Computer Simulation on Transformation Process of Steel on Rapid Heating (Report I)†

– Formation of Austenite from Pearlite –

Katsunori INOUE*, Etsuji OHMURA** and Shoichi IKUTA***

Abstract

The transformation of pearlite to austenite on rapid heating was studied by a two-dimensional carbon diffusion model. The finite difference method was introduced to simulate the transformation process. The simulated results were shown in the pseudo-color images on the display, and the growth rate of austenite was also investigated. It was shown that the dissolution velocity of the cementite is more than 3.5 mm per second for the heating rates above 10^3 K per second, and the dissolution of a pearlite colony with grain size 80μm is completed in 20 ms at most on such rapid heating.

KEY WORDS: (Phase Transformation) (Computer Simulation) (Pearlite Dissolution) (Rapid Heating) (Carbon Steel) (Carbon Diffusion) (Finite Difference Method) (Laser Materials Processing)

1. Introduction

Materials processing with laser beams has progressed markedly in recent years. In the industrial use of them, not only a thermal model but also a metallurgical model are very useful to predict the experimental results previously for a given application and for a given steel. Capable mathematical models can be also applied to determine theoretically the best combination of the process variables: the power, size, and shape of the beam, the travelling velocity, and the chemistry and metallurgy of the steel. A finite-difference computer model[1] for the laser transformation hardening has been already developed to simulate the changes with time of the heat flow, the carbon redistribution in austenite and the microstructure in the heat-affected zone.

The first stage of structural changes of steel in laser materials processing is the transformation of austenite from pearlite. It is the purpose of this paper to develop a computer model to simulate the transformation process on rapid heating and to investigate the growth rate of austenite.

Nucleation of austenite in pearlitic structures occurs preferentially at the intersection of pearlite colonies, not at the interlamellar surfaces. Once austenite has nucleated in the pearlite, its subsequent growth is presumably controlled by carbon diffusion in the austenite[2]. Therefore, a two-dimensional carbon diffusion model is introduced in this paper instead of one-dimensional model[3]. The simulation is carried out using the finite difference method. The simulated results are shown in the pseudo-color images on the display and the growth rate of austenite is also investigated.

2. Analysis

Figure 1 illustrates the two-dimensional model which is used to determine the carbon diffusion from a layer of cementite into an adjacent layer of ferrite. The dissolution

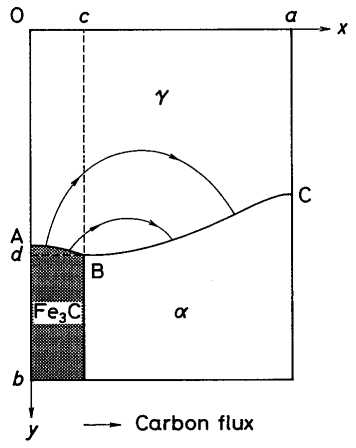

Fig. 1 Diffusion geometry for dissolution of pearlite.

† Received on May 6, 1987.
* Professor
** Research Instructor
*** Graduate Student of Osaka University

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of cementite starts at the point $(c, 0)$ in Fig. 1. The temperature at which the cementite starts to dissolve, that is, Ac_{1s} is dependent on the heating rate, and it is about 1063K (790°C) when the heating rate exceeds 200K per second or so[4].

Fick's Laws permit the concentration of a diffusion substance (carbon in this case) to be determined as a function of distance and time. The differential equation is:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}-\frac{1}{D}\frac{\partial}{\partial t}\right) C(x,y;t)=0\,. \qquad (1)$$

The boundary conditions are

$$\frac{\partial}{\partial x} C(0,y;t)=\frac{\partial}{\partial x} C(a,y;t)=0\,, \qquad (2)$$

$$\frac{\partial}{\partial y} C(x,0;t)=\frac{\partial}{\partial y} C(x,b;t)=0\,, \qquad (3)$$

$$\frac{\partial}{\partial x} C(c,y;t)=0\,,\quad d<y\leqslant b\,, \qquad (4)$$

and the initial condition is

$$C(x,y;0)=\begin{cases} C_{cm}\,, & 0\leqslant x\leqslant c \\ C_{\alpha}\,, & c<x\leqslant a \end{cases} \qquad (5)$$

where C and D are the carbon concentration and diffusion coefficient of carbon in austenite, respectively, and the substricts cm and α mean the carbon concentration of cementite and ferrite, respectively.

The diffusion coefficient of carbon is temperature dependent, and is given by

$$D=D_0 \exp\left(-\frac{Q_0}{RT}\right), \qquad (6)$$

where D_0 is frequency factor, Q_0 activation energy and R gas constant, 8.314J/(mol · K), and

$$D_0=0.167\times 10^{-4}\,\mathrm{m^2/s}\,,$$

$$Q_0=136.3\ \mathrm{kJ/mol},$$

for eutectoid steel[5]. Ferrite can contain 0.0218 wt. pct. of carbon at most[6], then it is assumed that the ferrite at the α/γ interface transfers to austenite if it contains more carbon.

