Mathematical Model to Predict Property of Plain Carbon Steel

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***Abstract*—This paper gives a mathematical model to predict certain properties mainly, mechanical properties like hardness, tensile strength, of a two component equilibrium system. Iron-carbon system has been chosen as an application to the proposed model and various properties have been discussed. The model is based on two major rules, the lever rule and the rule of mixtures. Lever rule can be applied for any two component system but rule of mixtures have certain limitations regarding its applicability, which have been due fully mentioned. A detailed method has been provided for deriving the equations. And, graphical representation of those equations is also shown.**

Keywords—Rule Of Mixtures; Hardness; Lever Rule; Tensile Strength; Morphology; Microconstituent

1. INTRODUCTION

Any material has its application based on its properties. Therefore, it is essential to know the property of material. Properties of any material can be calculated by performing destructive testing such as tensile testing, creep testing, hardness testing, impact strength and non-destructive testing like ultrasonic testing, eddy current testing, liquid penetrant testing, magnetic particle testing and many more. But these tests require many numbers of samples and also time. Later on if the property is not according to the requirement, the synthesis process is to be repeated with the required modification in the composition of the sample. Previously, some researches[1,2] have been done to predict mechanical properties of various materials before they are synthesized.

Plain carbon steel is an alloy of iron and carbon basically, but also some other elements, known as alloying element, may be present in small quantities. Plain carbon steels can be categorized as: hypo-eutectoid steels (0.008-0.8% C), eutectoid steel (0.8% C), and hyper-eutectoid steels (0.8-2% C). Steels with carbon percentage higher than 2% C are called cast irons.

The final property of the material depends strongly on the microstructure of that material. The microstructure, on the other hand depends on the phases present, which depends on composition, temperature and pressure, the three degrees of freedom. In material science, pressure is often considered to be constant, therefore the Gibbs phase rule for two-component system is reduced to F = C – P + 1, where F is the degree of freedom, C is the number of components and P is the number of phases in equilibrium. The **lever rule** is a tool used to determine weight percentages of each phase of a binary equilibrium phase diagram. It is used to determine the percent weight of liquid and solid phases for a given binary composition and temperature that is between the liquidus and solidus. Lever rule is very helpful in determining the microstructure of the sample.

A general idea to calculate the property of any material is obtained by using the rule of mixtures. Rule of mixtures[3,4] is widely used for calculating the property of composites. An advantage of rule of mixtures is that the property can be added or subtracted or even reciprocated depending upon the effect, which the property would have on the final material. The component that would dominate depends upon its properties, the relative volume fractions present and the fabrication process used. While applying Rule of Mixtures to composites, the properties of reinforcement and the matrix is taken into account. While for metal alloys the phases formed by the two individual elements, its morphology and distribution, mostly decides the properties such as tensile strength, hardness, etc. Hence, the rule of mixtures is to be used with due recognition to the fact that not all two component systems, will comply the rule of mixtures. Henceforth, a model has been proposed to apply rule of mixtures to two component systems, specifically iron-carbon equilibrium diagrams.

2. RULE OF MIXTURES

'Rule of Mixtures' are mathematical expressions which gives a property of the material in terms of the properties and quantity of its constituents.

Assume a material with n number of phases or components, as 1, 2, 3,….., n and their respective volume fractions as V_1, V_2, V_3, ….., V_n. Let their individual property be Q_1, Q_2, Q_3, ….., Q_n respectively and the total property of the material be Q.

By rule of mixtures, the property of the material can be given by

$$Q = \frac{Q_1 . V_1 + Q_2 . V_2 + Q_3 . V_3 + \cdots + Q_n . V_n}{V_1 + V_2 + V_3 + \cdots + V_n}$$

As, the sum of all volume fraction is equal to 1, the equation is reduced to,

$$Q = Q_1 . V_1 + Q_2 . V_2 + Q_3 . V_3 + \cdots + Q_n . V_n$$

Note that, even weight fractions can be used instead of volume fractions. Also, the sum of all weight fractions is equal to 1.

