A Continuum Approach to Transformation Kinetics of Metals

A Continuum Approach to Transformation Kinetics of Metals

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A continuum model for the solid-solid transformation kinetics of diffusion type is proposed. The theoretical procedure to figure the continuous cooling transformation diagram (C-C-T diagram) and the time-temperature-transformation diagram (T-T-T diagram) is discussed. Some numerical results are given for the austenite-pearlite transformation of steels.

1. Introduction

The phase transition, or the phase transformation, problem is one of the most attractive problems not only in physics but also in the practical engineering field. Limiting to the industrial attention, for example, the effective thermo-mechanical treatment in the plastic forming of metals, such as the ausforming, is possible only when plenty of knowledge about the solid-solid phase transformation is assumed.[1] The continuous casting in the steel industry is just a case of the solidification processes.[2]

The phenomena, of course, attracted the attention of the continuum mechanists. Their studies cover from the soft phonon mode of lattice vibration to the heat treatment of steels, and also from rational mechanics to the finite element formulation.[3)-9]

The phase transformation problems in engineering are always the coupled problems in such fields as mechanics, thermodynamics and, above all, metallurgy. This complicates the situation greatly when the problems are studied from the point of continuum mechanics. This might be the main reason why, except few excellent studies[5),6], the transformation kinetics could not help sometimes, in fact, leaving untouched, and at other times being assumed to be too simple, although the thermomechanical consideration was often done minutely and strictly.

In this paper a continuum model for the solid-solid transformation kinetics is proposed. It is shown that the model employed can well describe the metallurgical reality.[10)-12] The theoretical procedure to figure the continuous cooling transformation diagram (C-C-T diagram) and the time-temperature-transformation diagram (T-T-T diagram)[13] is discussed when the material experiences the uniform temperature histories. As an application of the theory presented, some numerical calculations are conducted for the austenite-pearlite transformation of steels.

2. Continuum Model of Solid-Solid Phase Transformations

2.1 General formulation

Let us consider a material in the course of solid-solid phase transformation.

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Of course, the phase transformation discussed here is not necessarily limited to the transformations between two phases but could be the transformations among the multi-phases.

We assume that the phenomenological aspect of the solid-solid phase transformation of metals is characterized by a set of equations;

$$\dot{\boldsymbol{\xi}}=\boldsymbol{\Xi}(\boldsymbol{\xi}, \theta, \dot{\theta}, \mathscr{T}; \boldsymbol{x}), \tag{2.1}$$

where $\boldsymbol{\xi}$ represents a set of scalar variables, which describes the extent of phase transformation. It is worth noting that $\boldsymbol{\xi}$ should not be regarded as the fractions of each phases only. In fact later we will illustrate a case in which the other additional variables are necessary to describe the system rationally by means of Eq. (2.1). The variables θ and $\dot{\theta}$ stand for the temperature and the temperature rate, respectively, while $\mathscr{T}$ represents all other factors that might take effect on the progress of phase transformation. The stress tensor or the strain tensor induced in the material is very likely included in $\mathscr{T}$ when the stress assisted transformation or the strain-induced transformation is discussed.[1] The argument $\boldsymbol{x}$ in Eq. (2.1) means that the transformation might be inhomogeneous in nature. In later discussion, however, the inhomogeneity is not considered.

When the material experiences a uniform temperature history;

$$\theta(\boldsymbol{x}, t)=\vartheta(t) \tag{2.2}$$

and, therefore,

$$\dot{\theta}(\boldsymbol{x}, t)=\frac{\mathrm{d}}{\mathrm{d}t}\vartheta(t)\equiv\Theta(t), \tag{2.3}$$

Equation (2.1) reduces to

$$\dot{\boldsymbol{\xi}}(\boldsymbol{x}, t)=\boldsymbol{\Xi}(\boldsymbol{\xi}(\boldsymbol{x}, t), \vartheta(t), \Theta(t), \mathscr{T}(\boldsymbol{x}, t)). \tag{2.4}$$

The variable $\boldsymbol{x}$ is omitted in the following discussions, since it plays only a role of parameter. Assuming that differential equation (2.4) can be solved for an appropriate initial condition, we get a solution

$$\boldsymbol{\xi}(t)=A(t; \vartheta, \Theta). \tag{2.5}$$

The arguments ϑ and Θ mean that the solution depends on the temperature history experienced by the material.

