Modeling Pearlite Transformation in Super-high Strength Wire Rods: I. Modeling and Simulation in Fe–C–X Ternary Alloys

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A computer model was developed to simulate pearlite transformation in Fe–C base near-eutectoid alloys during isothermal holding, continuous cooling and patenting in view of its application to high carbon super-high strength wire rods. The model is based upon Johnson-Mehl-Avrami theory; it consists of calculation of nucleation and growth rates and conversion of the extended to real volume as well as calculation of lamellar spacing from the well-known correlation with undercooling. Calculated pearlite start and finish temperatures, number and size of nodules and lamellar spacing were in good agreement with those obtained from Gleeble thermomechanical simulation.

KEY WORDS: high carbon steel; pearlite; patenting; lamellar spacing; modeling; nucleation; growth.

1. Introduction

High strength steel wire is widely used in many areas of construction and transportation, such as steel strands for prestressed concrete (PC) and steel tire cord etc. The extremely high strength of these steels, usually more than 1.5 GPa, is achieved primarily from fine pearlitic microstructure in steels of near-eutectoid composition, which can be reduced eventually to a few tens of nm by heavy drawing.1) In recent years marked advancements have been made in high carbon steel wire. For instance, a steel cord of automobile tire having ultimate strength as high as 4 GPa was developed.2) Such a high strength can be achieved from the optimum combination of alloying additions and cooling conditions, preservation of lamellar structure during bluing or galvanization and minimization of the formation of grain-boundary network of proeutectoid cementite or ferrite and strengthening if it was formed.3) Among these we focus our attention on alloying addition and cooling condition during patenting and develop a computer model to calculate lamellar spacing, pearlite nodule size and size distribution given the steel composition and cooling conditions. Results are compared with those obtained from Gleeble thermomechanical simulation.

2. Modeling

2.1. Basic Formulation

The pearlite transformation consists of nucleation and growth of pearlite nodules. At early times Johnson-Mehl-Avrami (JMA) equation was employed to calculate the isothermal transformation curve of pearlite.4) Before we apply the JMA type analysis, a couple of points are noted. In the first, the theory can take into account the effects of hard impingement by extended volume and phantom nuclei. However, the effects of soft impingements are not taken into account*. The growth of pearlite is controlled by carbon diffusion ahead of pearlite nodule/austenite boundaries in eutectoid Fe–C alloys with expedition by boundary diffusion.5) However, it is reported that the extent of diffusion zone ahead of the boundary is not large at larger undercoolings, e.g. ~10 nm at a temperature 70°C below the eutectoid temperature.6) Hence, it is expected that the effect of soft impingement is not very large and the JMA type analysis is applicable to the transformation in the present alloys. In the second, Mehl and Dubé7) noted that the morphology, size relative to the matrix grain size and distribution of pearlite nodules varied considerably with reaction temperature. At higher temperatures where the ratio of nucleation to growth rate was small, the nodule sizes became greater than the grain size and nucleation was taken to occur almost at random. At low temperatures, however, nodules were aligned more or less along the grain boundary, impinged within the boundaries at earlier stages and grew toward the center of the matrix like a sector. In this experiment the matrix grain size was relatively small (d ≤ 20 μm) due to deformation prior to transformation. Hence, we assume that the high temperature regime of the shape and distribution of nodules expanded to a lower temperature where patenting was performed.

We begin with calculation of extended volume \( V_{ex} \), the sum of the volumes of pearlite nodules growing without hard impingement. We divide the entire course of heat treatment into n time steps. Let \( V_{ex}^{n} \) be the extended volume of

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*Hard impingement means that the growth is hindered due to direct contact of nodules, and soft impingement implies the slow down of growth due to overlap of carbon diffusion fields between nodules growing in the neighborhood.
Pearlite nodules nucleated at the i-th time step (henceforth, denoted the i-th group) at the end of heat treatment. It is expressed as,

$$V_j^{ext} = N_i \frac{4\pi}{3} R_m^3$$ \hspace{1cm} (1)

where \(N_i = J_i \Delta t\) is the number of nodules in the i-th group, \(J_i\) is the nucleation rate and \(\Delta t\) is the width of time step. \(R_m\) is the radius of nodules at the end of heat treatment, i.e. n-th time step, which is given by the equation,

$$R_m = \sum_{j=1}^{n} g_{ij} \Delta t$$ \hspace{1cm} (2)

where \(g_{ij}\) is the growth rate of nodules of the i-th group at the j-th time step. The total extended volume \(V^{ext}\) and the fraction transformed \(Y\) are given by the equation,

$$V^{ext} = \sum_{j=1}^{n} V_j^{ext}$$ \hspace{1cm} (3)

and,

$$Y = 1 - \exp(-V^{ext})$$ \hspace{1cm} (4)

respectively.