The property of any material depends on many factors as: property of phases present, volume fraction of phase present, defects and dislocations, co-herency, structure dependent, morphology of phases, etc. When the influence of

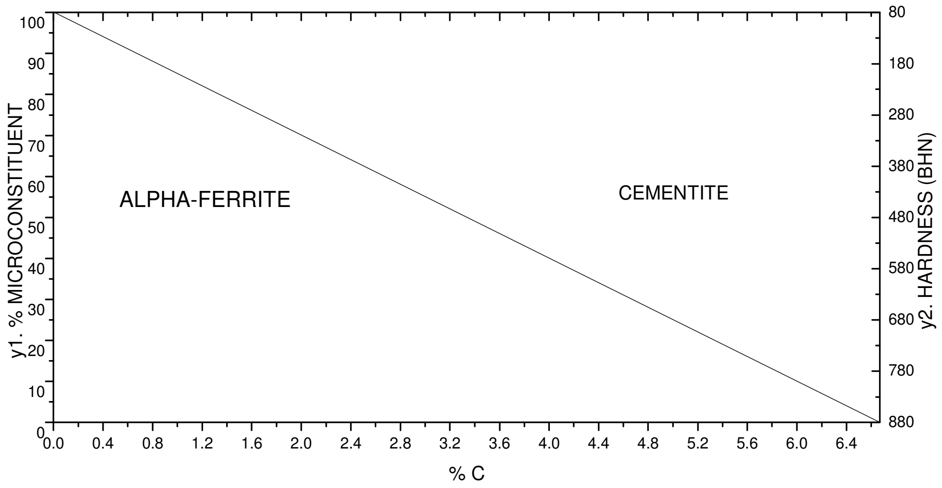

Fig. 1 A plot to show variation of amount alpha-ferrite and cementite with percentage carbon.

morphology is negligible and factors like defects and dislocations, coherency, etc. are side-lined, the property can be approximated as the average of the individual properties of the microconstituent.

The rule of mixtures explained above is hereby, applied for iron-carbon equilibrium diagrams and the following points have been emphasized. In this paper, an attempt is made to correlate (a) percentage microconstituent with percentage carbon by using lever rule, (b) percentage carbon and property with the help of lever rule and rule of mixtures. An effort is also made to establish mathematical equations so as to predict certain properties such as hardness, tensile strength to make the further fabrication process easy. A graphical presentation based on the equations is also given which can be used for predicting properties.

3. *Graphical modeling for Iron-carbon equilibrium system:-*

Lever rule is applied at various carbon percentages in iron-carbon equilibrium diagrams, to calculate the weight fractions of alpha-ferrite and cementite and subsequently a graph is plotted. Fig. 1.a gives the amount of ferrite and cementite phases present as against the percentage of carbon content. The y1 axis gives the percentage weight fraction of alpha-ferrite at room temperature. The percentage weight fraction of cementite can be calculated by subtracting the percentage weight fraction of alpha-ferrite from 100.

Upto 0.008%C, we have 100% ferrite phase. Gradually, it decreases and cementite phase increases. At 6.67%C, ferrite is reduced to zero and cementite is 100%.
This can be given by the equation,

$$y = 100\ (\%) \quad \ldots\ldots (1.a)$$

$$y = -14.99 * x + 100\ \ (\%) \quad \ldots\ldots (1.b)$$

where, x is the percentage of carbon,
y is the percentage of alpha-ferrite,
100 – y is the percentage of cementite.

Eqn. 1.a represents the graph from 0% to 0.008% C, which is straight line. Eqn. 1.b represents the line in respect to y1 axis and has a negative slope of 14.99, as shown in Fig. 1.

For predicting hardness:-

The hardness[5] of 100% ferrite is 80 BHN. From the graph, it is quite evident that with increase in carbon content, percentage of ferrite decreases, resulting in an increase in cementite. As the cementite is a hard phase of 880 BHN[5], the final hardness of plain carbon steel increases from 80 BHN to 880 BHN. Since, property of cementite strongly depends on the microstructure. Therefore, after 2% C the value of final hardness is not consistent with each specimen but maybe found to belong to a range. An equation can be written as follows:

$$\text{Average Hardness} = -8 * f + 880\ (\text{BHN}) \quad \ldots\ldots (2)$$

where, f is the percentage of ferrite present.