Let us write the solution for the constant rate cooling history

$$\theta=\vartheta(t)=T-\alpha t, \ (T, \alpha\text{: constant}) \tag{2.6}$$

as

$$\boldsymbol{\xi}(t)={}_{\mathrm{C}}A(t; T, \alpha). \tag{2.7}$$

The C-C-T diagram is no other than the curves of Eq. (2.7) plotted in the plane of θ(linear scale)$-t$(logarithmic scale) with $\boldsymbol{\xi}$ as a parameter. When we put $\alpha=0$ in Eq. (2.7), the solution reads

$$\boldsymbol{\xi}(t)={}_{\mathrm{T}}A(t; T). \tag{2.8}$$

This solution for various values of T figures the T-T-T diagram in the same plane.

In order to present a clear continuum mechanical view for the phase transformation problems we disregard the dependence of $\mathscr{F}$ in Eq. (2.1) in the following study. In other words the phase transformation discussed here is not coupled with the other phenomena, such as, for example, the mechanical behavior of materials. Moreover, only the case in which Eq. (2.1) has a structure

$$\dot{\xi} = {}_{\xi}\Xi(\xi, \dot{\theta}) \cdot {}_{\theta}\Xi(\theta, \dot{\theta}) \tag{2.9}$$

will be treated. Cahn started his discussion on the transformation kinetics from this type of equation but with no $\dot{\theta}$-dependence.[14]

Before going further it is worth noting here that the Johnson-Mehl type transformations[10),12)];

$$\begin{aligned} p &= 1 - \exp(-V_e) \\ V_e &= \int_0^t \frac{4}{3}\pi G^3 \dot{N}(t-\tau)^3 d\tau \end{aligned} \tag{2.10}$$

is fully expressible by means of the governing equation proposed here; Eq. (2.1). In Eq. (2.10) p stands for the fraction of the phase produced by the transformation, while G and $\dot{N}$ mean the growth rate of the product and the rate of nucleation per unit volume of matrix, respectively. Generally both G and $\dot{N}$ depend on the temperature strongly. In the case of isothermal phase transformation, Eq. (2.10) is reduced to a familiar form

$$p = 1 - \exp\left(-\frac{1}{4} \cdot \frac{4}{3}\pi G^3 \dot{N} t^4\right). \tag{2.11}$$

When the material experiences a general temperature history (2.2), the time differentiation of Eq. (2.10) gives

$$\dot{p} = \int_0^t 3\left(\frac{4}{3} G^3 \dot{N}\right)(t-\tau)^2 d\tau\,(1-p), \tag{2.12}$$

which is rewritten by means of the additional state variables q, r and s as

$$\begin{aligned} &\dot{p} = q(1-p), \quad \dot{q} = r, \\ &\dot{r} = s, \quad \dot{s} = 6\left(\frac{4}{3}\pi G^3 \dot{N}\right). \end{aligned} \tag{2.13}$$

This is in fact no other than a special form of Eq. (2.1), but with no $\dot{\theta}$-dependence in this case. Let us emphasize here the following fact: The way of reducing a higher-order differential equation to a set of first-order differential equations by introducing the additional state variables is very familiar in mechanics.[15),16)]

2.2 Phase transformation of steels

In order to illustrate how the theory proposed so far works in practice, we apply it to the phase transformation of steels. When the steel is cooled from the temperature above the eutectoid temperature, or the equilibrium transformation temperature, the initial phase, the austenite, transforms to such phases as the felite, the pearlite (ferrite+cementite), the bainite and the martensite. In this study we model the actual transfromation of steels as follows:

1. The phases produced by the transformation are the pearlite and the martensite only.
2. The martensitic transformation takes place at a certain temperature, the martensitic transformation point, with an infinitely large speed.

The C-C-T and the T-T-T diagrams are then derived theoretically for the pearlite transformation in the temperature range between the eutectoid temperature and the martensitic transformation point.