### 2.2. Nucleation and Growth Rate of Pearlite Nodule

Pearlite nucleates on prior austenite grain boundaries. Whether ferrite or cementite nucleates first may depend on the alloy composition and transformation temperature. In a study by Mangan and Shiflet\(^{9}\) cementite plays a major role in both hypoeutectoid and hypereutectoid steels. Another notable feature of pearlite nucleation is that nucleation rate increases with time, of which two possibilities were discussed. One was based upon the idea of incubation period,\(^{4}\) and the other was ascribed to the increase of the surface area of the 1st nucleating phase (ferrite or cementite) on which the other phase (cementite or ferrite) nucleates.\(^{9}\) Mehl and Hagel\(^{9}\) reported nucleation rates averaged over a certain time range in a wide temperature range (560–700°C). Thus, we assume that the nucleation rate of pearlite \(J\) is described phenomenologically by the following equation,

$$J = AD_{\gamma} \exp \left( \frac{-B}{T (T_m - T)^2} \right)$$ \hspace{1cm} (5)

where \(A\) and \(B\) are constants, \(D_{\gamma}\) is the carbon diffusivity in austenite, \(T_m\) is the eutectoid temperature. In comparison with the time-dependent nucleation rate equation,\(^{40}\) coefficient \(A\) contains nucleation site density, Zeldovich factor and a factor representing time-averaged nucleation rate etc, whereas coefficient \(B\) contains the nucleus/matrix interfacial energy and latent heat of pearlite transformation. The expression of carbon diffusivity in austenite by Kaufman et al.\(^{11}\) was used in this calculation. As shown in Fig. 1, a regression analysis of a ln \(J/D_{\gamma}\) vs \(1/T (T_m - T)^2\) plot showed a good linear relationship with a slope \(B = 1.01 \times 10^{7}\) K\(^3\), which yielded the interfacial energy between pearlite nodule and the austenite matrix \(\sigma \approx 0.02\) J/m\(^2\), close to the value reported in Ref. 4).

Data at low temperatures deviate significantly from the straight line, which might be related to the difference in the distribution of pearlite nodules mentioned earlier.

Several equations were proposed for the growth rate of pearlite which assumes carbon volume diffusion control in austenite. According to Zener,\(^{12}\) the growth rate is given by,

$$g = A' D_{\gamma} (T_m - T)$$ \hspace{1cm} (6)

where \(A'\) is a proportionality constant. One can evaluate \(A'\) from the data in Fig. 9 of Ref. 7). However, this procedure yielded growth rates more than one order of magnitude greater than experiment in alloys studied (Table 1).

Tewari and Sharma\(^{13}\) proposed an equation of growth rate for partitioned and no-partitioned growth of pearlite. While in the present alloys Cr and Mo are partitioned at high temperatures, the extent of partitioning decreases rapidly at lower temperatures.\(^{5,14}\) Although Si continues to partition at low temperatures,\(^{15}\) patenting is performed below the nose temperature of TTT-curves which typically lies around 650°C. Accordingly, the equation proposed for no-partitioned growth,

$$g = 2.61 \frac{D_{\gamma}}{S} \left( x_c^{\gamma/a} - x_c^{\gamma/c} \right)$$ \hspace{1cm} (7)

is used in the subsequent simulations. Here, \(S\) is the interlamellar spacing, \(x_c^{\gamma/a}\) and \(x_c^{\gamma/c}\) are the carbon concentrations in austenite in equilibrium with ferrite and cementite, respectively.

### 2.3. Interlamellar Spacing

The interlamellar spacing of pearlite is one of the most important parameters which affect the strength of super-high strength wire rods. Indeed, a decrease in a few tens of percent in lamellar spacing may lead to an increase of a few hundreds of MPa in tensile strength after heavy drawing. Theoretically, the interlamellar spacing is inversely proportional to the amount of undercooling as,

$$S = \frac{4\pi T_m V_m}{\Delta H (T_m - T)}$$ \hspace{1cm} (8)

where \(\sigma\) is the energy of nodule/matrix boundary, \(V_m\) is the molar volume of pearlite and \(\Delta H(= 82\) kJ/kg\) is the latent heat of pearlite transformation.\(^{16}\) Indeed, a good correlation is reported between lamellar spacing and the amount of undercooling in an Fe–C eutectoid alloy unless the transformation temperatures are too low.\(^{31}\) It is also reported that the
slope of a $1/S$ vs $(T_eu - T)$ plot is similar (0.16 $\mu$m$^{-1} \cdot $K$^{-1}$) in many alloyed steel except in Fe–C–Si, Ni and Mo alloys; in Si alloys (0.11 $\mu$m$^{-1} \cdot $K$^{-1}$) it is presumably ascribed to the formation of partitioned pearlite (ortho-pearlite) in a wide range of temperature.$^{15}$

