General Method of Phase Transformation Modeling in Advanced High Strength Steels

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In the present paper, a new modeling approach is proposed for the austenite to ferrite and bainite transformation kinetics in transformation induced plasticity (TRIP) and complex phase (CP) steels. Based on experimental data obtained by dilatometry during continuous cooling, Rios' method has been successfully applied assuming additivity to calculate the parameters for the Johnson–Mehl–Avrami–Kolmogorov (JMAK) model, *i.e.* exponent n and the rate parameter k. Limitations of the Rios' method have been identified when k is a function of both temperature T and fraction transformed X. For these cases that are in particular relevant for the bainite transformation, a new modeling method has been developed to investigate the exact relationship of k with T and X. The new method has been used to describe the transformation kinetics in a TRIP and a CP steel. Good agreement has been obtained between the calculated and measured transformation data. The proposed new modeling method provides a general modeling approach that promises to be useful in predicting the complex phase transformation kinetics during industrial processing of advanced high strength steels (AHSS).

KEY WORDS: TRIP steel; complex-phase steel; phase transformation; mathematical model; JMAK equation; additivity rule.

1. Introduction

Advanced high strength steels (AHSS) derive their superior mechanical properties from transformation hardening that results in combining high strength with good ductility and formability as well as an increased capacity for impact energy absorption.[1,2] The required complex microstructures consist of at least two different transformation products, including ferrite, bainite, martensite and retained austenite, and their formation necessitates an increased complexity of the cooling process with tight processing windows. Among all AHSS, dual-phase (DP) steels with ferrite–martensite microstructures have gained the widest application because of the relative ease of making them. However, the complexity of processing is magnified when bainite is an important part of the final microstructure. For example, cooling transformation-induced plasticity (TRIP) steels too rapidly may result in extensive martensite transformation thereby deteriorating the unique TRIP properties that are related to the presence of carbide-free bainite and retained austenite. Therefore, in order to design optimal control of the cooling process, in-depth knowledge on the phase transformation kinetics is paramount. Based on the JMAK equation and the additivity rule, a number of mathematical models,[3–8] which were constructed from continuous cooling transformation data, have been proposed for DP, TRIP and complex-phase (CP) steels. However, no further detailed information on the determination of the model parameters and their potential limitations were provided.

Basically, there are two types of methods for the modeling of phase transformation during continuous cooling: (i) the mathematical method developed by Pont[9] and Malinov,[10] and (ii) the theoretical method developed by Rios.[11] As a continuation of previous work,[12] the present paper examines further the applicability and limitations of Rios' method to develop a more general method for the modeling of complex phase transformation processes in AHSS. An extension of the model is proposed for the case where the rate parameter k in the JMAK equation is not only a function of temperature but also a function of the fraction transformed.

2. Experimental Procedure

The steels for this study were supplied in the form of forged bars with a cross section of 60×200 mm. **Table 1** shows the chemical compositions of the present steels. Using ThermoCalc with the Fe2000 database, the Ae_3 temperatures have been determined to be 860°C and 832°C for

Table 1. Chemical compositions of the investigated steels (mass, %)

Steel Grade	C	Mn	Si	S	P	Nb	Mo	Al	N
CP	0.05	1.88	0.04	0.007	0.005	0.048	0.49	0.05	0.004
TRIP	0.19	1.5	1.6	-	-	-	0.2	-	-

TRIP and CP steels, respectively.

The dilatometric tests were carried out on a Gleeble 3500 thermo-mechanical simulator using tubular specimens with an outer diameter of 8 mm, a length of 12 mm and 1 mm wall thickness for continuous cooling transformation (CCT) tests from undeformed austenite and solid specimens with a cylindrical working zone with a diameter of 6 mm and a length of 10 mm for CCT test from work-hardened austenite. After austenitization to obtain a desired austenite gain size, D_γ, the samples were cooled to a predetermined temperature in the non-recrystallization region where the solid samples were deformed in axisymmetric compression to a prescribed true strain, ε, of up to 0.6. Then the samples were cooled to 200°C at different constant cooling rates ranging from 1 to 100°C/s. The experimental work and results were described in detail elsewhere.[7,8]

3. Rios' Method

3.1. A Brief Introduction of Rios' Method[11]

The basics of Rios' Method [11] can be described using the example of ferrite formation in the CP steel from work-hardened austenite with a grain size of 8 μm and an applied true strain of 0.6. **Figure 1** shows a typical contour plot $X(q, T)$ where q represents the cooling rate and X is the normalized fraction transformed for a given transformation product, *i.e.* here either ferrite (α) or bainite (B), which can be calculated from

$$X_\alpha = \frac{X_\alpha^{\text{true}}}{X_\alpha^{eq}} \quad \text{................................(1)}$$

$$X_B = \frac{X_B^{\text{true}}}{1 - X_\alpha^{\text{true}}} \quad \text{.............................(2)}$$

where X_α^{true} and X_B^{true} represent the true ferrite and bainite fraction transformed and X_α^{eq} is the ferrite equilibrium fraction at any given temperature.

