A Kinetics Model for Martensite Transformation in Plain Carbon and Low-Alloyed Steels

SEOK-JAE LEE and CHESTER J. VAN TYNE

An empirical martensite kinetics model is proposed that both captures the sigmodial transformation behavior for alloy steels and remains computationally efficient. The model improves on the Koistinen and Marburger model and the van Bohemen and Sietsma model with a function that better represents the transformation rate, especially during the early stages. When compared with existing models, the proposed model exhibits better predictions of volume fraction of martensite. The proposed model also predicts various other transformation properties accurately, such as M_{90} temperatures and retained austenite.

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I. INTRODUCTION

MARTENSITE is an important steel microstructure that contributes greatly to the final mechanical properties of steel after heat treatment because of its high strength and hardness. To predict steel microstructures accurately that result from the decomposition of austenite, a reliable kinetics model of martensite transformation is necessary. This model needs to calculate the volume fraction of martensite quantitatively and accurately as a function of temperature below martensite start (M_s) temperature. The martensite transformation is a time-independent (diffusionless) transformation, and the amount of martensite produced depends on the degree of undercooling below the M_s temperature. Research over the last 60 years has shown that the degree of undercooling below M_s temperature acts as a driving force to form martensite. Many investigations have related data about the amount of undercooling and the amount of martensite formed these relationships into various empirical kinetics models to predict the martensite transformation quantitatively in different types of steels.[1–7] The most well-known and widely used empirical model is one proposed by Koistinen and Marburger[5]

$$V_M = 1 - \exp[-K \cdot (M_s - T)] \quad [1]$$

where V_M is the volume fraction of martensite, T is the temperature in Kelvin, M_s is the martensite start temperature, and K is a constant. Koistinen and Marburger determined the value of the constant from plots of retained austenite obtained by X-ray analysis at room temperature after undercooling down to 194 K (–79 °C) in four carbon steels that had different carbon contents (*i.e.,* 0.37, 0.50, 0.81, and 1.10 wt pct C). From their analysis, the value of 0.011 was found for the constant (*i.e.,* $K_{KM} = 0.011$). The term "KM model" will be used when this value for the constant is used in Eq. [1]. For more than 60 years, Eq. [1] has been used widely to model martensite transformation in steels. The KM model has been used not only in the metallurgical research field but also in the field of mechanics (primarily by the finite-element method) to calculate the overall volume change of martensite during the heat-treatment processes of various steels.

The KM model was derived by considering only the undercooling effect on martensite formation. However, the undercooling degree below M_s temperature is not the only factor that can affect martensite transformation. Several studies on the effect of prior austenite grain size (PAGS) on martensite transformation have been reported.[8–12] The PAGS affects M_s temperature strongly and directly, as decreasing the PAGS also decreases the M_s temperature. The grain boundaries of prior austenite could act as nucleation sites for martensite transformation.[10] It seems that the PAGS does not affect the martensite transformation kinetics directly once the transformation starts—the PAGS affects only the M_s temperature, where the transformation begins.

Other models for the martensite transformation characterize the physical features of the phase change. For example, a geometrical model proposed by Hornbogen[13] demonstrates the fundamental characteristics of fractal martensite. His model is based on the classic geometry of microstructural elements and local regions available for predicting growth and properties, *e.g.,* toughness, in Fe-Ni alloy and shape memory alloy; but this type of geometrical model cannot predict the overall volume change of martensite below the M_s temperature, as the KM model does.

The value of K_{KM} equal to 0.011 in the KM model was derived from Fe-C alloys; there may be some inaccuracies in using this constant value to model the martensite transformation in steels that contain other

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alloying elements such as Ni, Cr, Mo, *etc*. Lee and Lee[14] showed that the martensite kinetics varied because of different amounts of alloying elements in AISI 41XX and 4340 alloys, although the PAGS was fixed. Recently, van Bohemen and Sietsma[15] investigated the effect of alloying elements on martensite transformation based on various data present in the literature and proposed a relationship between alloying elements and the constant in the KM model as

$$K_{BS}(K^{-1}) = 0.0224 - 0.0107C - 0.0007Mn - 0.00005Ni - 0.00012Cr - 0.0001Mo \quad [2]$$

where the amount of each alloy is in weight percent. The term ''BS model'' will be used with the constant in Eq. [1] as determined from Eq. [2]. The BS model provides a better characterization of the martensite transformation in steels with alloying elements other than carbon.

