

PHASE TRANSFORMATION MODELING OF MEDIUM-CARBON FORGING STEEL

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Abstract. The kinetics of phase transformations in medium-carbon forging steels (MCFS) have been modeled based on CALPHAD multicomponent thermodynamics and the classical nucleation-growth theory. New treatments include the time dependency of parabolic growth rate of proeutectoid ferrite (α), which account for the soft impingement effect by carbon enrichment in austenite (γ). And a potential transition of γ/α interface equilibrium has also been considered depending on temperatures and velocity of the moving interface. To make a realistic prediction of the onset of pearlite (P) transformation, a normal distribution of γ grain size has been assumed and successive $\alpha \rightarrow P$ transformation kinetics in each grain size have been summated.

The developed program coupled with thermodynamic solver, '*ThermoCalc*', calculated the isothermal kinetics of MCFS and has been found to predict well the effect of minor difference of chemical composition / holding temperatures.

INTRODUCTION

Medium carbon steels containing 0.2~0.5 mass percent carbon are used in a large quantity as materials for hot forging parts. A prediction of the microstructure consisting of proeutectoid ferrite (α), pearlite (P), and bainite (B) has long been a desired technology, which would be the basis for balancing mechanical properties and good machinability of final products.

The $\alpha/P/B$ fraction after forging is mainly affected by both carbon and manganese content, austenite (γ) grain size (AGS), and cooling schedules. Thermodynamics in Fe-Mn-C ternary system have been well discussed in terms of partitioning of Mn, and the parameters describing diffusion-controlled transformation can now be calculated by CALPHAD method for the ternary and even higher-order system. However, there is still discussion on the type of equilibrium operating at the real interface between α and γ . On the other hand, AGS and cooling rate are strongly related to hot working conditions and have been evaluated in the course of thermal-mechanically coupled FEM analysis. Senuma et al.[1] reported experimental equations for AGS for low carbon steel based on the relationship between rolling conditions and fractions of dynamic/static recrystallized γ grain, and Yogo[2] et al. recently modified the equation to be applicable to forging process.

A lot of work has been devoted to understand the kinetics of α , P and B transformations in the framework of the classical nucleation-growth theory, and there are some integrated models[3-6] reported to be able to predict the evolution of complex $\alpha+P+B$ structure. These models so far have been developed for low-carbon steel strips, and therefore, focused on the prediction of α grain size as

well as the fraction of widmanstätten α or B . In view of the circumstances, we have firstly constructed an integrated physical model of the successive $\alpha \rightarrow P$ transformation for medium-carbon forging steel (MCFS). And a trial program empowered by CALPHAD method has been developed to evaluate the usefulness of such computerized predictions.

This article presents the newly introduced features of treating the above diffusion-controlled phenomena in the model, together with the current status in predicting $\alpha \rightarrow P$ transformation behaviors of MCFS by the program. The possible B transformation from the remaining γ are also to be considered and will be included in a separate paper.

MODEL DESCRIPTION

Thermodynamic Calculations. Besides C content it is important to calculate the thermodynamic effect of Mn and/or Cr that exerts, through the strong interaction with C in γ , a decisive influence on the microstructure of MCFS. The CALPHAD method is a standard tool worldwide for calculating multicomponent thermodynamics. One of the commercial packages, *ThermoCalc*, was introduced in the present modeling work with the help of programming interface, *TQ-i*.

Linking dynamically with *ThermoCalc* and the steel database *TCFe3*, driving force of α and cementite (θ), equilibrium compositions with γ , and other thermodynamic parameters were always calculated for Fe-C-Si-Mn-Cr system. It should be mentioned that the newest version of *TQ-i* has been upgraded to manage para-equilibrium (PE) constraint. As discussed later, the interface compositions were also calculated under negligible-partitioned local equilibrium (NPLE).