In Rios' method it is assumed that the isothermal transformation can be described with the Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation, *i.e.*

$$X = 1 - \exp(-kt^n) \quad \text{.............................(3)}$$

where k and n are parameters. In order for the transformation to be isokinetic, *i.e.* additive, n must be a constant. According to Rios, the value of n can be calculated from continuous cooling transformation data by

$$\ln\ln\left(\frac{1}{1-X}\right)$$
$$= \ln\left(k(T)\cdot\left(\left|q(X_0,T)\right|\cdot\left(\frac{\partial T}{\partial q}\right)_{X_0}\right)^n\right) - n\cdot\ln\left(\left|q(X,T)\right|\right)$$
$$\text{..(4)}$$

i.e. $\ln\ln(1/(1-X))$ should be a linear function of $\ln(|q(X, T)|)$ for a fixed temperature and this slope should be independent of temperature. The derivative $(\partial T/\partial q)_{X_0}$ is cal-
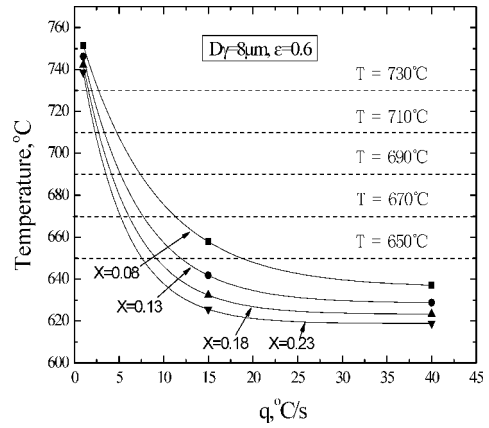

Fig. 1. Typical contour plot of $X(q, T)$ for ferrite transformation in the CP steel from work-hardened austenite with a grain size of 8 μm and an applied strain of 0.6.
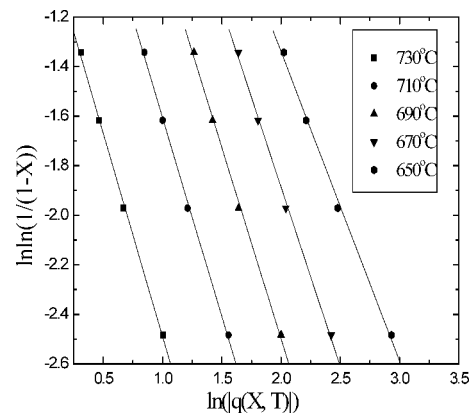

Fig. 2. Rios' analysis for the data shown in Fig. 1 to determine n.

culated from the curves in Fig. 1 for a selected, fixed volume fraction, X_0, at each temperature T. **Figure 2** shows the plots according to Eq. (4) that result from the data shown in Fig. 1. To a very good approximation the slope of these curves is independent of temperature, *i.e.* n is indeed a constant and for the given example an average n value of 1.4 is obtained.

By setting $X = X_0$ in Eq. (4), a simplified form for the calculation of $k(T)$ is obtained such that

$$k(T) = \frac{\ln(1/(1-X_0))}{((\partial T/\partial q)_{X_0})^n} \quad \text{.......................(5)}$$

At each temperature, a number of X_0 values can be selected to determine the values of k. The family of the k curves as a function of temperature is shown in **Fig. 3** for the example data of Fig. 1. Clearly, k is for this example in a good approximation independent of X_0 just a function of temperature. Taking an average value of k at each temperature, $k(T)$ can be proposed as shown in **Fig. 4**. Here data are summarized with different levels of applied strain indicating that k is also a function of the initial austenite microstructure.

3.2. Analysis and Discussion of Rios' Method

In the calculation for the ferrite and bainite transformation in the CP steel using Rios' method, the iso-X curve in the contour plot of all the cases have the same shape as pre-
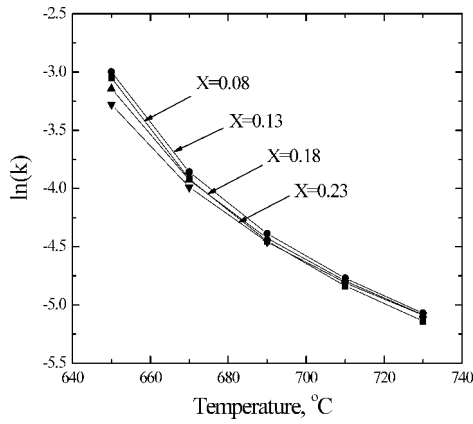
Fig. 3. Relationship between $\ln(k)$ and temperature for ferrite transformation in the CP steel with $D_\gamma=8\,\mu$m and $\varepsilon=0.6$ based on the data from Fig. 1.
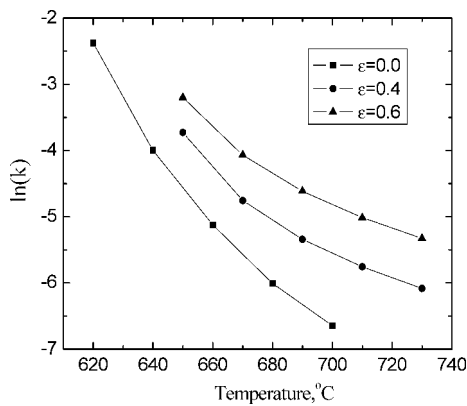

