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Application of Johnson-Mehl-Avrami-Kolmogorov type equation in non-isothermal phase process: Re-discussion

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ABSTRACT

A new non-isothermal phase kinetic equation which keeps the form of Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation is established. This non-isothermal JMAK type equation is expressed as $X(t)=1-\exp[-(Kt)^n]$, $K=K_0\exp\left(-\frac{Q}{RT_0}\right)$ T_0 can be given a linear relationship with transformation temperature T in relatively large parameter fluctuation ranges. The applications of non-isothermal JMAK type equation in $\gamma\rightarrow\alpha$ phase process of Fe-0.002 wt%C alloy under linear cooling process and welding thermal process do show its good agreements with the experimental data.

1. Introduction

The famous kinetic equation which deals with a phenomenological model and describes the isothermal phase process, also known as Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation, has been used and overused until nowadays since it has been put forward in the beginning of 1940s [1,2]. The JMAK equation gives a very simple expression between phase fraction transformed, time and temperature (see below, Eq. (1)) based on some assumptions [3]. Though many researchers questioned the validity of the JMAK theory in the last few decades [4–6], experimentalists kept using the original JMAK equation for its good agreement with the experimental results and simple interpretation for phase transformation [7–9]. The JMAK equation is given by

$$X(t)=1-\exp[-(Kt)^n],\ K=K_0\exp\left(-\frac{Q}{RT}\right) \tag{1}$$

where $X(t)$ is the fraction transformed after transformation time t, n the growth exponent, K_0 the pre-exponent coefficient, R the gas constant, T transformation temperature and Q the overall or apparent activation energy.

Many theoretical researchers have also tried to develop the non-isothermal phase kinetics. Sahay et al. [10,11] used the JMAK equation directly in conjunction with the functional relationship to predict the experimental non-isothermal phase process. They assumed a linear relationship between activation energy and the cooling rate to fit experimental results. Though these applications were persuaded weakly in theory, they advanced a simple approach to calculate phase kinetics. An interesting work is presented by Nakamura et al. [12] who proposed a general expression to extend JMAK equation in linear cooling process with the form of

$$X(t)=1-\exp\left\{-\frac{1}{\Phi^n}\left[\int_{T_s}^{T}k(T)dT\right]^n\right\},\ \int_{T_s}^{T}k(T)dT=K_0'(T-T_0')\exp\left(-\frac{Q}{k_BT}\right) \tag{2}$$

where Φ is the heating rate and k_B the Boltzmann constant. Blázquez et al. [13] fitted the value of T_0' and applied the kinetics to two different alloy systems. Sahay and Nakamura successfully proposed relatively simple methods to calculate phase kinetics in linear cooling process. Inspired by their works, a new non-isothermal JMAK type equation is developed in the present work. The advances of this non-isothermal JMAK type equation are i) it keeps the form of isothermal JMAK equation, ii) it deduces from the existing theories and iii) it has wider application ranges including linear cooling process.

2. The establishment of non-isothermal JMAK type equation

Phase transformation with random site-saturated nucleation,

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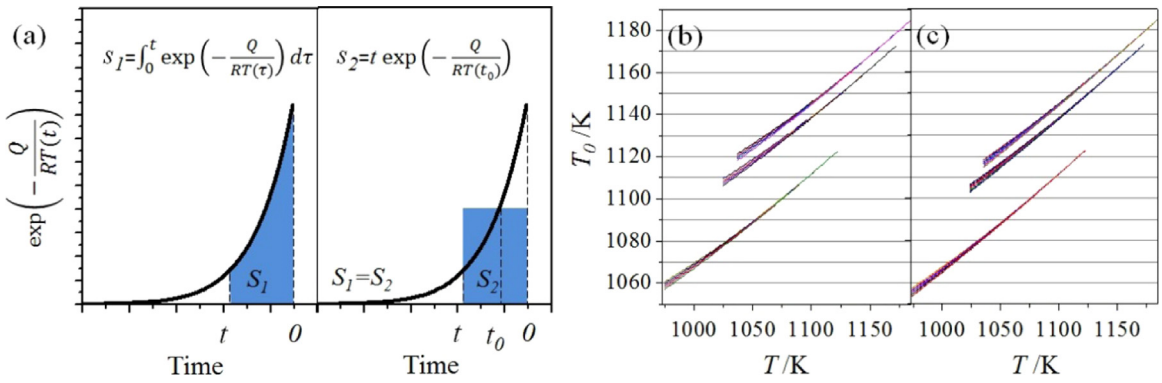

Fig. 1. (a) An average growth rate suggested in calculation; the relationship between T_0 and T (b) in linear cooling process (Q=140/130/120/110/100 kJ mol^{-1}, T_s=1185/1175/1123 K), (c) in welding thermal process (Rykalin-3D mode) (E=100/200 kJ cm^{-1}, T_p=1573 K, λ=0.4 J cm^{-1} s^{-1} K^{-1}, Q=140/130/120/110/100 kJ mol^{-1}, T_s=1185/1175/1123 K).