II. LIMITATIONS OF CURRENT MARTENSITE MODELS

The constant 0.011 in the KM model was obtained by X-ray peak analysis for the volume fraction of retained austenite from room-temperature–quenched and subzero-quenched samples. Their experimental method was not an *in situ* analysis with respect to temperature change; thus, it would be almost impossible to confirm the continuous change of martensite volume fraction. Koistinen and Marburger used an exponential function to fit their experimental data. This type of function typically is used to express diffusional transformation kinetics in a Johnson–Mehl–Avrami equation. Because of the constant, the resultant martensite transformation model is somewhat inflexible. For example, the volume fraction of martensite will be 0.5 at 63 K (–210 °C) below M_s, 0.9 at 209 K (–64 °C) below M_s, and 0.99 at 419 K (146 °C) below M_s. The value of the constant in the KM model does not allow for composition to affect the martensite transformation, and it requires significant undercooling for the transformation to reach near completion.

Although the volume fraction of martensite predicted based on the exponential function in Eq. [1] increases quickly with a C-shaped curve, different variations in the martensite volume fraction as a function of undercooling below M_s have been obtained from dilatometric analysis of low-alloyed steels.[14] Although Eq. [2] can account for some alloy effects on the transformation, the dilatometric results indicate that the functional form of the volume fraction of martensite formation at times resembles a sigmoidal shaped curve more closely with respect to temperature. The sigmoidal shape indicates that the transformation goes to completion with lower undercooling (*i.e.,* at higher temperatures). There is a limitation to obtaining a proper model for the martensitic transformations that exhibit a sigmoidal shaped behavior, either by using the original KM model or by modifying the KM model through changing the constant value K as in the BS model.

To overcome these limitations of the KM model, Lee *et al*.[16] proposed a new kinetics model of martensite transformation for low-alloy steels based on a dilatometric analysis. The change of martensite volume fraction was obtained from converted dilation data, which examines the kinetics of the martensite transformation in a macroscopic rather than a microscopic sense.[17] Such a converting technique, although well accepted in phase transformation kinetics studies, cannot reveal the physical details of martensite formation on a microstructural scale, namely, with respect to lath thickness, block size, *etc*. Dilatometer curves were converted to volume fraction of martensite for various low-alloy steels with different PAGS. Their model uses an ordinary differential function to express a sigmoidal curve behavior with consideration of the effects of the PAGS and alloying elements such as C, Ni, Cr, and Mo on the undercooling term. A numerical analysis must be used to solve the ordinary differential function, which makes it more difficult to use compared with the KM or BS models. The KM model's ease of use seems to be one of the primary reasons why many continue to use it despite its limitations.

III. PROPOSED MODEL

In the current study, we propose a new kinetics model for martensite transformation—not only to overcome some of the limitations that are present in the previous models but also to allow easier calculations. Our proposed model is an exponential function with two parameters that can be adjusted to account for the various effects of composition on the kinetics. The proposed model is

$$V_M = 1 - \exp[-K_{LV} \times (M_s - T)^{n_{LV}}] \quad [3]$$

where V_M is the volume fraction of martensite and T is the absolute temperature. The two parameters K_{LV} and n_{LV} are functions of the steel chemical composition.

Table I shows the volume fractions of martensite as calculated by using the differential model[16] for wide range of steel chemical compositions.

The previous ordinary differential model was derived from experimental data of steels whose chemical composition range matched exactly the compositions indicated in Table I. The range of chemical composition in Table I includes representative plain carbon and low-alloy steel series, such as AISI 10XX, AISI 41XX, AISI 4340, AISI 51XX, and AISI 86XX. The amounts of Mn and Si in the steel series are in a tight range; their amounts were fixed at the average values. Also, the fixed

Table I. Available Chemical Composition Range for the LV Model (wt pct)

C	Ni	Cr	Mo	Mn	Si
0.2–1.2	0.0–2.1	0.0–1.2	0.0–0.3	0.75*	0.25*

*The amounts of Mn and Si are fixed as average values of plane carbon and low alloyed steels.

PAGS value corresponding to 25 μm was used because the PAGS has little direct effect on martensite transformation kinetics below the M_s temperature.

To obtain the start of the transformation, the M_s temperature, suggested by Capdevila *et al.*[18] was used. Their equation is

$$\begin{aligned} M_s(K) = {} & 764.2 - 302.6C - 30.6Mn - 14.5Si \\ & - 16.6Ni - 8.9Cr + 2.4Mo - 11.3Cu \\ & + 8.58Co + 7.4W \end{aligned} \quad [4]$$

where the amount of each alloy is in weight percent.