Fig. 4. Relationship between $\ln(k)$ and temperature for ferrite transformation in the CP steel with an initial austenite grain size of $8\,\mu$m and different levels of applied strain.

(a)

(b)

Fig. 5. Contour plot of $X(q,T)$ for ferrite transformation in TRIP steel with (a) $D_\gamma=24\,\mu$m, $\varepsilon=0.0$; (b) $D_\gamma=24\,\mu$m, $\varepsilon=0.6$.

Fig. 6. Schematic TTT diagram.

sented in Fig. 1. However, as shown in **Fig. 5**, the shape of these plots is different for the ferrite transformation in the TRIP steel.

These differences can be rationalized by considering the underlying TTT diagram that provides the information on the required isothermal transformation time τ to reach a particular fraction transformed X at a given temperature T, as schematically illustrated in **Fig. 6**. Rios proposed in his method the following relationship for isokinetic reactions

$$\tau(X,T)=\left(\frac{\partial T}{\partial q}\right)_X \quad\text{..........................(6)}$$

and the cooling rate to obtain a fraction transformed X at temperature T during continuous cooling can be obtained from

$$q(X,T)=\int_{Ae_3}^{T}\frac{d\Theta}{\tau(X,\Theta)}\quad\text{.......................(7)}$$

It can be seen in Fig. 6 that for a fixed X, $(\partial T/\partial q)_X$ can fall into two regimes, i.e. it either decreases or increases with temperature depending whether the temperature is above or below the nose temperature, respectively. Using Eq. (7) the hypothetical contour plot can be constructed for a generalized continuous cooling transformation, as illus-
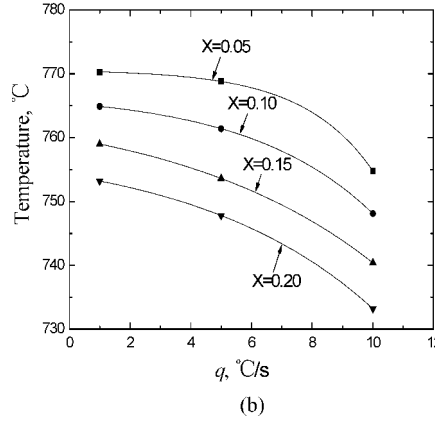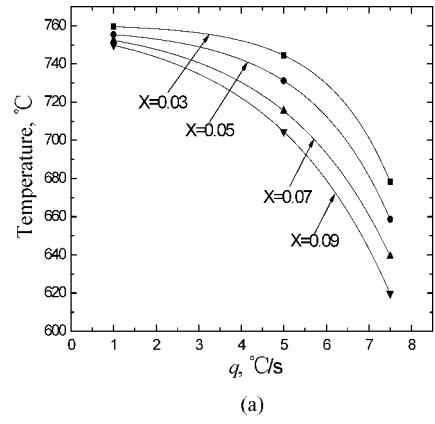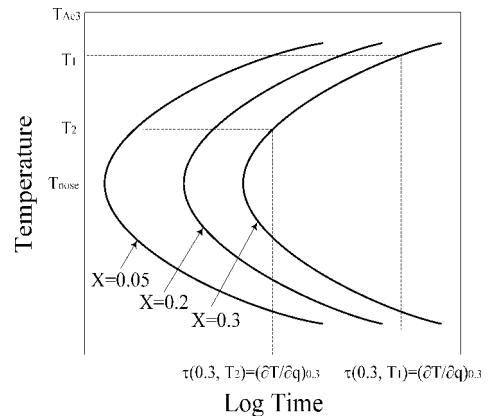
trated in **Fig. 7**. This analysis reveals the general shape of iso-X curves for all potential transformation scenarios. These curves show a typical inflection point that falls close to the nose temperature of the TTT diagram. The differences in the shape of the contour plots of the examples shown in Fig. 1 and Fig. 5, respectively, can then be rationalized as follows. For the CP steel the transformation occurs at temperatures that fall onto the upper branch of the general iso-X curves whereas for the TRIP steel the transformation occurs at temperatures that fall on the lower branch of the general iso-X curves.