The average interlamellar spacing $2a$ and the average diameter b of standard pearlite colonies are assumed to be 480 nm[6] and 80μm, respectively, which are the values of standard pearlite colonies in eutectoid steel.

The ratio of c to a in Fig. 1 can be determined by the following equation:

$$\rho_{cm}\, c\, C_{cm}+\rho_{\alpha}\,(a-c)\,C_{\alpha}=\rho_P\, a\, C_P\,, \qquad (7)$$

where ρ is density and the substrict P means the properties of pearlite. In Eq. (7), ρ_{cm}, ρ_{α} and ρ_P are nearly equal each other and C_{α} is nearly equal to zero, then

$$c : a = C_P : C_{cm}\,. \qquad (8)$$

Substituting C_{cm} = 6.67 wt. pct. and C_P = 0.77 wt. pct. into Eq. (8), the ratio of c to a is obtained as 3 : 26 approximately. Using this ratio, C_{α} is determined as 0.0004wt. pct. from Eq. (7), and it is lower than 0.006wt. pct. which is the maximum carbon content of ferrite in the room temperature[6].

In order to consider the temperature dependence of the diffusion coefficient of carbon in austenite, the finite difference equations are derived using the alternating direction implicit (ADI) method. **Figure 2** shows the grid system used. The grid spacings Δx_1, Δx_2 and Δy are expressed as follows:

$$\Delta x_1=\frac{2c}{2m_1-1} \qquad (9)$$

$$\Delta x_2=\frac{2(a-c)}{2(m-m_1)-1}\,, \qquad (10)$$

$$\Delta y=\frac{b}{n-1}\,, \qquad (11)$$

The finite difference equations for the grid (i, j) in the area of $0\leqslant i\leqslant m_1-2$ or $m_1+1\leqslant i\leqslant m-1$, and $0\leqslant j\leqslant n-1$, for instance, can be written in the following forms:

(i) $t_1\rightarrow t_2\ (=t_1+\Delta t)$

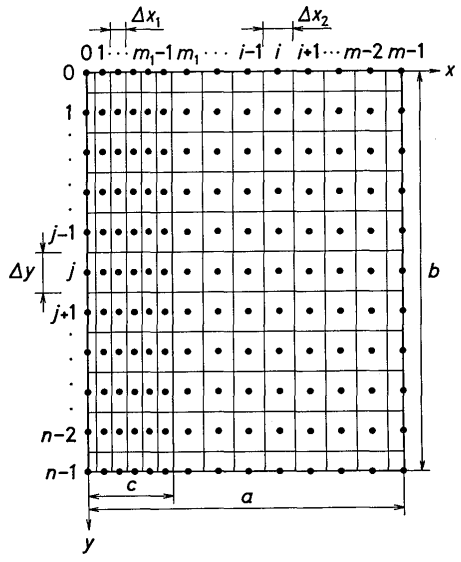


Fig. 2 Grid system.

$$-F_x^{(k)}(t_2)C_{i-i,j}(t_2)+\left\{1+2F_x^{(k)}(t_2)\right\}$$
$$\times C_{i,j}(t_2)-F_x^{(k)}(t_2)C_{i+i,j}(t_2)$$
$$=F_y(t_1)C_{i,j-1}(t_1)+\left\{1-2F_y(t_1)\right\}C_{i,j}(t_1)$$
$$+F_y(t_1)C_{i,j+1}(t_1)\,,\quad k=1,2 \qquad (12)$$

(ii) $t_2 \rightarrow t_3\ (=t_2+\Delta t)$

$$-F_y(t_3)C_{i,j-1}(t_3)+\left\{1+2F_y(t_3)\right\}$$
$$\times C_{i,j}(t_3)-F_y(t_3)C_{i,j+1}(t_3)$$
$$=F_x^{(k)}(t_2)C_{i-i,j}(t_2)+\left\{1-2F_x^{(k)}(t_2)\right\}$$
$$\times C_{i,j}(t_2)+F_x^{(k)}(t_2)C_{i+i,j}(t_2)\,,\ k=1,2 \qquad (13)$$

where $C_{i,j}$ is the carbon concentration at the grid (i, j),

$$F_x^{(k)}(t)=\frac{D(t)\cdot\Delta t}{(\Delta x_k)^2}\,,\quad k=1,2 \qquad (14)$$