Based on the volume fraction of martensite at different temperatures, the optimized K_{LV} and n_{LV} were obtained as a function of alloying elements as follows:

$$\begin{cases} K_{LV}(K^{-1}) = 0.0231 - 0.0105C - 0.0017Ni \\ \quad + 0.0074Cr - 0.0193Mo \\ n_{LV} = 1.4304 - 1.1836C + 0.7527C^2 - 0.0258Ni \\ \quad - 0.0739Cr + 0.3108Mo \end{cases} \quad [5]$$

where the amount of each alloy element is in weight percent. The coefficients in Eq. [5] were determined by optimization using the Newton-Raphson method. Because of the nonlinear aspect of the optimization, the possibility of the multiple solutions for K and n was investigated. No other solutions were found in the available chemical composition range given in Table I. The new kinetics model based on Eq. [3] with the optimized parameters in Eq. [5] will be referred to as the "LV model."

The constant parameter K (*i.e.*, 0.011) used in the original KM equation was obtained by fitting the volume fraction of retained austenite in iron-carbon alloys with different carbon levels. The constant was modified to account for different alloy steel compositions in the BS model. The LV model accounts not only for compositional effects on the constant but also for the compositional effects on the transformation curve shape by allowing the exponent to have a variation in composition. In all three cases, the models are based on results from experimental data. As more steels are analyzed, other terms can be added to Eq. [5] to account for other alloying elements. Also, as the compositional ranges are increased beyond those given in Table I, the coefficients in Eq. [5] might be modified slightly because of the interactions of the various alloying elements. Nevertheless, the functional form of the LV model is computationally efficient and provides a solid framework as the martensite transformation is investigated experimentally in other steels.

IV. COMPARISON OF MODELS

Figure 1 shows the comparison of the volume fractions of martensite predicted by both the KM and LV models with the measured volume fraction of martensite.[2,15,19] The experimental data for plain carbon steels containing different carbon levels were used in Figure 1(a), whereas the experimental data for low-alloy steels were used in Figure 1(b). Both the LV model and the KM model show relatively good correspondence for the experimentally determined martensite volume fractions for the plain carbon steels. However, the predicted volume fraction of martensite when calculated by the LV model is more accurate compared with that calculated by the KM model for low-alloy steels in Figure 1(b).

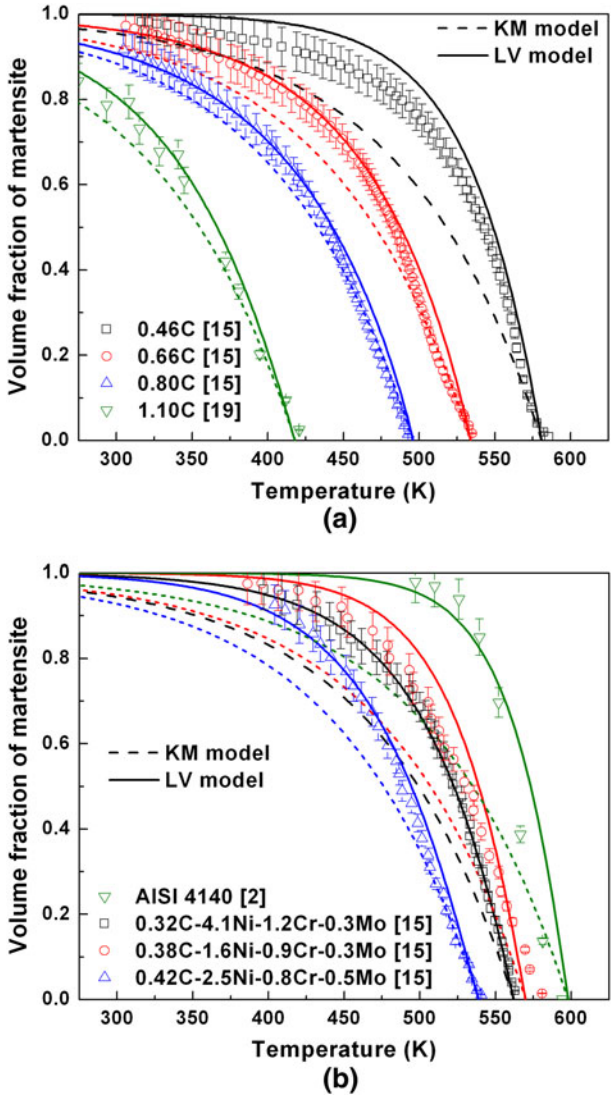
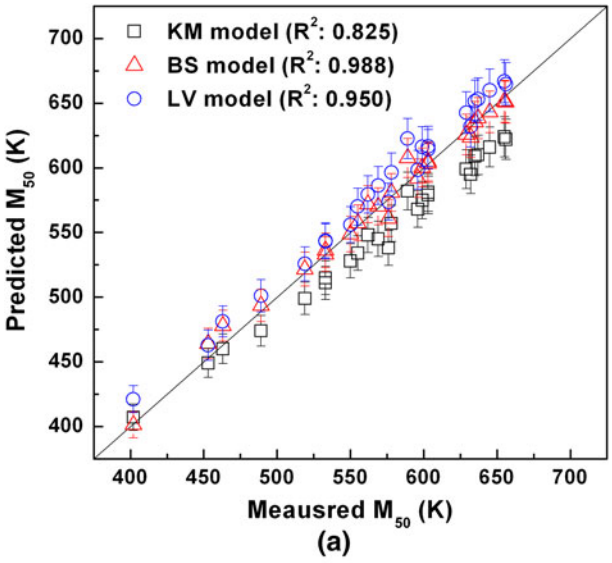