Further, the generalized function of the rate-parameter $k(T)$ is shown in **Fig. 8** indicating that k displays a characteristic maximum at the nose temperature. The data for the ferrite transformation in the CP steel (see Fig. 3) fall on the
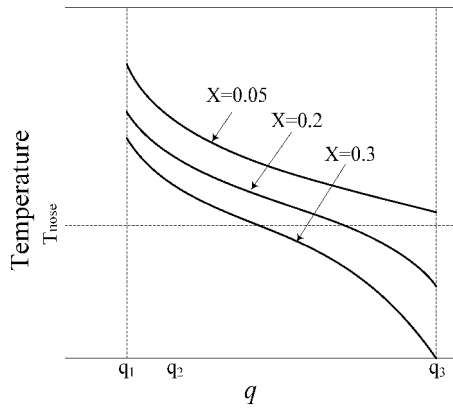
Fig. 7. Contour plot of $X(q, T)$ determined from theoretical deduction of Rios' method using a hypothetical TTT diagram.
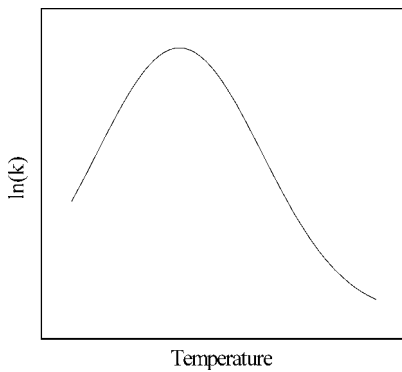

Fig. 8. General relationship between $\ln k$ and T based on a typical TTT diagram.

(a)

(b)

Fig. 9. Results from Rios' analysis showing its limitations for the bainite transformation in the CP steel: a) $D_\gamma = 20\,\mu m$ and $\varepsilon = 0.0$; b) $D_\gamma = 62\,\mu m$ and $\varepsilon = 0.0$.

higher temperature part of the generalized $k(T)$ curve. However, analyzing the data for the bainite transformation in the CP steel and the ferrite transformation in the TRIP steel reveals that the Rios' method is not applicable in these cases, *i.e.* either n shows an apparent temperature dependence or k is not a unique function of temperature when considering different values for X_0, as shown in **Fig. 9** for the bainite transformation. In essence, k becomes a function of X as well and this is in violation of the inherent assumptions made in Rios' method and may also lead to the apparent temperature dependence of n. Thus, an extension of this method will be considered to also find a suitable modeling strategy for this more complex transformation behavior.

4. New Method

4.1. Formulation of New Method

It was shown by Lusk[13] that the rule of additivity is valid for isokinetic reactions, *i.e.* the transformation rate must be of the form

$$\dot{X} = F(T) \cdot G(X) \quad \text{..........................(8)}$$

Provided k is not a function of X, the transformation rate based on the JMAK equation is given by

$$\dot{X} = k(T)^{1/n}\{n(1-X)[-\ln(1-X)]^{(n-1)/n}\} \quad \text{........(9)}$$

Thus, the transformation is additive as long as the exponential n is a constant. However, the carbon redistribution during ferrite and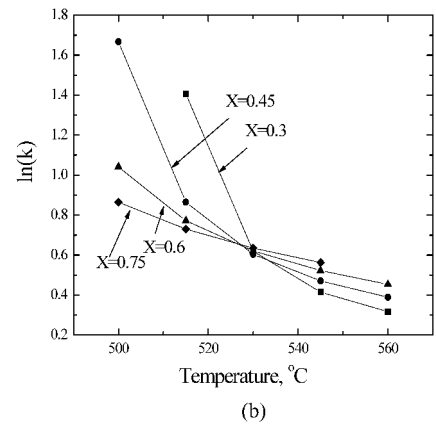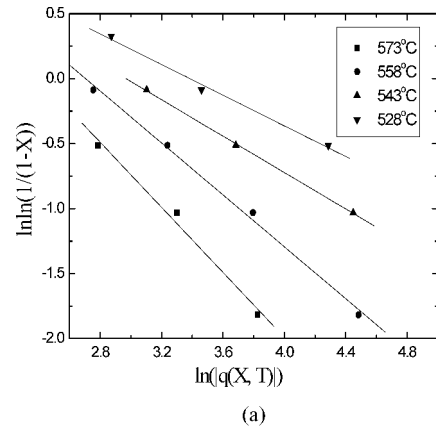 bainite transformation is considered to affect the transformation kinetics since the un-transformed austenite is stabilized due to carbon enrichment. Higher carbon concentration in untransformed austenite, which is determined by the transformed fraction, X, results in reduced driving pressure and higher demand for carbon redistribution, as is particularly pronounced for the bainite transformation in the CP steel and the ferrite transformation in the TRIP steel. Therefore, the more general case of $k = k(X, T)$ is considered here and conditions can still be specified where additivity is fulfilled. In this general case, the transformation rate may be written

$$\dot{X} = \frac{k(X,T)^{1/n}\{n(1-X)[-\ln(1-X)]^{(n-1)/n}\}}{1 + (1-X)\dfrac{dk}{dX}\left[\dfrac{\ln(1-X)}{k}\right]} \quad \text{....(10)}$$