Incubation Time. The incubation time (τ) of isothermal α transformation was calculated in *Eq. 1* according to the pillbox model[7]. The diffusivity of carbon in γ (D_C^γ), and the maximum driving force available for α nucleation (ΔG_V) were input from the above thermodynamic solver. The γ/α interfacial energy ($\sigma^{\gamma/\alpha}$) of 0.705J/m² and the volume occupied by iron atom (V^α) of 8.785x10⁻³⁰m³ were taken as constants, while the average lattice parameter a was estimated from the experimental equations[8] including effect of alloying elements. X_C^0 is the initial C content and other symbols have the usual meanings.

$$\tau = \frac{12kTa^4 \cdot \sigma^{\gamma/\alpha}}{D_C^\gamma X_C^0 \cdot V_\alpha^2 \cdot \Delta G_V^2} \quad (1)$$

Growth of Proeutectoid Ferrite. The nucleation rate of α (I_f) on γ boundary surface was calculated following the classical nucleation theory. The fitting parameters were taken from Liu's work[9].

Assuming carbon-diffusion-controlled growth of α , the parabolic growth rate constant (α_l) was expressed in *Eq. 2*, and numerically solved *via* the subroutine by Capdevila[10]. The choice of interface carbon composition set ($X_C^{\gamma/\alpha}$, $X_C^{\alpha/\gamma}$) has been controversy, and those in PE constraint would be the most reasonable for an interface moving at higher velocities under high supersaturations. Hillert[11] suggested, however, at a later stage of isothermal transformation, there may be a gradual shift of the interface equilibrium from PE to the one with a spiky partitioning of Mn.

The treatment here proposed is that the transition from PE to NPLE occurs when the velocity of

$$2 \left(\frac{D_C^\gamma}{\pi} \right)^{1/2} \frac{X_C^{\gamma/\alpha} - X_C^\gamma}{X_C^{\gamma/\alpha} - X_C^{\alpha/\gamma}} = \alpha_1 \exp \left\{ \frac{\alpha_1^2}{4D_C^\gamma} \right\} \operatorname{erf} \left\{ \frac{\alpha_1}{2\sqrt{D_C^\gamma}} \right\} \quad (2)$$

interface (v^α) becomes lower compared to Mn diffusivity. Although the boundary diffusivity of Mn is not known, it was estimated as 5 times as the bulk one in γ (D_{Mn}^γ). Thus the critical ratio p for the transition was defined in Eq. 3 where t is holding time.

$$p = \frac{5D_{Mn}^\gamma}{v^\alpha} = \frac{10D_{Mn}^\gamma \sqrt{t}}{\alpha_1} \quad (3)$$

The soft impingement effect (SIE) is pronounced and have to be properly modeled for the α growth of MCFS. Andrés[12] proposed a 1-D analytical model after Gilmour's work, but in the present model a regressive SIE treatment has been implemented to consider C enrichment caused by a 3-D " α -shell" growing from γ grain boundary. In Eq. 2, the C content away from interface (X_C^γ) should increase if considered in a finite γ grain. This could be conveniently monitored by the change in the average C content in remaining γ (X_{bar}^γ) from the volume fraction of transformed α (V_f) as shown in Eq. 4.

$$X_{bar}^\gamma = \frac{X_C^0 - V_f X_C^{\alpha/\gamma}}{1 - V_f} \quad (4)$$

The increase of V_f increases X_{bar}^γ and makes α_1 time-dependent. In this sense, I_f and D_C^γ were recalculated every time of updating X_{bar}^γ .

