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Kinetic Model of ε-Cu Particle Dissolution in Welding-Induced HAZ of Copper-Containing Steel

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Abstract: The kinetics of ε-Cu particle dissolution in the matrix of heat affected zone (HAZ) during welding of a copper-containing steel was determined by assembling the welding temperature-time program into a modified Whelan's solution. The particle dissolution dependence on the degree of "superheating" above the equilibrium transformation is demonstrated from the model. In terms of volume fraction of particle dissolution, the HAZ may be classified into three zones, including the undissolving zone, the partially dissolving zone, and the completely dissolving zone, respectively. The numerical solution was in good agreement with the experimental examination finding. The results of model can be used to quantitatively map the ε-Cu dissolution zone dependence on the peak temperature of welding thermal cycles and understand the evolution of this transformation during welding.

Key words: ε-Cu; particle dissolution; kinetics; welding; steel

The precipitation of Cu-rich particles, depending on alloy composition, can make a significant contribution to the overall properties of high strength low alloy (HSLA) steels[1,2]. Highly weldable and corrosion-resistant copper-containing steels with high-level strength and toughness have been developed for naval and defense applications[3]. However, when the steels are welded, the copper precipitates may dissolve partly or completely into the matrix and as a result, a softened heat affected zone (HAZ) may occur accordingly, which has been experimentally examined in as-welded HSLA100 steel by Yoo J Y, et al[4] and in HSLA80 steel by Dunne D[5]. From the viewpoint of safety and integrity in engineering structures, considerable attention must be paid to mapping the particle dissolution distribution over the whole HAZ, which is mainly characterized by the non-isothermal temperature-time program during welding of this type of steel.

The particle dissolution can be understood and described more thoroughly and accurately by modeling this transformation. Using Fick's second law and invariable boundary conditions, Whelan M J[6] presented an analytical approach to estimate the dissolution rate of particles in spherical shape in relation to an isothermal process. However, the particle/matrix interface concentration is severely dependent on the temperature-time program and the boundary conditions, since the diffusion field near the particle actually varies with time. Thus, an analytical approach that is often simplified for the application of an isothermal process cannot be directly adopted by a non-isothermal phase transformation behavior unless it satisfies the additivity law or isokinetic condition defined by Christian J W[7] and further clarified by Grong Ø and Bjørneklett B I[8,9].

This attempt seeks to quantitatively understand the welding-induced dissolution of ε-Cu particles into the matrix of the HAZ by modeling work. An integral equation representing the particle volume fraction dependence on the heating peak temperature was determined from a modified Whelan's equation by assembling the welding thermal programs, and a numerical solution in the form of dissolution map was obtained by concreting the thermal histories of the HAZ produced by manual arc welding (MAC)

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into it. A comparison was made between the modeling results and the experimental data.

1 Mathematical Formulation

Regarding Whelan's model, the dissolution of spherical particles embedded in an infinite matrix in the case of isothermal heating is governed only by the solute diffusion from the static precipitate/matrix boundary into the adjacent matrix and can be described by the following equation[6].

$$\frac{\mathrm{d}r}{\mathrm{d}t} = -k\left[\frac{D_{\mathrm{m}}}{r} - \sqrt{\frac{D_{\mathrm{m}}}{\pi \cdot t}}\right] \tag{1}$$

where r and t represent the particle radius and time, respectively; and D_{m} is the bulk diffusion coefficient of copper atom in matrix. $k = (C_{\mathrm{i}} - C_{\mathrm{b}})/(C_{\mathrm{p}} - C_{\mathrm{i}})$ is a dimensionless variable indicating the systematic constituent gradient near the particle/matrix interface as schematically shown in Fig. 1.

In Fig. 1, C_{i} represents the concentration of copper located at the precipitate/matrix interface, and C_{b} is the bulk concentration of copper in the matrix. C_{p} refers to the concentration of copper in the ε-Cu particles and has been confirmed to be 100% by other's study[10].