Provided

$$k = h(T) \cdot l(X) \quad \text{...............................(11)}$$

and, therefore

$$\frac{dk}{dX} = h(T)\frac{dl}{dX} = k\left(\frac{dl/dX}{l(X)}\right) \quad \text{..............(12)}$$

such that then Eq. (10) fulfills the general relationship of Eq. (8) for the reaction to be additive. Rewriting Eq. (11) as

$$\ln k = H(T) + L(X) \quad \text{...........................(13)}$$

and inserting into Eq. (4) yields

$$\ln \ln \left(\frac{1}{1-X} \right) = H(T) + L(X) + \ln \left[\left| q(X_0,T) \right| \cdot \left(\frac{\partial T}{\partial q} \right)_{X_0} \right]^n$$
$$- n \cdot \ln \left[\left| q(X,T) \right| \right] \quad ....(14)$$

For a fixed temperature, a series of equations can be generated for different values of X as indicated below

$$\begin{cases} \ln \ln \left(\frac{1}{1-X_1} \right) = L(X_1) - n \cdot \ln \left[\left| q(X_1,T) \right| \right] + C \\ \ln \ln \left(\frac{1}{1-X_2} \right) = L(X_2) - n \cdot \ln \left[\left| q(X_2,T) \right| \right] + C \quad .....(15) \\ \quad ... \\ \ln \ln \left(\frac{1}{1-X_m} \right) = L(X_m) - n \cdot \ln \left[\left| q(X_m,T) \right| \right] + C \end{cases}$$

where

$$C = H(T) + \ln \left[\left| q(X_0,T) \right| \cdot \left(\frac{\partial T}{\partial q} \right)_{X_0} \right]^n \quad ....(16)$$

In this more general case of $k = k(X,T)$, a complex numerical approach needs to be applied to find n and the functions $L(X)$ and $H(T)$. Using the examples of ferrite transformation in the TRIP steels and bainite transformation in the CP steels the application of this new methodology will be illustrated in the next Section.

4.2. Application of New Method

Using the JMAK equation and assuming additivity in the generalized case of $k(X,T)$ the fraction transformed X_i at a particular temperature T_i during continuous cooling can be written such that

$$X_i = 1 - \exp \left\{ - \left[\frac{1}{q} \int_{Ae_3}^{T_i} k(X,T)^{1/n} dT \right]^n \right\} \quad ......(17)$$

Re-arranging of Eq. (17) yields

$$q[-\ln(1-X_i)]^{1/n} = \int_{Ae_3}^{T_i} k(X,T)^{1/n} dT \quad ....(18)$$

which is of a suitable form to evaluate $k(X,T)$ for a given value of n. Assuming a specific value of n, e.g. $n=1$, the associated k can be determined for given combinations of X_i and T_i, i.e.

$$k_i(X_i,T_i) = \frac{I_i - I_{i-1}}{T_i - T_{i-1}} \quad ....(19)$$

where. $I_i = q \cdot [-\ln(1-X_i)]^{1/n}$. This procedure can be repeated for different n values until a suitable relationship for $k(X,T)$ has been found. In cases where this is not possible one would have to conclude that the assumption of n=const. is not fulfilled even in a first approximation such that the reaction would not be additive. However, in the
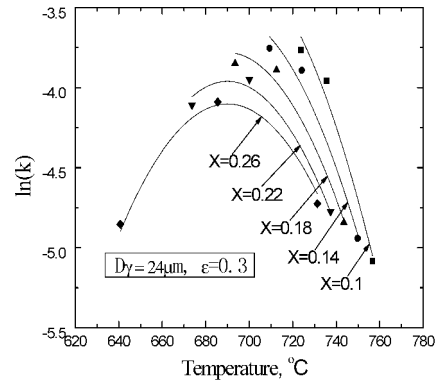
(a)
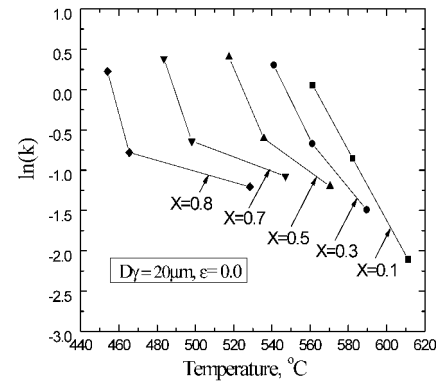
(b)

Fig. 10. Representative results of relationships between $\ln k$ and T for (a) ferrite transformation in TRIP steel; (b) bainite transformation in CP steel.

present cases, $k(X,T)$ can be brought into the form required by Eq. (13) when taking $n=1$ for ferrite transformation in the TRIP steel and $n=0.85$ for the bainite transformation in the CP steel, respectively.