Onset and Growth of Pearlite. The transformation of P from the interface between preceding α and γ has been modeled based on Capdevila's comprehensive work[13]. The critical velocity (v^θ) of moving γ/α interface that allows θ nucleation was given by Eq. 5 in which the lattice parameter of

$$\left. \begin{aligned} v^\theta &= \frac{-(a^\gamma)^3 D_C^\gamma \cdot X_C^{\gamma/\theta} (\Delta G_V^\theta)^3}{16(1 - \cos \psi) \sqrt{\pi k T (\sigma^{\alpha/\theta})^5 K}} \\ \cos \psi &= \sigma^{\gamma/\alpha} / 2\sigma^{\alpha/\theta} \end{aligned} \right\} \quad (5)$$

γ (a^γ), the driving force (ΔG_V^θ), and α/θ interfacial energy ($\sigma^{\alpha/\theta}$) of 0.68J/m² were included. In general, C content in γ necessary for the nucleation of θ is represented by the equilibrium content ($X_C^{\gamma/\theta}$) and the previous models had determined the end of α and the start of P when the two conditions were fulfilled;

$$\begin{aligned} * \text{ thermodynamic condition} & \quad X_C^{\gamma/\theta} < X_{bar}^\gamma \\ * \text{ kinetic condition} & \quad v^\alpha < v^\theta \end{aligned}$$

However, X_{bar}^γ is just an average and does not necessarily corresponds to the one at θ nucleation site. And it would be more likely a situation that the smaller γ grain size (AGS) is, the faster X_{bar}^γ increases even if the same thickness of α covers γ grain surface. Thus in our model, the critical enrichment factor C has been introduced in the new thermodynamic condition. Simply assuming a normal distribution, Eq. 6 has been checked for discrete AGS around the average with 2.5 μm increment.

The nucleation rate of pearlite (I_p) was formulated in the similar way as proposed by Reed and Bhadeshia[14]. For the growth of P , diffusion-controlled mechanism in Fe-Mn-C system have been discussed extensively[15,16], and the two growth rate in LE or NPLE mode (G_{LE} , G_{NPLE}) were

$$C(X_C^{\gamma/\theta} - X_C^0) \leq X_{bar}^\gamma - X_C^0 \quad (6)$$

proposed to operate depending on temperature. These are given in Eq. 7 and Eq. 8, respectively. The expressions for lamellar spacing S , S_{crit} and parameters in G_{LE} including Mn partitioning coefficient (K_p) were taken from ref.[17].

$$G_{NPLE} = \frac{D_c^\gamma}{0.72} \frac{S}{S_\alpha S_\theta} \frac{X_C^{\gamma/\alpha} - X_C^{\gamma/\theta}}{X_C^{\theta/\gamma} - X_C^{\alpha/\gamma}} \left[1 - \frac{S_{crit}}{S}\right] \quad (7)$$

$$\left. \begin{aligned} G_{LE} &= 12K^p D_{Mn}^B \delta \frac{1}{S_\alpha S_\theta} \frac{X_{Mn}^{\gamma/\alpha} - X_{Mn}^{\gamma/\theta}}{X_{Mn}} \left[1 - \frac{S_{crit}}{S_0}\right] \\ K^p D_{Mn}^B \delta &= 2.223 \cdot 10^{-7} \exp\left(-\frac{14940}{RT}\right) \end{aligned} \right\} \quad (8)$$

One of the two growth rates was selected depending above or below the "NPLE eutectoid temperature" at which $X_C^{\gamma/\alpha}$ equals to $X_C^{\gamma/\theta}$ under NPLE constraint.

Calculation of Integrated Kinetics

Isothermal transformation kinetics has been calculated basically according to the procedure by Umemoto[6]. An ellipsoidal α having an aspect ratio of 3:1 was assumed to grow at the parabolic rate of $3\alpha_l$ along γ grain boundary. As discussed, α_l changes with time and so that increases of α radius in every time increments were summated to get a present radius. Details of calculating volume fraction are in the literature and would not be repeated here.

