<td>0.014</td>
<td>-</td>
<td>-</td>
<td>1.51</td>
<td>-</td>
<td>0.0051</td>
</tr>
<tr>
<td>1.0Cu - Ti - B</td>
<td>0.04</td>
<td>1.48</td>
<td>0.42</td>
<td>0.02</td>
<td>0.013</td>
<td>0.047</td>
<td>0.0025</td>
<td>1.09</td>
<td>-</td>
<td>0.0065</td>
</tr>
<tr>
<td>1.5Cu - Ti - B</td>
<td>0.05</td>
<td>1.63</td>
<td>0.47</td>
<td>0.02</td>
<td>0.014</td>
<td>0.047</td>
<td>0.0015</td>
<td>2.17</td>
<td>-</td>
<td>0.0062</td>
</tr>
<tr>
<td>1.5Cu - Ti - B - Ni</td>
<td>0.03</td>
<td>1.68</td>
<td>0.53</td>
<td>0.02</td>
<td>0.013</td>
<td>0.032</td>
<td>0.0012</td>
<td>1.55</td>
<td>0.79</td>
<td>0.0058</td>
</tr>
</tbody>
</table>

**Table 2.** The maximum, minimum, average value and standard deviation of the parameters for determining the CCT diagrams.

<table>
<thead>
<tr>
<th>Variables</th>
<th>Maximum Value</th>
<th>Minimum Value</th>
<th>Average Value</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (wt%)</td>
<td>0.30</td>
<td>0.015</td>
<td>0.1221</td>
<td>0.0624</td>
</tr>
<tr>
<td>Mn (wt%)</td>
<td>2.33</td>
<td>0.320</td>
<td>1.1432</td>
<td>0.4381</td>
</tr>
<tr>
<td>Si (wt%)</td>
<td>1.20</td>
<td>0.150</td>
<td>0.4286</td>
<td>0.2664</td>
</tr>
<tr>
<td>Cu (wt%)</td>
<td>1.86</td>
<td>0.000</td>
<td>0.1575</td>
<td>0.3467</td>
</tr>
<tr>
<td>B (wt%)</td>
<td>0.01</td>
<td>0.000</td>
<td>0.0009</td>
<td>0.0023</td>
</tr>
<tr>
<td>Ti (wt%)</td>
<td>0.18</td>
<td>0.000</td>
<td>0.0148</td>
<td>0.0447</td>
</tr>
<tr>
<td>V (wt%)</td>
<td>0.37</td>
<td>0.000</td>
<td>0.0699</td>
<td>0.0844</td>
</tr>
<tr>
<td>Cr (wt%)</td>
<td>5.75</td>
<td>0.000</td>
<td>0.5634</td>
<td>1.0896</td>
</tr>
<tr>
<td>Ni (wt%)</td>
<td>3.48</td>
<td>0.000</td>
<td>0.5787</td>
<td>0.7557</td>
</tr>
<tr>
<td>Mo (wt%)</td>
<td>0.96</td>
<td>0.000</td>
<td>0.2509</td>
<td>0.2554</td>
</tr>
<tr>
<td>Tan (°C)</td>
<td>1350.00</td>
<td>850.00</td>
<td>967.4118</td>
<td>114.0165</td>
</tr>
<tr>
<td>CR (°C/s)</td>
<td>167.30</td>
<td>0.020</td>
<td>17.0297</td>
<td>31.2520</td>
</tr>
<tr>
<td>Fs (°C)</td>
<td>904.44</td>
<td>329.00</td>
<td>681.3865</td>
<td>112.8964</td>
</tr>
<tr>
<td>FF (°C)</td>
<td>791.00</td>
<td>329.00</td>
<td>604.6251</td>
<td>77.4782</td>
</tr>
<tr>
<td>Ps (°C)</td>
<td>791.00</td>
<td>329.00</td>
<td>604.6251</td>
<td>77.4782</td>
</tr>
<tr>
<td>Pf (°C)</td>
<td>745.00</td>
<td>329.00</td>
<td>584.1760</td>
<td>72.7409</td>
</tr>
<tr>
<td>Bs (°C)</td>
<td>745.00</td>
<td>329.00</td>
<td>569.3752</td>
<td>72.9863</td>
</tr>
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<td>BF (°C)</td>
<td>703.33</td>
<td>205.00</td>
<td>445.2575</td>
<td>112.0200</td>
</tr>
</tbody>
</table>

650

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are the maximum and minimum values of $x$ respectively. The composition of the eight alloys, described in Table 1, have been used finally to compare and explain the CCT diagrams, developed through dilatometric method and through the model prediction method in order to demonstrate the reliability of the model.