Representative results of the relationship between k and temperature for these transformations are shown in **Fig. 10**. Clearly k depends on X but its temperature dependence resembles that expected from the general plot shown in Fig. 8. For the ferrite transformation in the TRIP steel the transformation occurs around the nose temperature and a parabolic relationship of $\ln K$ with T may be used as a first approximation, i.e.

$$\ln k = A_1 (T-T_0)^2 + A \quad ....(20)$$

Here, A_1, T_0 and A are adjustable parameters. For a given initial austenite microstructure, the parameters A_1 and T_0 must be constant whereas A can be taken as a function of the fraction transformed in order to still have the additivity criteria fulfilled. For the ferrite and bainite transformation in the CP steel the transformation takes place above the nose temperature such that a linear dependence of $\ln k$ with temperature can be used such that[14]

$$\ln k = A_1 \cdot T + A \quad ....(21)$$

The critical step now is whether or not the additivity criteria are fulfilled and A can be determined as a function of X. **Figure 11** illustrates that this can be attained for the two transformations analyzed. For the ferrite transformation in the TRIP steel, A decreases linearly with X whereas a loga-
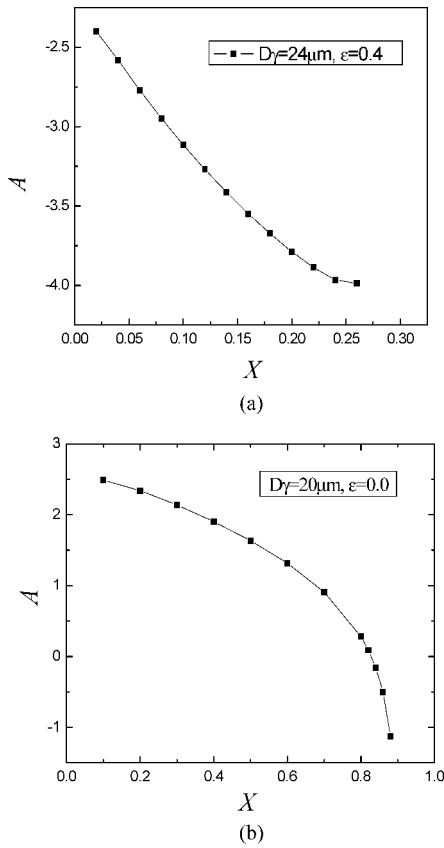
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Fig. 11. Parameter A plotted as a function of X for (a) ferrite transformation in TRIP steel; (b) bainite transformation in CP steel.

Table 2. JMAK-parameters for ferrite transformation of CP steel.

Rate parameter: $\ln(k) = A_1 T + A_2 \ln\left(D_{eff}\right) + A_3$			
$A_1(°C^{-1})$	A_2*	A_3	n
-0.032	-1.546	20.08	1.4

*For D_{eff} in μm

Table 3. JMAK-parameters for ferrite transformation of TRIP steel.

Rate parameter: $\ln(k) = A_1\left(T - T_0\right)^2 + A_2 \ln\left(D_{eff}\right) + A_3 \cdot X + A_4$					
$A_1(°C^{-2})$	A_2*	A_3	A_4	$T_0(°C)$	n
-4.14×10^{-4}	-2.75	-5.11	5.96	688	1

*For D_{eff} in μm

Table 4. JMAK-parameters for bainite transformation of CP steel.

Rate parameter: $\ln(k) = A_1\left(T - T_0\right)^2 + A_2\left(c_{rem}\ln\left(D_{eff}\right)\right) + \ln\left(A_3 - X\right) + A_4$					
$A_1(°C^{-2})$	A_2*	A_3	A_4	$T_0(°C)$	n
-9.7×10^{-5}	-19.4	0.907	5.78	400	0.85

*For D_{eff} in μm

rithmic relationship of A with X can be proposed for the bainite formation in the CP steel.