In Fig. 2, considering in terms of pearlite, we have 100% pearlite at 0.8%C, this splits the graph into two areas. In the first area from 0.008%-0.8%C (Hypo-eutectoid Steel), proeutectoid ferrite and pearlite are the microconstituents, while in the second area from 0.8%-6.67%C (Hyper-eutectoid steel), proeutectoid cementite and pearlite are the major ones.

As said previously, percentage of ferrite is 100% from 0 to 0.008% C, so percentage of pearlite is zero. For carbon content from 0.008% to 0.8%, the percentage weight fraction of pearlite (y) for line 1 can be approximately calculated using the equation,

$$y = 125 * x\ (\%) \quad \ldots\ldots (3)$$

While for y for line 2, the equation is

$$y = -17.03 * x + 113.63\ \ (\%) \quad \ldots\ldots (4)$$

where, x is the percentage of carbon present in the steel.

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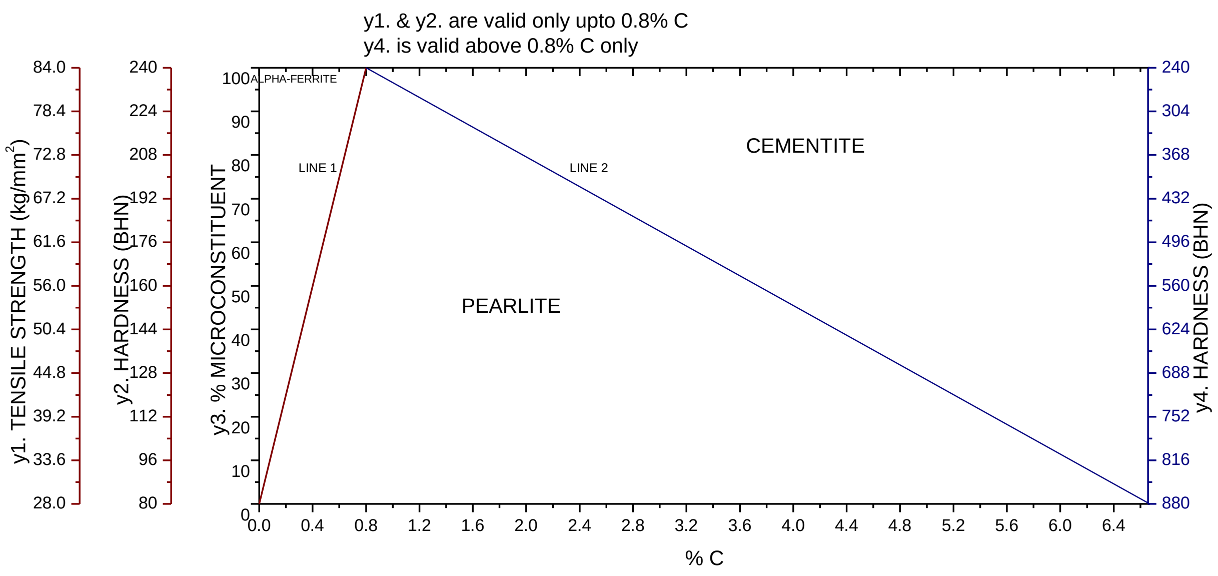

Fig. 2 A plot to show variation of amount of alpha-ferrite and cementite with percentage carbon

100-y gives the percentage weight fraction of the other constituent, which are proeutectoid ferrite and proeutectoid cementite for line 1 and line 2 respectively.

In Fig. 2, the axis y3 is to be referred to calculate the percentages of ferrite and cementite graphically.

(a) Hardness prediction of hypo-eutectoid plain carbon steel:-

To calculate the hardness of hypo-eutectoid steel, the rule of mixtures can be applied, as hardness is not morphology sensitive.

Let p and f be the percentages of pearlite and proeutectoid ferrite in hypo-eutectoid steel.

$$p + f = 100 \quad \ldots\ldots. \text{(i)}$$

Average Hardness = (Hardness of pearlite * p + Hardness of ferrite * f) / 100 …… (ii)

The hardness[5] of pure ferrite and pearlite is 80 BHN and 240 BHN.