Fig. 1—Predicted volume fraction of martensite using the KM model and the LV model and comparing the model results with experimental data for (*a*) plain carbon steels and (*b*) low-alloy steels.

The M_{50} and M_{90} temperatures, where the martensite fractions are 50 and 90 vol pct, respectively, were obtained from the published isothermal transformation diagrams[20] of 25 plain carbon and low-alloy steels to allow a more reliable comparison between the models. The chemical compositions of the selected steels were in the range of chemical compositions of Table I. Figure 2 shows a comparison among the three models, as well as the experimentally measured M_{50} and M_{90} temperatures. All models show insignificant differences for the



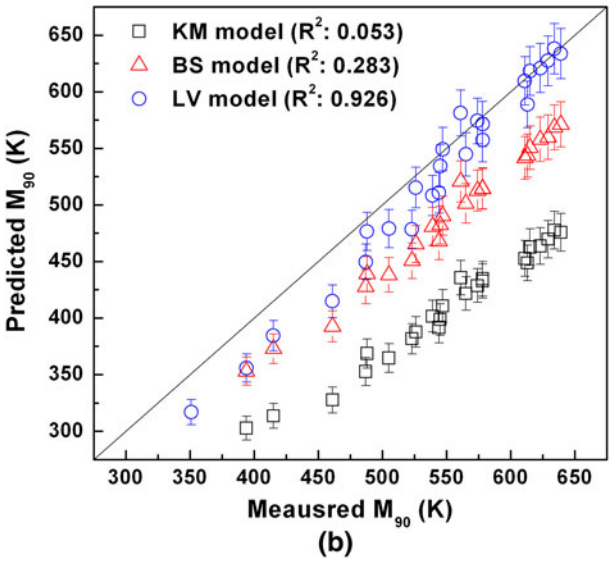


Fig. 2—Comparison among three models (KM model, BS model, and LV model) with the measured values of (*a*) M_{50} and (*b*) M_{90} temperatures, respectively.

M_{50} temperature, whereas the LV model exhibits much better agreement with the measured M_{90} temperatures.

Figure 3 shows the comparison of retained austenite predicted by three different models with measured retained austenite[5,21] for the Fe-C alloys at room temperature. Increasing the carbon content increases the thermodynamic stability of austenite; as a result, the amount of retained austenite after quenching is increased at room temperature. It is well known that the presence and amount of the retained austenite plays an important role in designing steels by providing increased ductility. Compared with the other models, the amount of retained austenite calculated by the LV model predicts the measured values more accurately. The amount of retained austenite found in the KM model does not predict accurately the measured retained austenite,[5] which was used to derive the KM model itself. Equation [4] for M_s temperature was used in the