In the analyzed cases it has been possible to include the dependence of the transformation kinetics on the initial austenite microstructure as part of the function for parameter A. In a first approximation, the functionality of A vs. X is independent of the initial austenite microstructure and the overall form of A can be written as combination of two functions that either depend on X or the initial austenite microstructure such that

$$A = a(X) + b(D_{eff}) \quad\quad\quad\quad (22)$$

where the initial austenite microstructure can be represented by an effective grain size[15]

$$D_{eff} = D_\gamma \exp(-\varepsilon) \quad\quad\quad\quad (23)$$

In case of bainite, the transformation may start from an austenite–ferrite dual-phase microstructure. Then the effective grain size refers to that of the remaining austenite assuming that the original austenite grain size is reduced by an outer shell of ferrite that occupies a volume fraction in an average grain that is equal to the overall fraction of ferrite at bainite start. Further, A can then also depend on the carbon enrichment of austenite that results from the ferrite transformation and can be approximated by

$$c_{rem} = \frac{c_o}{1 - X_f} \quad\quad\quad\quad (24)$$

where c_o is the average carbon content and X_f is the ferrite

fraction when the bainite transformation commences. The functions $k(X, T)$ with their detailed parameters as determined for the ferrite transformation in the CP steel (follows Rios' method, *i.e.* k is independent of X) and in the TRIP steel ($n=1$) as well as the bainite transformation in the CP steel ($n=0.85$) are summarized in **Tables 2**, **3** and **4**, respectively.

Figure 12 shows the calculated results for the ferrite transformation kinetics in the TRIP steel and the comparison with the measured results. The ferrite and bainite transformation kinetics were calculated and compared with the measured results for CP steel as shown in **Fig. 13** and **Fig. 14**, respectively. In general good agreement is obtained adopting additivity as described for the proposed model methodology either by Rios' method or its extension when k becomes also a function of X. The results for the ferrite portions of the austenite decomposition confirm previous findings that ferrite formation can accurately be described with the JMAK approach and assuming an additive reaction. The bainite model provides good fits for small austenite grain sizes (*i.e.* 20 μm and below). The fit quality is reduced when the transformation leads just to rather small fractions of a particular transformation product which in general can be considered of minor importance for practical applications. In case of the bainite reaction in the CP steel, rather large discrepancies have been obtained between calculated and measured kinetics for the larger austenite grain size of $D_\gamma = 62\,\mu$m. This can be primarily attributed to the fact that with increasing austenite grain size additional nucleation modes are expected for the bainite reaction, *i.e.* sympathetic nucleation. A shift from nucleation at the austenite–ferrite interfaces to sympathetic nucleation may lead to a change in the n-value which would suggest a non-additive transformation.[8] However, in the present case, this change is primarily related to the change in initial austenite
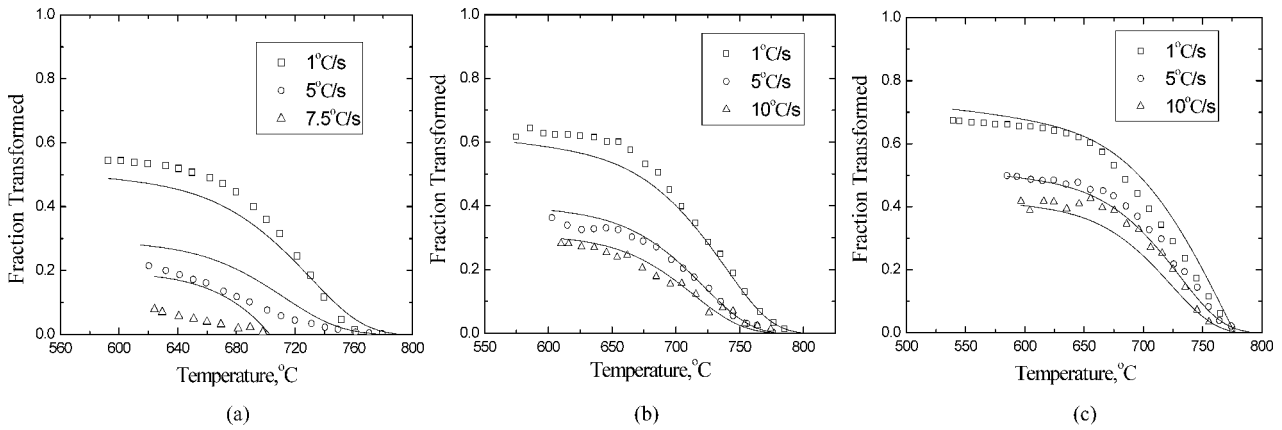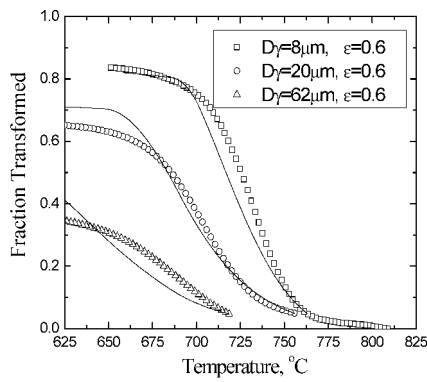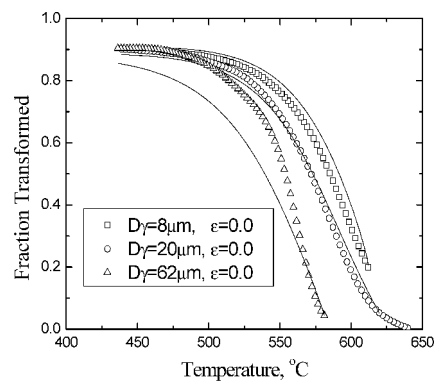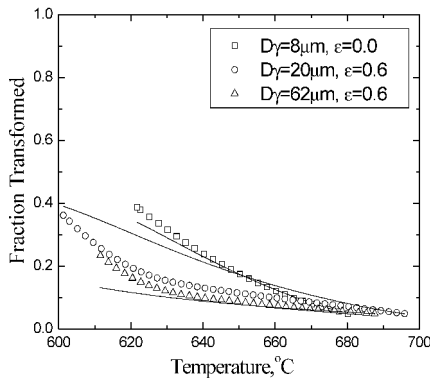
Fig. 12. Comparison between measured (symbols) and calculated (solid line) ferrite fractions in the TRIP steel with an initial grain size of 24 μm and an applied true strain of (a) 0.0; (b) 0.4; (c) 0.6.
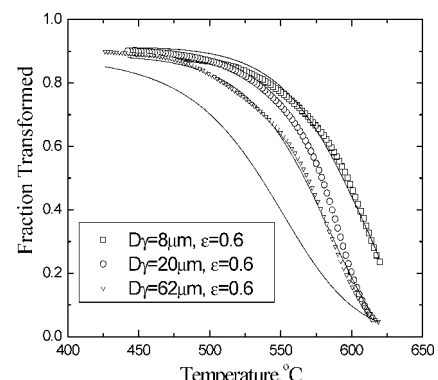