2.4. Influence of Latent Heat on the Progress of Transformation

A large amount of heat is generated during pearlite transformation. Whereas Gleeble simulator is controlled to keep the cooling rate, the latent heat will raise significantly the local temperature near the pearlite nodule/austenite boundary. Indeed, it is reported that recalescence has a significant effect as long as the specimen size is greater than 1 mm.$^{17}$ Accordingly, the amount of recalescence was calculated from the equation,

$$
\Delta T = \frac{\Delta H \cdot \Delta Y}{C_p \cdot r} \quad \text{(9)}
$$

where $C_p = 699 \text{ J/K·kg}$ is the specific heat of iron at 600°C$^{18}$ and $\Delta Y$ is the increase in fraction transformed per time step. $r$ is the fraction of heat used to raise the temperature of the boundary region, which could be evaluated if the a cooling curve is available. Here, $r$ was assumed to be 0.1.

3. Experimental Procedure

Alloys were vacuum induction melted using electrolytic iron, high purity carbon, silicon, chromium and molybdenum and were cast into 80 kg ingot. The ingot was forged into rods, 15 mm in diameter and 110 mm in length. They were then machined for heat treatment by means of Gleeble 3 800 thermomechanical simulator as illustrated in Fig. 2. Specimens were austenitized at 1 070°C for 10 min, cooled to 960°C at a cooling rate of 5°C/s and 50% deformed at a strain rate of 3/s, and were cooled to 910°C in 3 s. In continuous cooling experiment they were then cooled to room temperature at a cooling rate varying from 0.5 to 50°C/s (dashed line). In isothermal holding experiment they were cooled to the holding temperature (550–625°C) at 80°C/s, where the specimens were held for varying times. Specimens were then cooled to room temperature at a rate faster than 50°C/s (solid line). These are schematically illustrated in Fig. 3. The pearlite start ($P_s$) and finish temperature ($P_f$) for CCT or TTT curves were determined from the points at which a dilatometric curve deviated from the straight line, as described elsewhere.$^{19}$

After specimens were polished and etched by 4% nital, the size and number of pearlite nodules were measured by software of quantitative analysis of 2D microstructure (ImagePro Plus) on the specimen surface of area $1.12 \times 10^6 \mu$m$^2$. Brown and Ridley$^{20}$ evaluated nucleation rates by counting the number of nodules greater than a certain value and measuring the increasing rate of these numbers with time. In this report the Schwartz-Saltykov analysis was applied to evaluate the total number of pearlite nodules from the relationship,

$$
N = \frac{1}{\Delta} \sum_{i=1}^{\Delta} \alpha_i \cdot n_i \quad \text{(10)}
$$

where $\Delta (= 3 \mu$m) is the width of size group, $n_i$ is the number of nodules of the $i$-th size group per unit area of polished surface, and $\alpha_i$ is the coefficient determined from the stereological analysis.$^{21}$

The interlamellar spacing was measured by surveying colonies for a minimum spacing. This method is widely used because the probability of lamellae being nearly perpendicular to the specimen surface is relatively high.$^{22}$

4. Results and Discussion

4.1. Fraction Transformed and Number of Nodules

Figures 4(a) through 4(c) show optical micrographs of three alloys isothermally held at 575°C for 1–2 s. It is immediately seen that the transformation occurred considerably

![Fig. 2. Specimen used for Gleeble thermomechanical simulation.](image)

![Fig. 3. Schematic illustration of heat treatment by means of Gleeble thermomechanical simulator. Solid and dashed lines are respectively for isothermal holding and continuous cooling experiment.](image)

![Fig. 4. a) Optical micrograph of Fe–C–Si alloy isothermally held at 575°C for 1 s. b) Fe–C–Cr alloy isothermally held at 575°C for 1.4 s, and c) Fe–C–Mo alloy isothermally held at 575°C for 0.5 s. Grey and black areas are pearlite nodules.](image)
faster in the Fe–C–Si alloy than in the other two alloys. It is noted that the transformation did not start during cooling to the holding temperature except in the Si alloy in which a small amount of pearlite (~1%) was observed in a specimen quenched from 910°C. Calculated transformation curves are compared with experiment at 575°C in Figs. 5(a) through 5(c). These figures were used to determine coefficient A in the nucleation rate equation in the alloys studied. Whereas alloying elements are reported to reduce nucleation rate except Co,4) the A values were many orders of magnitude greater than that in Fe–C alloy as shown in Table 2. Since coefficient A depends on the nucleation site density, this is probably because the specimens were deformed at 960°C before cooled to the reaction temperature.