Let the fraction of the pearlite be p. The production rate of pearlite $\dot{p}$ takes the form from Eq. (2.9) as

$$\dot{p}={}_pP(p, \dot{\theta})\, {}_\theta P(\theta, \dot{\theta}). \tag{2.14}$$

We assume that the material functions ${}_pP(p, \dot{\theta})$ and ${}_\theta P(\theta, \dot{\theta})$ are expressed by

$$\begin{aligned} {}_pP(p, \dot{\theta}) &= \left(\ln\frac{C}{C-p}\right)^{3/4}(C-p), \\ {}_\theta P(\theta, \dot{\theta}) &= 4[D\pi(\theta)]^{1/4}, \end{aligned} \tag{2.15}$$

where the material constants C and D are the functions of the temperature rate only;

$$C=C(\dot{\theta}),\ D=D(\dot{\theta}). \tag{2.16}$$

The form of the function $\pi(\theta)$ will be discussed later minutely.

When the constant cooling process (2.6) is chosen as the temperature history, the differential equation (2.14) is solved for the initial condition $p(0)=0$ to give

$$p(t)=C(\alpha)\left[\left[1-\exp\left[-D(\alpha)\left\{\int_0^t(\pi(T-\alpha t))^{1/4}d\tau\right\}^4\right]\right]\right]. \tag{2.17}$$

Equation (2.17) together with Eq. (2.16), *i.e.*,

$$C=C(\alpha),\ D=D(\alpha) \tag{2.18}$$

in our present context enables us to construct a C-C-T diagram.

For isothermal history, $\alpha=0$, Eq. (2.17) reduces to

$$p(t)=C(0)[1-\exp\{-D(0)\pi(T)t^4\}]. \tag{2.19}$$

This figures a T-T-T diagram in the temperature-time plane.

It is important to stress here the following fact: Comparison of Eq. (2.19) with Johnson-Mehl's Eq. (2.11) reveals the physical meaning of the function $\pi(\theta)$ as

$$\pi(\theta)=\frac{4}{3}\pi G^3\dot{N} \tag{2.20}$$

and

$$C(0)=1,\ D(0)=1/4. \tag{2.21}$$

For further characteristic of the material functions $\pi(\theta)$ and $C(\dot{\theta})$, let us examine the general features of the T-T-T and the C-C-T diagrams of the steels. The T-T-T diagram, the thin lines in Fig. 2.1, could be characterized as follows[13];

1. It figures like the letter C in shape.
2. The pearlite transformation completes perfectly in the temperature range between

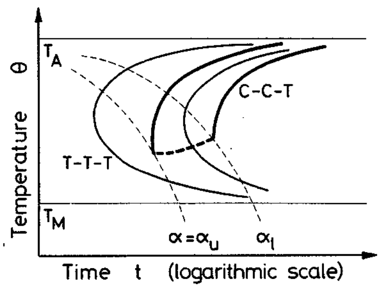

Fig. 2.1 T-T-T and C-C-T diagrams; Schematic representation.

the eutectoid temperature (T_A) and the martensitic transformation point (T_M). This leads us to the following estimation of $\pi(\theta)$:

$$\pi(\theta)\to 0 \quad \text{for } \theta\to T_A \text{ or } T_M. \tag{2.22}$$

We might, therefore, assume $\pi(\theta)$ to have a form

$$\pi(\theta)=a\left(\frac{T_A-\theta}{A}\right)^{n_A}\left(\frac{\theta-T_M}{M}\right)^{n_M}, \tag{2.23}$$

where a, A, n_A, M and n_M are the material constants. The general feature of C-C-T diagram, the thick lines in Fig. 2.1, could be summarized as follows[13]:

1. The transformation does not always complete. In fact along the thick broken line in Fig. 2.1, the transformation stops.
2. There exist the upper critical cooling rate (α_u) and the lower critical cooling rate (α_l).
3. Compared to the T-T-T diagram, the diagram shifts to the larger-time side as a whole.

The characteristics 1. and 2. state that for the cooling rate between α_l and α_u, the transformation stops on its way and therefore the austenite is retained. Now we could conclude that

$$\begin{aligned} C(\alpha)&=1 \quad ; \quad \alpha\le\alpha_l\,,\\ 0<C(\alpha)&<1 \quad ; \quad \alpha_l<\alpha<\alpha_u\,,\\ C(\alpha)&=0 \quad ; \quad \alpha\ge\alpha_u\,. \end{aligned} \tag{2.24}$$

In other words, provided that the material constant is given, the equations

$$C(\alpha)=0 \quad \text{and} \quad C(\alpha)=1 \tag{2.25}$$

determine the upper and the lower critical cooling rates, respectively.