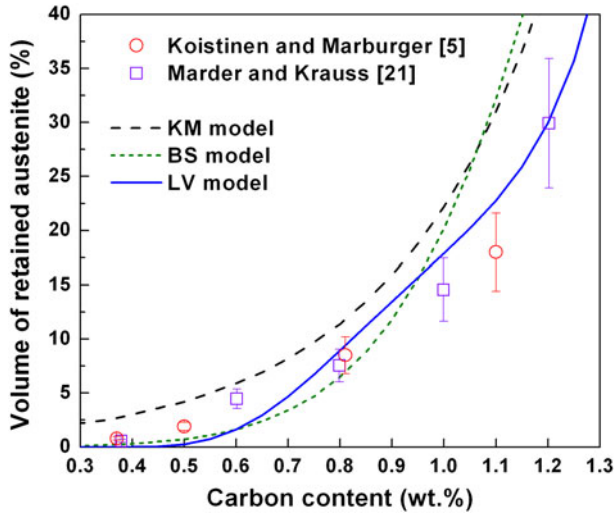
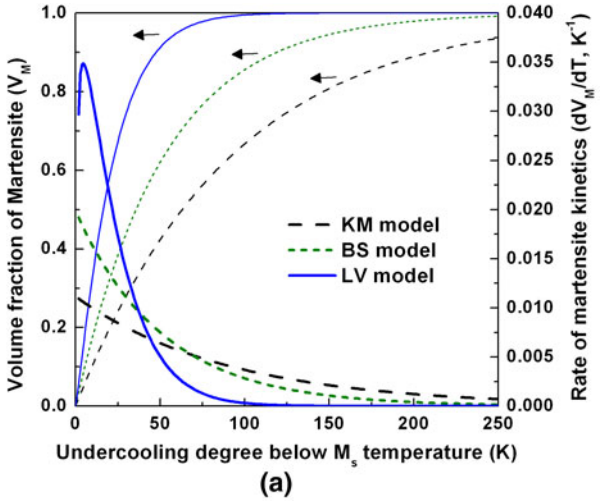


Fig. 3—Predicted retrained austenite by the three different models (KM model, BS model, and LV model) as a function of carbon content and comparison with experimental data for Fe-C alloys.

current study, whereas the M_s data obtained by Digges[22] and Greninger[23] was used for deriving the KM model.

V. AN EXAMPLE APPLICATION: QUENCH DISTORTION SIMULATION

The influence of the kinetics model of martensite transformation can be observed also by examining the amount of distortion that occurs after quenching the steel. To illustrate this effect, the distortion in an AISI 5120 steel cylinder has been calculated using the finite-element software ABAQUS (SIMULIA, Providence, RI) and subroutines related to phase transformation.[16] These simulations used the three models for the martensite transformation. The cylindrical sample geometry was designed to investigate the quench distortion affected by transformation strain and geometrical thermal strain. Figure 4(a) shows the changes of volume fraction and rate of transformation kinetics in martensite formation of AISI 5120 steel as a function of the undercooling below the M_s temperature of 113 K (386 °C). For both the KM model and the BS model, the transformation rate decreases continuously as the martensite transformation progresses. The rate of transformation for the LV model increases until the amount of martensite reaches approximately 15 vol pct, and then decreases. The change in the kinetics rate reveals the characteristics of a sigmoidal-shaped curve for the martensite transformation, which is predicted by the LV model with the exponent value, n_{LV}. The martensite transformation rate depends on the chemical composition of the steel. For example, Fe-Ni alloys whose M_s temperatures are below 273 K (0 °C) show burst martensitic transformation because of the high Ni content.[24] The relatively slow transformation rates of the KM and BS models are also observed in the lower predicted values of the M_{90} temperatures in Figure 2(b).



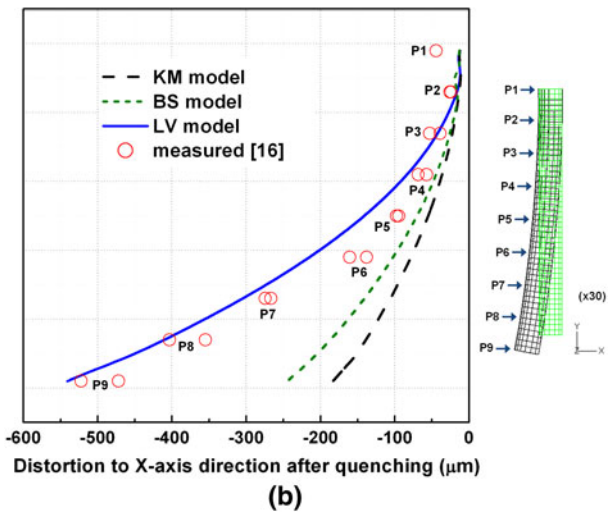


Fig. 4—(*a*) Predicted volume fraction and rate of transformation kinetics by three different martensite models for AISI 5120 steel and (*b*) effect of martensite kinetics on the final distortion after oil quenching. The measured values at P1-P9 were reported in a previous study.[16]

Figure 4(b) shows the importance of having a correct martensite kinetics model. This figure shows the final distortion in the asymmetric 5120 cylindrical sample. The deviation from the initial location (green color) is increased because of the faster kinetics of martensite transformation, as captured by the LV model. As a calculation note, the computation time for running this distortion simulation using the LV model (or the KM or BS models) was only 7 pct of the time required for the calculations using the ordinary differential function for the martensite transformation.