During fast welding thermal cycle, however, since the particle dissolution takes place in a very short term, and the diffusion fields among the adjacent particles may not impinge each other, the invariant-field solution is valid for a short period of time[11]. By neglecting the transient item $(D_{\mathrm{m}}/\pi t)^{1/2}$, the radius r and the volume fraction f of particle dependence on the heating time t are obtained respectively as:

$$r^2 = r_0^2 - 2k \cdot D_{\mathrm{m}} \cdot t \tag{2}$$

and

$$f = f_0\left[1 - \frac{2k \cdot D_{\mathrm{m}} \cdot t}{r_0^2}\right]^{3/2} \tag{3}$$

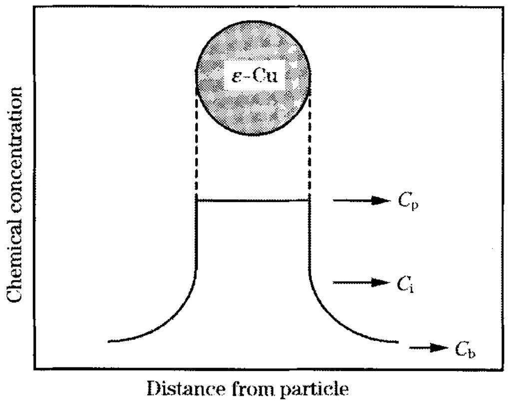

Fig. 1 Schematic demonstration of the systematic constituent gradient near the particle/matrix interface

where r_0 and f_0 represents the initial average radius and the volume fraction of the particles. Depending on the heating temperature, the time t_{d}, in which a particle of initial radius r_0 dissolves completely into the matrix, can be therefore described by the following equation:

$$t_{\mathrm{d}} = \frac{r_0^2}{2k \cdot D_{\mathrm{m}}} \tag{4}$$

By introducing the state variable p, which is defined in the following equation:

$$p = \left[1 - \left(\frac{f}{f_0}\right)^{2/3}\right] = \frac{2k \cdot D_{\mathrm{m}} \cdot t}{r_0^2} = \frac{t}{t_{\mathrm{d}}} \tag{5}$$

the volume fraction variation $\mathrm{d}f$ in a unit time interval $\mathrm{d}t$ can be obtained:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\mathrm{d}f}{\mathrm{d}p} \cdot \frac{\mathrm{d}p}{\mathrm{d}t} = \frac{\mathrm{d}f}{\mathrm{d}p} \cdot \frac{1}{t_{\mathrm{d}}} \tag{6}$$

In terms of Christian's definition, Eqn. (6) confirms that the welding-induced dissolution is of an isokinetic process and satisfies the additivity law.

To generate a numerical solution to the kinetic equation, however, the welding thermal program may be simplified and constituted by two stages. The heating stage is described by a linear temperature-time program:

$$T = T_0 + vt \tag{7}$$

where v is the heating rate, and the cooling stage is computed from Christensen's equation[12]:

$$T = T_0 + (T_{\mathrm{p}} - T_0)\exp(-Bt) \tag{8}$$

where T, T_0, and T_{p} represent the instantaneous temperature at time t, the initial temperature prior to welding, and the peak temperature, respectively, of a welding thermal cycle. B is defined as:

$$B = \frac{T_{\mathrm{p}} - T_0}{t_{8/5}}\left[\frac{1}{773 - T_0} - \frac{1}{1\,073 - T_0}\right] \tag{9}$$

where, $t_{8/5}$ is the time in which a certain location of HAZ is cooled from 1 073 K to 773 K.

Consequently, the dependence of volume fraction of particles in the specific HAZ on the peak temperature T_{p} can be obtained by introducing integration throughout the temperature-time history, and can be described using the following equations:

$$\frac{f}{f_0} = \left\{1 - \frac{2}{r_0^2}\left[\int_{T_1}^{T_{\mathrm{p}}} \frac{k \cdot D_{\mathrm{m}}}{v}\mathrm{d}T - \int_{T_{\mathrm{p}}}^{T_1} \frac{k \cdot D_{\mathrm{m}}}{B(T - T_0)}\mathrm{d}T\right]\right\}^{3/2} \tag{10}$$

where T_1 is the minimum temperature at which the precipitates start to dissolve into the matrix, which can be derived by assuming that f/f_0 is equal to 1.

Using Eqn. (10), it is now possible to evaluate the ε-Cu dissolution throughout the HAZ where the thermal cycles with different peak temperatures are