Fig. 13. Comparison between measured (symbols) and calculated (solid line) ferrite fractions in the CP steel for cooling rates of (a) 1°C/s; (b) 5°C/s.

Fig. 14. Comparison between measured (symbols) and calculated (solid line) bainite fractions in the CP steel for cooling rates of: (a) 15°C/s; (b) 40°C/s.

microstructure rather than a change in transformation temperature for a given initial austenite condition. Thus, n and other parameters can be made a function of the effective austenite grain size. For example taking $A_2 = -33$ and $A_4 = 9$ while keeping all other parameters as shown in Table 4 provides a satisfactory fit for the bainite transformation kinetics from an austenite grain size of 62 μm. This suggests that the dependence of the rate parameter k on the prior austenite microstructure is more complex than proposed with the relationship given in Table 4. However, adding additional parameters to formulate more complex relationships is beyond the scope of this work as it would be of little relevance for run-out table cooling conditions. A further

complication of the bainite model is that *via* the parameter T_0 the nose temperature is set to be 400°C even though measurement data were not available for temperatures in this range. Thus, the extension of the bainite model to these lower temperatures may have limited predictive capabilities.

From a practical perspective, it is important to propose bainite transformation models for cooling paths on the run-out table of a hot mill and during continuous annealing (or hot dip galvanizing). Here, the fine grained pancaked austenite with grain sizes of 20 μm or below that is expected at finish mill exit or, alternatively, fine-grained austenite–ferrite microstructures resulting from intercritical

annealing (usually below $10\,\mu m$) are of primary significance. The proposed bainite model with a constant n value for these initial microstructures promises to provide a useful tool for industrial process models.

Recent experimental investigation of the phase transformation in the CP steel that combine continuous cooling with coiling simulations indicate that the extent of the bainite transformation depends on the coiling temperature.[16] For coiling temperatures above 550°C, carbide precipitation may occur during coiling and this appears to affect the bainite transformation kinetics. Thus, corrections to the bainite model will be needed to capture these observations by combining the bainite model with a carbide precipitation model. However, from a pragmatic perspective of process model development this seems to be of little significance as the complex-phase steels of interest derive their unique properties from transformation hardening that is enabled by low coiling temperature practices rather than precipitation strengthening.

5. Conclusions

A new modeling method was developed for continuous cooling transformation when the JMAK rate parameter k is a function of the transformed fraction X. For this purpose, the Rios' method where it is assumed that k is only a function of temperature has been modified. Provided n is constant and k can be written as a product of a function that depends solely on temperature and a function that only depends on fraction transformed the additivity principle is still fulfilled. This extension permits to describe the ferrite transformation in a TRIP steel and the bainite transformation in a CP steel during continuous cooling where the original Rios method could not be successfully applied.

This new approach is in particularly useful in evaluating the limits of the additivity principle for bainite transformation in advanced high strength steels. In general, the bainite transformation must be considered as non-additive as nucleation conditions may change as a function of transformation temperature thereby making n a function of temperature. However, for cases that are of practical interest for industrial processing (*e.g.* during run-out table cooling) a constant n value can be assumed with k being a suitable function of X and T. Further, n can be taken as a function of

the prior austenite or austenite–ferrite microstructure before the start of the bainite formation. This provides further versatility to include the bainite reaction into industrial process models.

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