3.2. Formation of Model Committee Through Optimization of Network Architecture

In the present study, optimization of the number of hidden units and hidden layers was achieved by using hyperbolic tangent function considering its inherent flexibility. Several network architectures were configured by varying the number of hidden layers and number of neurons in it. The developed models were trained separately with an aim to identify the most appropriate one according to their prediction error.

The networks with different complexities were trained with Scaled Conjugate Gradient (SCG) and Levenberg–Marquardt (LM) algorithms, which are found to be superior to other algorithms in earlier studies. Although the networks trained with LM algorithm provides better results with 4 and 5 hidden layers, for comparable number of architecture, SCG algorithm seems much superior for minimizing the error level for such a complicated problem as well as exhibits better prediction capacity than LM algorithm. Taking this into account, a committee was formed with few best models and the mean prediction of the models was used to describe the input–output relationship. This exercise usually minimizes the prediction error of any individual model. In line with the earlier studies formation of the committee was carried out by ranking the models for each training algorithms in order of the error levels occurred in the course of their predictions. Finally, the exercise resulted into a committee comprising three models trained with SCG algorithm and one model trained with LM algorithm.

3.3. Model Performance and Reliability

The models performances were verified for each transformation temperature (start and finish) separately through the correlation coefficient study between the predicted and observed temperature. It may be mentioned here that in each case the correlation coefficient was above 0.8. Figure 1 presents the example of one such scatter plot showing the correlation between bainitic transformation start temperatures predicted by the model and experimentally observed bainitic transformation start temperature. The marker in the scatter diagram represents the performance of the trained network on the total data set including training, testing and in-process validation data. From the same figure it is also evident that the prediction performance of the model is satisfactory within the domain of applicability of the model defined by its statistical history presented in Table 2. Table 1 presents the compositions of eight alloys used for comparison of CCT diagram developed through the models and compare with those developed through the dilatometric method. These new alloys are completely unknown to the model and isolated from the model development environment. Despite that, close convergence of the predicted model and the experimental CCT diagram further substantiates the reliability of the model.

4. Results and Discussion

4.1. Validation of the Model of CCT Diagram

To assess the accuracy in predictability of the CCT diagram by the committee a predicted CCT diagram was compared with an experimental one for an 0.09C–1.48Mn–0.25Si–0.06S–0.014P–0.01Cr–0.01Ni–0.01Mo–0.04V–0.01Cu–0.047Al (wt%) steel, austenised at 950°C. The comparison of the diagrams presented in Fig. 2 confirms that the model predicted ferritic, pearlitic and bainitic transformation temperatures with reasonable accuracy.

4.2. Determination of CCT Diagram

Figures 3(a) to 3(d) demonstrate the effect of Ti (0.032 wt%), B (0.0008 wt%), Ti (0.028 wt%) + B (0.009 wt%) and Cu (1.51 wt%) on the transformation temperature ranges concerning the formation of different phases. Corresponding results obtained from dilatometric investigations are also appended in the figures. It is evident that the exper-
Fig. 3. Comparison of the experimental (symbols connected by solid lines) and the predicted (dashed lines) CCT diagrams for (a) Ti, (b) B containing steels, (c) Ti–B and (d) 1.5 wt% Cu containing steels.
Experimental results reasonably match with the predicted results in terms of initiation and completion of the austenite transformation. It is interesting to note that while the dilatometric results failed to capture the temperature ranges concerning pearlitic and bainitic transformations for the chosen cooling rates, the present model has clearly delineated the same. The influence of B is exhibited in terms of widening the temperature range for bainitic transformation and Cu extends the bainitic transformation domain towards much slower cooling rates. Figure 3(c) clearly reveals the synergistic effect\(^{[3]}\) for the combined addition of Ti and B in terms of lowering the Ac\(_3\) and Ac\(_1\) temperatures. Lowering of the austenite transformation temperatures is more prominently captured in the results predicted by ANN modeling.