VI. DISCUSSION OF LV MODEL

Currently, the empirical LV model is based on the dilation curves, where various noncompositional factors affecting the martensite transformation are contained implicitly. It would be highly beneficial if the LV model could be based on fundamental aspects of thermodynamics and kinetics. However, the LV model can describe the transformation characteristics of martensite kinetics effectively from a macroscale perspective.

Several studies on the factors that affect martensite transformation kinetics in steels have been reported. For example, the grain size of prior austenite has little effect on the martensite transformation kinetics below the M_s temperature. Although the rate of martensite transformation kinetics (dV_M/dT) is sensitive to the PAGS, the change of total volume faction of martensite below the M_s temperature is not influenced strongly by the PAGS.[14] Therefore, a grain size parameter does not need to be considered directly in the LV model because it is captured in the M_s value used in the equation. Previous work provided an equation for the M_s temperature that considers the effect of the prior austenite grain size and a wide range of chemical compositions.[16] This proposed M_s temperature equation is used to include the effect of PAGS implicitly in the LV model.

The free energy change depends strongly on chemical composition and the nonchemical energy changes related to interfacial energy, elastic strain energy, and shear energy for dislocation movement affecting the martensite transformation.[24] The austenite strength can be affected by applying a large external stress to the sample, *e.g.,* accumulative roll bonding process. This stress induces a smaller grain size, which results in a decrease in the M_s temperature.[25] These factors affect directly the differences of the free energy changes between austenite and ferrite. The thermodynamic transformation energy determined by comparing chemical and nonchemical energy changes shows a nonlinear relationship as a function of undercooling below the M_s temperature. Therefore, the exponent term in the LV model is the appropriate place to consider any modification to account for these noncompositional factors.

The LV model is suitable for typical plain carbon and low-alloyed steels, but it is not applicable currently to some highly alloyed steels, such as high-Ni alloy steel or high-Mn alloy steel. New composition parameters in Eq. [5] can be obtained for a broader and/or limited range of alloying steel compositions by analyzing the dilation data of additional steels. Typically, high-Ni alloy steels show an isothermal martensite transformation below the M_s temperature, which is caused by a totally different transformation mechanism compared with that of the iron-carbon based alloys. Recently, the transformation-induced plasticity steel and twinning-induced plasticity steel containing a high Mn content are being examined in automotive sheet research, but the austenite phase of these steels is stable at low temperatures after simple quenching. As a result, retained austenite can be present at room temperature. The retained austenite transforms into martensite by applied strain, such that a different type of martensite transformation occurs, *i.e.,* strain-induced martensite. A different equation is used widely to express the strain-induced martensite transformation with the parameters related to the external strain/stress effect.[26] The plain carbon and low-alloy steels used to derive the LV model have narrow ranges for Mn and Si, and thus have been treated as a constant in the current study.

Despite these limitations, the LV model provides a computationally efficient method of describing the martensite transformations accurately for a wide range of plain carbon and low-alloy steels. Additional work should be done to incorporate more fundamental factors into this model. Currently, the proposed LV model can be used for analyzing many commercially available steels. The empirical LV model will be useful in investigations of these types of steels.

VII. SUMMARY

The current study proposes a new empirical martensite kinetics model (LV model) based on an exponential function. The LV model overcomes one limitation of the KM model by considering the effects of chemical composition. It also improves on both the KM and BS models by using a function that better captures the kinetics rate. The effect of prior austenite grain size was assumed to be incorporated in the value of the M_s temperature and not in the transformation equation. The volume fraction of martensite obtained from experimental dilatometric curves over a wide range of chemical composition was used to determine the two parameters in the LV model. When compared with the other models, the LV model exhibits better predictions of volume fraction martensite. It was also better in calculating other properties, such as the M_{90} temperatures and retained austenite. For heat treatment simulations, it is anticipated that the LV model will provide more accurate and effective predictions when used to analyze plain carbon and low-alloy steels.

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