Figure 6 illustrates the size distribution measured in Fe–C–Cr specimens reacted at the same temperature. The smallest size group contained large number of black dots which might be etch pits or contamination. If black dots smaller than 0.5 and 1 μm were removed, the total number was ~20 and 50–65% less, respectively. Figure 7 shows the variation of nodule number (solid curve) calculated at 575°C in the Cr alloy. The dashed curve shows the number of nodules newly formed within the remaining matrix. It is seen that the numbers of nodules calculated with A in the table are in good agreement with measured ones.

Table 1. Chemical composition of alloys studied (mass%).

<table>
<thead>
<tr>
<th>Alloy</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Mo</th>
<th>Al</th>
<th>V</th>
<th>Ti</th>
<th>O</th>
<th>N</th>
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<tbody>
<tr>
<td>Fe–C–Si</td>
<td>0.86</td>
<td>0.02</td>
<td>0.884</td>
<td>0.008</td>
<td>0.003</td>
<td>0.02</td>
<td>0.007</td>
<td>0.003</td>
<td>0.004</td>
<td>0.006</td>
<td>0.0009</td>
<td>0.0026</td>
</tr>
<tr>
<td>Fe–C–Cr</td>
<td>0.87</td>
<td>0.04</td>
<td>0.013</td>
<td>0.008</td>
<td>0.004</td>
<td>0.50</td>
<td>0.005</td>
<td>0.003</td>
<td>0.004</td>
<td>0.001</td>
<td>0.0011</td>
<td>0.0030</td>
</tr>
<tr>
<td>Fe–C–Mo</td>
<td>0.76</td>
<td>0.03</td>
<td>0.031</td>
<td>0.008</td>
<td>0.005</td>
<td>0.02</td>
<td>0.51</td>
<td>0.002</td>
<td>0.002</td>
<td>0.011</td>
<td>0.0010</td>
<td>0.0029</td>
</tr>
</tbody>
</table>

* The austenite was not deformed.
4.2. Nodule Diameter

In Fig. 8 are plotted the maximum and mean nodule diameters against holding time. The former is the diameter of nodules nucleated at the first time step $R_{1j}$, and the latter is given by,

$$\bar{R} = \frac{\sum_{j=1}^{J} R_{kj}N_k}{\sum_{k=1}^{K} N_k} \quad \text{(11)}$$

These plots are valid only at earlier stages at which hard impingement has not occurred extensively. It is seen in the figure that calculated mean nodule diameter is in good agreement with measurement. On the other hand, the observed maximum diameter was as large as ~20 $\mu$m (not shown), very large compared to calculation. This is presumably because more than one nodule nucleated close to each other and impinged during growth.

4.3. TTT and CCT Curves

Figure 9 shows the comparison of calculated TTT curves of 1 and 99% transformation with experiment in the Cr alloy. Data on $P_f$ were not secured due to rapid transformation. It is seen that the nose temperature is around 620°C in this alloy.

Figures 10(a) and 10(b) illustrate CCT and transformation curves in the Mo alloy continuously cooled at a cooling rate from 3 to 50°C/s. Pearlite transformation was almost completed at cooling rates smaller than 5°C/s. At faster cooling rates where the transformation was not completed $P_f$ was defined as the temperature (or time) at which the fraction transformed reached 90% of the final fraction transformed. It is seen that the agreement between calculated and measured $P_s$ and $P_f$ is satisfactory.

4.4. Simulation of Interlamellar Spacing

The lamellar spacing of pearlite formed during isothermal holding was simulated incorporating recalescence and results are shown in Figs. 11(a) through 11(c). Dashed curves indicate the instantaneous lamellar spacing of newly formed nodules and solid curves, the lamellar spacing averaged over all nodules formed by that time. Although the local temperature will soon cool down to the holding temperature, this was not taken into account. It is seen that in all alloys measured lamellar spacings are somewhat greater.
than those expected at the holding temperature. This seems to indicate that the temperature in the local region can be raised 20–30°C by latent heat in these specimens.

5. Summary

A computer model of pearlite transformation in Fe–C base alloys during cooling and/or isothermal holding was developed in view of its application to the transformation during patenting of super-high strength wire rods. The model was based upon Johnson-Mehl-Avrami theory in which the effects of hard impingement was taken into account. The nucleation rate was calculated phenomenologically incorporating data in an Fe–C eutectoid alloy and an adjustable parameter. The growth rate was calculated using the equation proposed by Tewari and Sharma. The number and size of pearlite nodules, fraction transformed, TTT- and CCT-curves and interlamellar spacings were simulated in near-eutectoid Fe–C–Cr, Si and Mo alloys. Results were in good agreement with experiment. Whereas Gleeble simulator was controlled to keep the specified cooling rate or holding temperature, the influence of latent heat may not be totally ignored, particularly in simulation of lamellar spacings.

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REFERENCES