In contrast the growth rate of P is constant and, using Eq. 9[13], the volume fraction (V_P) was analyzed for a semi-spherical geometry. γ grain boundary area (S^γ) per unit volume was estimated for a truncated octahedron grain and related to α/γ interface area ($S^{\alpha/\gamma}$) with a simple expression; $S^\gamma(1-V_P)^{2/3}$. V_P^{eq} is the equilibrium volume fraction of P and ϕ is an integral constant given by y/G where y is a distance from α/γ interface.

$$\left. \begin{aligned} V_P &= V_P^{eq} \left[1 - \exp\left\{S_V^{\alpha/\gamma} G t f(G, I_P, t)\right\}\right] \\ f(G, I_P, t) &= \int_0^1 [1 - \exp\left\{\frac{\pi}{3} I_P G^2 t^3 (1 - 3\phi^2 - 2\phi^3)\right\}] d\phi \end{aligned} \right\} \quad (9)$$

Inside the program, first a normal distribution of AGS and corresponding volume contributions (f_d) are generated from an input of average AGS. Linking *Thermocalc*'s functions, thermodynamic parameters, incubation time, nucleation and growth rates are deduced and then the calculation of V_f starts on the smallest AGS. It runs recursively inputting new D_c^γ , I_f , α_l , X_{bar} and checking the PE to NPLE transition with p . Once the conditions for the onset of P are fulfilled, the V_p calculation is invoked and it finishes if the total volume fraction exceeds f_d . After completion of the same procedures on all discrete AGS, volume fractions are summated along the calculated time series to get the whole transformation kinetics.

RESULTS AND DISCUSSION

An evaluation of the foregoing models was carried out first for 0.37C-0.56Si-1.45Mn-0.04Cr (mass%) of which isothermal kinetics was investigated in detail[10]. The calculated and observed volume fraction are compared in Fig. 1. Experimentally, the α growth in (a) at slightly above its eutectoid temperature (968K) shows a much slower kinetics than the constant parabolic law. At a later stage, the growth is especially retarded and the calculation reproduces the kinetics due to both the SIE model and PE to NPLE transition.

At a lower temperature in **(b)**, a period of simultaneous α retarding and gradual P development is expressed in the calculation and the experiment reveals such a behavior. The final volume fraction at the end of isothermal holding agrees reasonably well with the observed one. Contrary to **(a)**, the program predicts no transition of γ/α interface equilibrium in **(b)**. At present, p and C are fitted and constant throughout the prediction. These values need to be related to physical quantities deduced from atomistic diffusion theory.

In **Fig. 1(c)** and **(d)**, a comparison of kinetics at 928K has been made on similar steels within the same compositional standard. It should be pointed out that a minor deviation of Mn content yields a noticeable difference of kinetics. The current program only calculates the thermodynamic effect of Mn, which slows diffusional growth by changing equilibrium C concentration of γ in particular under NPLE constraint. Even so the agreements are passable in both steels and prove the usefulness for