growth and impingement modes is given by [14,15].

$$X(t)=1-\exp\left\{-gI_0\left[\int_0^t v_0\exp\left(-\frac{Q}{RT(\tau)}\right)d\tau\right]^n\right\} \tag{3}$$

where I_0 is the number of pre-existing nuclei per unit volume, v_0 the pre-exponential factor for growth, g a geometrical constant, n the growth dimensions. An average growth rate is suggested in calculating the transcendental integral function in Eq. (3), as illustrated in Fig. 1(a).

$$\int_0^t \exp\left(-\frac{Q}{RT(\tau)}\right)d\tau=t\exp\left(-\frac{Q}{RT(t_0)}\right) \tag{4}$$

Take $T(t_0)$ as T_0. The relationship between T_0 and Q, T_s (phase start temperature) and T can be calculated under a given $T(t)$. Submitting Eq. (4) into Eq. (3), the non-isothermal JMAK type equation is given by

$$X(t)=1-\exp\left[-(Kt)^n\right],\ K=K_0\exp\left(-\frac{Q}{RT_0}\right) \tag{5}$$

Eq. (4) is rewritten as

$$\exp\left(-\frac{Q}{RT_0}\right)=\frac{\int_0^t \exp\left(-\frac{Q}{RT(\tau)}\right)d\tau}{t}=V(t) \tag{6}$$

$V(t)$ is average growth rate factor. T_0 is then calculated with

$$T_0=-\frac{Q}{R\ln V(t)} \tag{7}$$

The value of $\ln V(t)$ which leads to the best fitting depends on the value of T_s, Q and expression of $T(t)$. An approximate straight line in limit phase transformation temperature range and activation energy range can be fitted for $1/\ln V(t)$. Then the final expression of T_0 can be given by

$$T_0(T_s)=aT+b\mathrm{K} \tag{8}$$

where a and b are fitted constants under a corresponding T_s. Take two typical cooling processes of linear cooling process and welding thermal process for examples. Transformation temperature function in linear cooling process is expressed as

$$T(t)=T_s-rt \tag{9}$$

where r is the cooling rate. Temperature function of Rykalin-3D mode is given by [16].

$$T'(\theta)=\frac{E}{2\pi\lambda\theta}\exp\left(-\frac{E}{2T_p\lambda\pi e\theta}\right) \tag{10}$$

where E is the heat input, θ the thermal time, λ the thermal conductivity and T_p the peak temperature. Assume $T'(\theta')=T_s$ in the cooling process, thus transformation temperature function is written as

$$T(t)=T'(\theta'+t) \tag{11}$$

The relationship between T_0 and T in linear cooling process and welding thermal process are shown in Fig. 1(b) and (c), respectively. It can be seen three beams of lines can be fitted by three approximate paralleled lines. So in limit phase start temperature range ($T_s+\Delta T$ to T_s), a relationship also can be given as

$$T_0(T_s+\Delta T)=a(T+\Delta T)+b\mathrm{K}=T_0(T_s)+a\Delta T \tag{12}$$

3. Application of the non-isothermal JMAK type equation to γ→α phase process

The Fe-0.002 wt%C alloy samples with chemical composition of Fe-0.0020C-0.0060Si-0.0160Mn-0.0060P-0.0040S-0.0100Al-0.01Cr-0.0100Ni-0.0100Cu (wt%) were cut from 30 mm-thick plates. Before simulation, samples were annealed at 1173 K for 5 h. Dumb-bell-shaped samples were machined from the central 10 mm section, 75 mm in length and 10 mm in diameter with the central section 10 mm in length and 4 mm in diameter. A Gleeble 3500 simulator was programmed to follow thermal cycles. Thermocouple wires were point welded on the center of Φ4 mm cylinder to conduct heat transfer. For linear cooling process, samples were heated up from room temperature to 1273 K at a rate of 1 K s^{-1} and kept for 300 s, then cooled continuously with rates of 10 and 20 K s^{-1} to 373 K, respectively. For welding thermal process, samples were heated to 1573 K at a rate of 100 K s^{-1} and then cooled continuously with Rykalin-3D (thick plate) modes which correspond to heat inputs of 100 and 200 kJ cm^{-1}, respectively. Then specimens were cut from the center of thermocouple welding points, polished, etched with 5 wt% picric acid solution and 4% nital solution and observed by optical microscopy (OM). All the grains on the cross-section of the samples on the magnification of 50× were counted to calculate ferrite grain nucleus density. The lever rule on dilatation-temperature curve was used to calculate phase kinetics.

Fig. 2 shows the grain boundaries after γ→α phase transformation. Estimations of the nucleus densities in linear cooling processes of 10 K s^{-1} and 20 K s^{-1} are about 7.03 × 10^{10} m^{-3} and