3. Numerical Illustration

3.1 T-T-T diagram

Following Inoue *et al*[6], we employ a numerical representation

$$\pi(\theta)=0.173\left(\frac{720-\theta}{195}\right)^{8.20}\left(\frac{\theta-380}{145}\right)^{6.80} \tag{3.1}$$

for $\pi(\theta)$. As was explained before, the eutectoid temperature and the martensitic transformation point are

$$T_A=720°\text{C} \quad \text{and} \quad T_M=380°\text{C}, \tag{3.2}$$

respectively, in this case. We have also mentioned in Eq. (2.21) that for the isothermal transformation

$$C=1 \quad \text{and} \quad D=1/4. \tag{3.3}$$

Equations (2.14) and (2.15) together with Eqs. (3.1) and (3.3) yield

$$p=1-\exp\left[-1/4 \cdot 0.173\left(\frac{720-T}{195}\right)^{8.20}\left(\frac{T-380}{145}\right)^{6.80} t^4\right]. \tag{3.4}$$

The numerical results by means of Eq. (3.4) for the several values of T between T_A and T_M are plotted in Fig. 3.1 to give a T-T-T diagram in the temperature-time plane. In this figure, and throughout this study, we regard that the beginning and the completion of the transformation are equivalent to the time corresponding to $p=0.01$ and $p=0.99$, respectively, as is done commonly in the metallurgical studies. The T-T-T diagram obtained demonstrates a very good applicability of the theory proposed here. An example of the progress of transformation is shown in Fig. 3.2 for $T=450°$C.

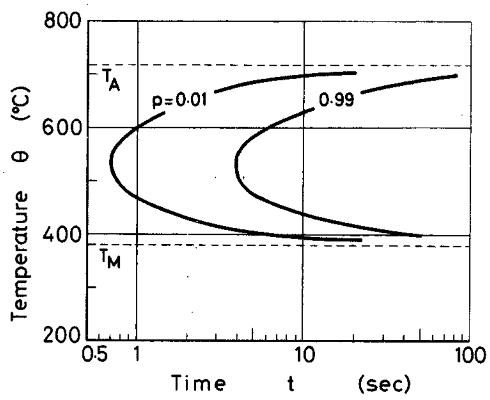

Fig. 3.1 T-T-T diagram.

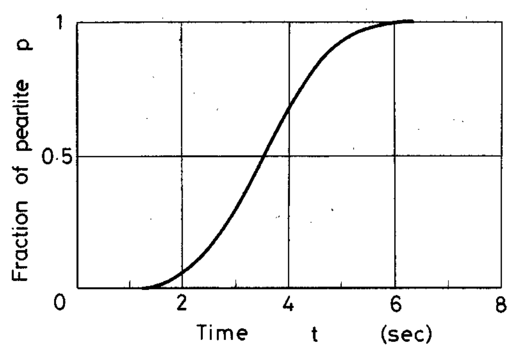

Fig. 3.2 Progress of transformation.

3.2 C-C-T diagram

Let assume that the material functions $C(\alpha)$ and $D(\alpha)$ have the form shown in Figs. 3.3 and 3.4, respectively. In other words, from the present practical version of Eq. (2.25),

$$C(\alpha_u)=0.01 \quad \text{and} \quad C(\alpha_l)=0.99, \tag{3.5}$$

we have $\alpha_u=200\,°\mathrm{C/sec}$ and $\alpha_l=30\,°\mathrm{C/sec}$. The C-C-T diagram for the constant rate cooling history

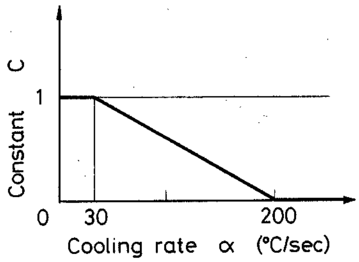

Fig. 3.3 Assumed form of *C*.