Comparison of Figs. 3(a) to 3(c) with Fig. 3(d) indicate that lowering of the Ac\(_1\) transformation temperature is most significant in the case of 1.5 wt% Cu-added sample. However, the predicted CCT diagrams do not reveal any variation in terms of temperature range related to the pearlitic transformation.

Figures 4(a) to 4(c) show the effect of variation in amount of Cu-addition (1.0–2.0 wt%) in Ti–B microalloyed steel. Comparison of results shown in Fig. 3(c) with Figs. 4(a) to 4(c) indicates that Ac\(_3\) and Ac\(_1\) temperatures are primarily influenced by Ti and B rather than Cu, at least up to 1.5 wt% Cu. Addition of 2.0 wt% Cu markedly reduces the transformation temperatures. It may be noted that the temperature range for pearlitic transformation has been nar-

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**Fig. 4.** Comparison of the experimental (symbols connected by solid lines) and the predicted (dashed lines) CCT diagrams for (a) 1.0 wt% Cu–Ti–B, (b) 1.5 wt% Cu–Ti–B and (c) 2.0 wt% Cu–Ti–B steels.
rowed down with increase in Cu concentration (>1.0 wt%). Moreover, a wide temperature range of bainitic transformation is achieved even at the lower cooling rates (say 0.1°C/s) for addition of Cu ≥1.5 wt% (Figs. 3(d), 4(b) and 4(c)).

It may be mentioned here that addition of Ni is recommended in the Cu-added steels to circumvent the occurrence of hot shortness during hot rolling.14) Therefore, it is reasonable to examine the influence of Ni on austenite transformation behavior of Cu-added Ti–B microalloyed steels. Figure 5 shows that Ni addition has completely eliminated the pearlite transformation with the chosen range of cooling rate and markedly reduced the transformation temperatures.

To understand the individual effect of Ni on pearlite transformation the steels containing only Ni and Ni with Ti and B are examined using the present ANN model. Figures 6(a) and 6(b) demonstrate that neither Ni only nor Ni in combination with Ti and B are effective to suppress the pearlitic transformation. The observation thus corroborates the combined role of Ni and Cu in suppressing pearlite formation as revealed in Fig. 5. The CCT diagrams clearly demonstrate the effect of the alloy content in retarding the γ→α transformation. Most interesting feature is the lower-

Fig. 5. Comparison of the experimental (symbols connected by solid lines) and the predicted (dashed lines) CCT diagrams for Ti–B microalloyed steel containing 1.5 wt% Cu and 0.79 wt% Ni.

Fig. 6. The predicted CCT diagrams (dashed lines) for steels containing (a) 0.77 wt% Ni in the absence of microalloying elements and (b) 0.81 wt% Ni with Ti–B microalloying additions.
ing of Ar₃ temperature in the case of Ni containing 1.5 wt% Cu-added alloy (Fig. 5). It may also be noted that although the predicted lowering of ferrite start temperature is more prominent than the experimental one at lower cooling rate, a reasonable agreement between experimental and predicted values are achieved at higher cooling rates (say, ≥5°C/s).

The experimental and predicted CCT diagrams hint upon the fact that alloys containing up to 2.0 wt% Cu without Ni addition fails to circumvent the pearlitic transformation. Moreover, the Ni containing 1.5 wt% Cu-added alloy provide optimum benefit in terms of achieving adequate austenite as well as retaining adequate amount of bainite in the microstructure under air-cooling condition. Therefore, the above results unambiguously suggest the possibility of obtaining a pearlite-free microstructure akin to the conventional ferrite–martensite dual phase steels.

### 4.3. Microstructure Formation in Dilatometric Samples

Figures 7(a) to 7(e) show the SEM micrographs of Ti–B microalloyed steel. For cooling rates from 0.1 to 5°C/s pearlitic regions are formed along the ferrite grain boundaries (Figs. 7(a) to 7(c)). At the cooling rates (CR) of 20°C/s and 100°C/s the equiaxed ferritic grains are almost absent (Figs. 7(d) and 7(e)). The microstructure is constituted by bainite (α°₂) and martensite (α') of lath morphology.