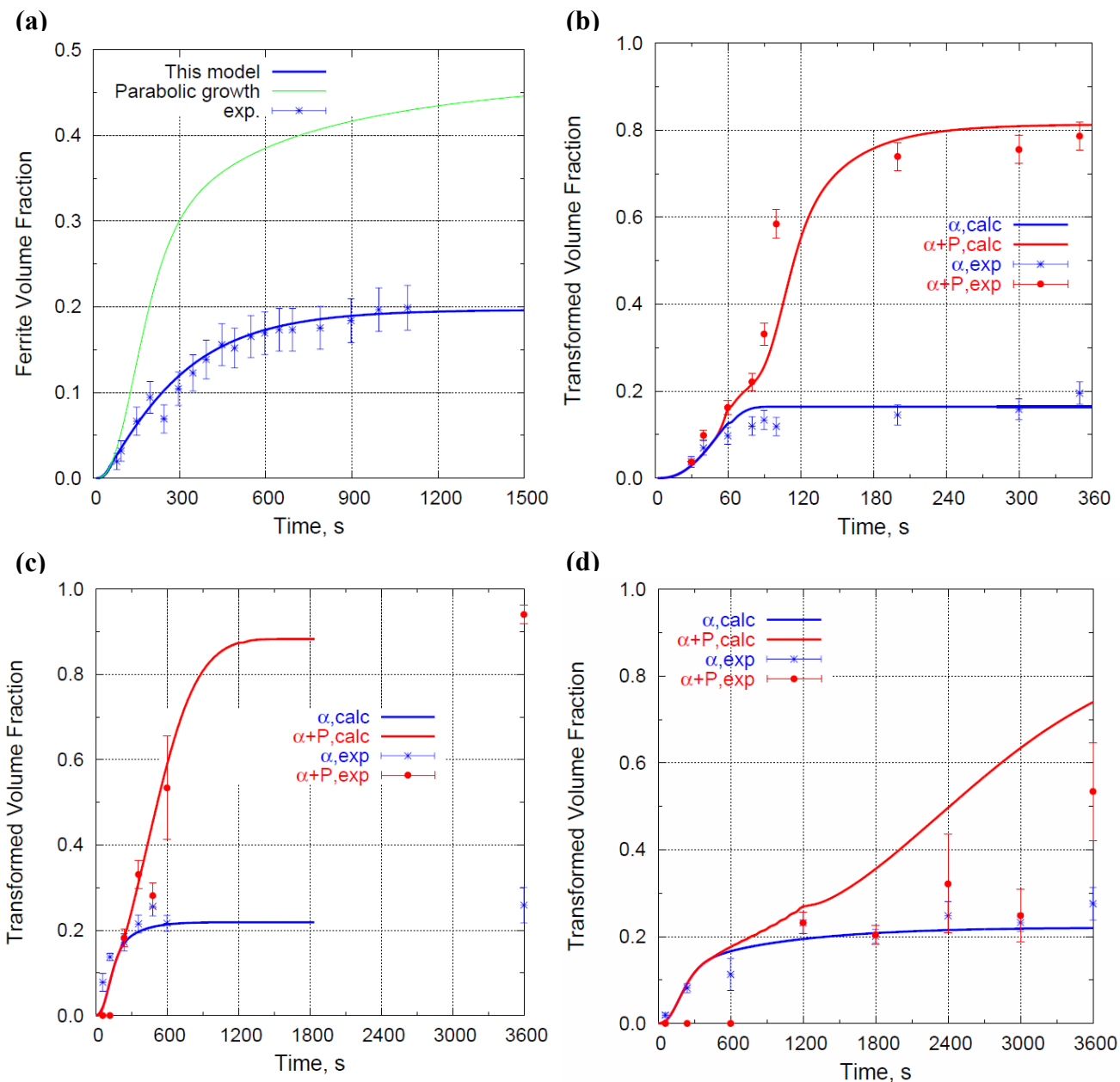


Figure 1 The comparison of calculated and measured change in volume fraction of proeutectoid ferrite and pearlite. **(a)** 0.39C-0.50Si-1.51Mn-0.14Cr at 973K, **(b)** the same steel at 914K, **(c)** 0.39C-0.51Si-1.29Mn-0.15Cr at 928K, and **(d)** 0.39C-0.50Si-1.51Mn-0.14Cr at 928K.

predicting difference among commercial distributing MCFS. Still the discrepancy is large for P in the case of higher Mn content. This suggests more modeling work is necessary in order to expand the applicable composition range and to make the program a lot more practical in predicting phase transformation.

SUMMARY

- (1) The integrated phase transformation model has been developed for medium-carbon forging steel. New treatments include the time-dependent growth rate of α in the SIE model and checking PE to NPLE constraint of γ/α interface. The both were made possible through the recursive evaluation of C enrichment in γ and the CALPHAD thermodynamics.
- (2) The calculation reproduced well the slow α growth above eutectoid temperatures, as well as the successive $\alpha \rightarrow P$ transformation kinetics by introducing a distribution of AGS. The program showed an ability of predicting the difference in transformation kinetics caused from a minor compositional deviation.

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