Combining (i) and (ii),

$$\text{Average Hardness} = 1.6 * p + 80 \text{ (BHN)} \quad \ldots\ldots (5)$$

In Fig. 2, this equation is represented by line 1 with respect to axis y2 and 1.6 indicates the positive slope of line.

(b) Tensile strength prediction of hypo-eutectoid plain carbon steel:-

Using a similar approach as used for calculating hardness, tensile strength can also be calculated. Tensile strength property is very morphology sensitive. And, hence the following equation gives only an estimate and not the exact strength.

$$\text{Average T. S.} = 0.56 * p + 28 \text{ (kg/mm}^2\text{)} \quad \ldots\ldots (6)$$

The tensile strength[5] of alpha ferrite is known as 28 kg/mm^2. In Fig. 2, this equation is represented by line 1 with respect to axis y1 and 0.56 is the positive slope of the line.

(c) Hardness prediction of hyper-eutectoid plain carbon steel:-

Unlike, for hypo-eutectoid steels, hyper-eutectoid steels are more brittle and therefore, more hard. Although, hardness for 100% cementite is 880 BHN, it varies with different samples as each have a different microstructure. The hardness for 100% pearlite[5] is 240 BHN. With the help of rule of mixtures, the following equation is formed:

$$\text{Average Hardness} = - 6.4 * p + 880 \text{ (BHN)} \quad \ldots\ldots (7)$$

In Fig. 2, this equation is represented by line 2 with respect to axis y4. Also, the negative sign of the slope, 6.4 indicates hardness increases with increasing carbon.

4. RESULTS AND DISCUSSION:-

With the carbon percentages known, the amount of microconstituents present can be calculated and thereby, predict the microstructure. Also, the mechanical properties like hardness or tensile strength can also be known either by using the graph or the equations, provided that the properties do not depend on the morphology. With varying carbon percentages, the change in property can be observed from Fig. 1 and Fig. 2.

In Fig. 1, a negative slope is observed for amount of total ferrite. As a result of which, hardness increases and so does total cementite present. Also, the value of hardness after 2% C is just a rough estimate due to increased influence of morphology.

The amount of pearlite increases for hypo-eutectoid steel (positive slope) and is maximum for eutectoid steel and then decreases (negative slope) from 100% to 0% in hyper-eutectoid steels, in Fig. 2. The other constituents, namely alpha-ferrite and cementite follow a reverse trend as of pearlite in the respective regions. From the hardness axes, it can be concluded that the value of hardness increases from 0-6.67% C. The predicted value of hardness is fairly accurate, but it is not so in the case of tensile strength. A simple reason may be given that the interaction between the two phases is neglected.

Upto 0.8% C, the absence of proeutectoid cementite helps in prediction of tensile strength of hypo-eutectoid steel. Beyond 0.8% C, the brittle nature of cementite is a major factor that does not allow any direct prediction of tensile strength feasible. Therefore, tensile strength has been calculated only for hypo-eutectoid steel and not for hyper-eutectoid steel.

The graph can be used to explore the viable options for different carbon percentages and different mechanical properties. The equations reduce the hassle of drawing a graph and directly give the value of the final property. Furthermore, the equations are derived using a solid reasoning and steps, therefore providing for its credentials. The above discussed model can be applied for any two component system if the system obeys rule of mixtures, although here it was used only for iron-carbon equilibrium diagram. Another point to be noted is that the process of manufacturing the sample must be same for any carbon percentage. That is, samples prepared with different rates of cooling cannot be used while predicting properties. The reason being the property of the individual constituents varies, as the morphology changes[6].

5. CONCLUSIONS:-

A mathematical model to predict the properties of plain carbon steel has been presented. Using the model, some equations have been derived and further using those, two graphs have also been plotted. These graphs give a direct relationship between the percentage of carbon and the amount of microconstituent present and the properties. However, there are certain limitations to the applicability like morphology sensitivity, manufacturing of specimen, etc.

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