Figures 8(a) to 8(e) show the SEM micrographs of Cu-added Ti–B microalloyed steel. The microstructure formed at a cooling rate of 0.1°C/s (Fig. 8(a)) comprises polygonal ferrite (αₚ) grains and pearlitic constituents at grain boundary and triple points similar to that obtained in the case of Ti–B steel at the same cooling rate. At a cooling rate of 1.0°C/s nominal amount of martensitic islands (α') are formed along the boundaries of polygonal ferrite (Fig. 8(b)). At a cooling rate of 5°C/s microstructure (Fig. 8(c)) shows nominal amount of equilibrium ferrite and marked presence of massive ferrite (αₚ₉) and lath like bainitic and/or martensitic phases. At the cooling rates of 20°C/s and 100°C/s, microstructure (Figs. 8(d) and 8(e)) is essentially constituted by lath martensitic (α') phases.

Figures 9(a) to 9(e) show the microstructures of dilatometric samples in the case of Cu and Ni-added Ti–B microalloyed steel. At a cooling rate of 0.1°C/s, the microstructure (Fig. 9(a)) is predominantly ferrite along with the presence of notable amount of pearlite. At a cooling rate of 1.0°C/s, the microstructure (Fig. 9(b)) reveals ferritic regions with islands of martensite formed at the grain boundary and triple point regions. It is imperative to mention that the microstructural features in Fig. 9(b) reveal close resemblance with ferrite–martensite dual phase microstructures. The microstructure (Fig. 9(c)) obtained at a cooling rate of 5°C/s shows considerable amount of bainite/martensite along with nominal amount of massive ferritic regions. At the cooling rates of 20°C/s and 100°C/s, the microstructure (Figs. 9(d) and 9(e)) is essentially lath martensitic in nature.

The microstructural observations clearly indicate that in the case of Ti–B steel pearlite formation from austenite is suppressed at a cooling rate >5°C/s and lath like phases evolve at higher cooling rates (20–100°C/s). However, Cu addition in the present Ti–B microalloyed steel has effectively suppressed the pearlitic decomposition of austenite at cooling rates >1°C/s. While microstructures of the Cu-added steels comprise nearly equiaxed ferrite grains and martensitic islands distributed along the grain boundaries.
and triple points for cooling rates from 1 to \( \times 20\,^\circ\text{C}/\text{s} \), cooling at higher rates form lath morphology of ferrite/bainite. The aforesaid results reasonably corroborate the phase evolution in the present alloys predicted by ANN model and dilatometric study. It is evident that Cu addition in Ti–B microalloyed steel is effective in suppressing pearlite formation. The Ni- and Cu-added microalloyed steel formed a ferrite – martensite microstructure akin to the conventional dual phase steel under a cooling rate close to air cooling condition.

4.4. Hardness Measurement

The hardness values obtained from the present alloys under different cooling rates are appended in the concerned CCT diagrams. Figure 10 shows the variation of hardness as the function of cooling rate for different alloys. Addition
of Ti resulted plateau in hardness curve above cooling rate of 10°C/s. For the other alloys, the plateaus are attained after a cooling rate of 50°C/s. At any given cooling rate, the hardness values vary with alloying in the order of Ti<B<Ti+B<Cu+Ti+B. Effect of B in increasing the hardness is remarkably greater than Ti particularly at higher cooling rates (20–100°C/s) and similarly Cu (1.5 wt%) is more effective than B. In the case of Cu-added microalloyed samples hardness values increase with increase in Cu.

Observed variation in hardness among different alloys particularly at higher cooling rates may be attributed to the fact that addition of increased amount of Cu and presence of Ni in the Ti–B microalloyed steel enhances the formation of low temperature transformation products. Attainment of plateau above a cooling rate of 50°C/s for all the alloys indicates that the saturation of displacive transformation.

5. Conclusions

(1) The predicted and experimental CCT diagrams established the scope of obtaining dual phase like microstructure in 1.5 wt% Cu and Ni-added steels at a cooling rate comparable to air-cooling condition.

(2) The microstructural investigation clearly demonstrated the absence of pearlite in the microstructure obtained in 1.5 wt% Cu-added Ti–B microalloyed steel in directly air-cooled condition (i.e., for cooling rate >0.1 °C/s). The effect is most prominent in Ni containing Cu-added Ti–B microalloyed steel and the microstructure formed therein is comparable with dual phase steels.

(3) The Cu containing alloys particularly at the higher cooling rate exhibit remarkable improvement in hardness.

(4) The results strongly suggest the necessity of experimental exercise to study the microstructural evolution and mechanical behavior of the directly air-cooled Cu-added Ti–B microalloyed steel.

REFERENCES