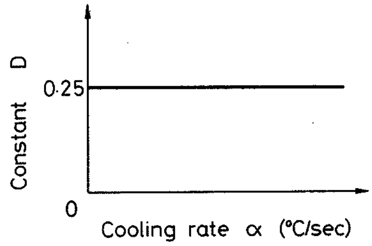

Fig. 3.4 Assumed form of *D*.

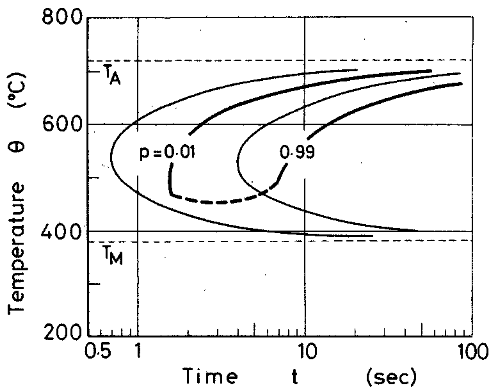

Fig. 3.5 C-C-T diagram.

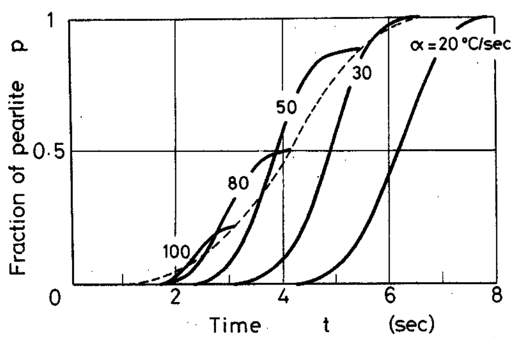

Fig. 3.6 Progress of transformation.

$$\theta = 720 - \alpha t \tag{3.6}$$

is now obtainable from Eq. (2.17) with Eq. (3.1). The result is shown in Fig. 3.5. The progress of transformation is illustrated in Fig. 3.6 with the cooling rate as a parameter. The thin broken line in Fig. 3.6 corresponds to the thick broken line in Fig. 3.5, where the transformation stops. The C-C-T diagram calculated well realizes the overall characteristics of the diagram listed in Sec. 2.2.

Figures 3.7 and 3.8 are the similar results when the function $D(\alpha)$ is replaced by a little more complex function as shown in Fig. 3.9.

The quantitative application of the theory to the practical engineering problems

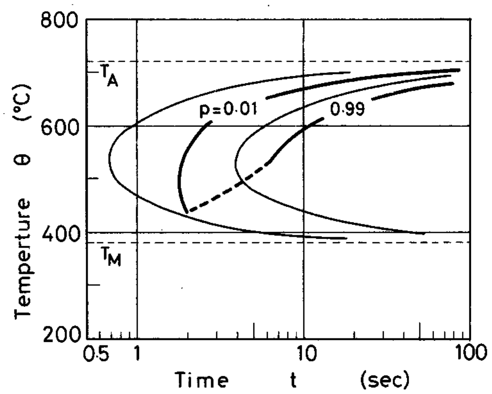

Fig. 3.7 C-C-T diagram.

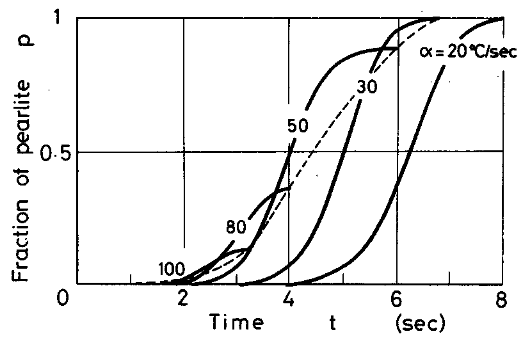

Fig. 3.8 Progress of transformation.

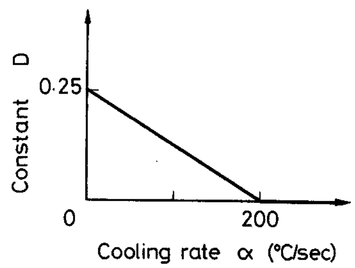

Fig. 3.9 Assumed form of D.

will be the subject of further research.

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