$$F_y(t)=\frac{D(t)\cdot\Delta t}{(\Delta y)^2}\,, \qquad (15)$$

and

$$C_{-1,j}(t)=C_{1,j}(t)\,,\quad 0\leqslant j\leqslant n-1 \qquad (16)$$

$$C_{m,j}(t)=C_{m-2,j}(t)\,,\quad 0\leqslant j\leqslant n-1 \qquad (17)$$

$$C_{i,-1}(t)=C_{i,1}(t)\,,\quad 0\leqslant i\leqslant m-1 \qquad (18)$$

$$C_{i,n}(t)=C_{i,n-2}(t)\,,\quad 0\leqslant i\leqslant m-1\,. \qquad (19)$$

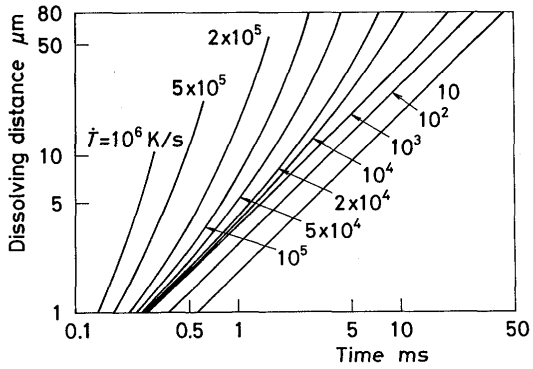
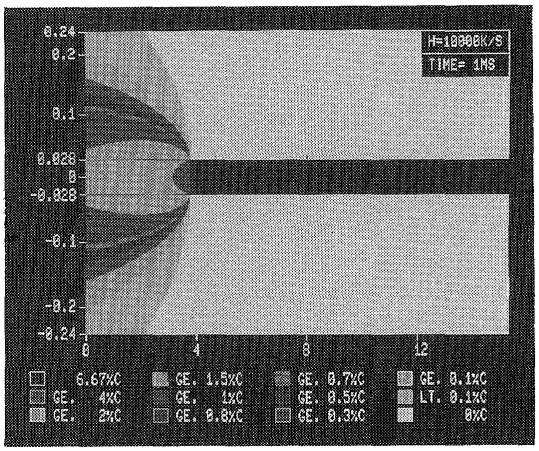
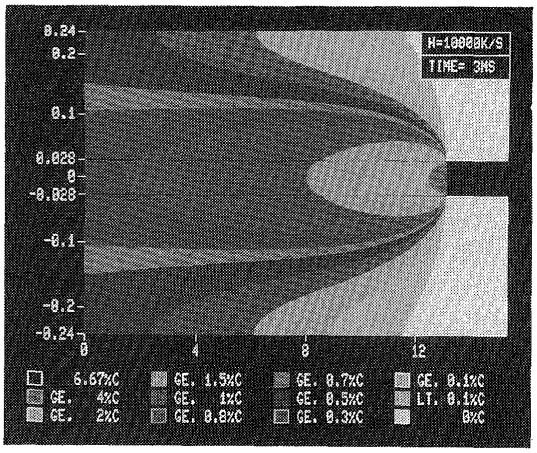


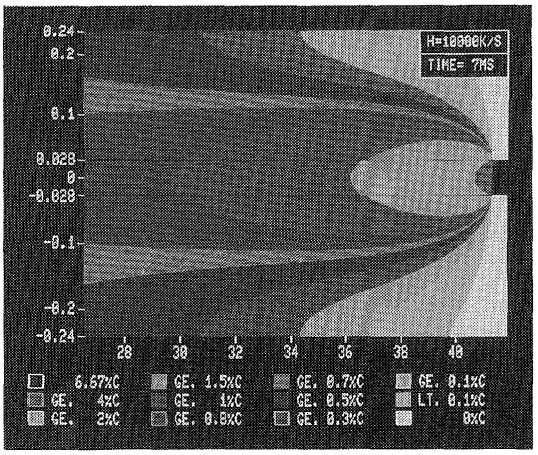
Fig. 3 Dissolving distance d in Fig. 1 with time at various heating rate.



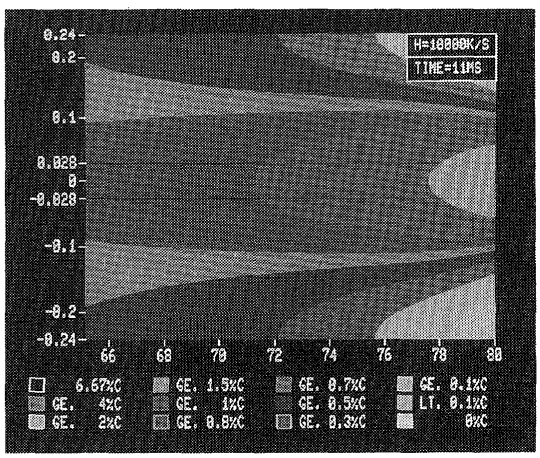
(a)



(b)



(c)



(d)

Fig. 4 Examples of the calculated results of the pearlite dissolution: (a) t = 1ms; (b) t = 3ms; (c) t = 7ms; and (d) t = 10.6ms. The unit of the abscissa and of the ordinate is μm.

3. Results

In this study, a mini-computer, HITAC E-800 was used to carry out the calculations of the pearlite dissolution, and the calculated results on the carbon content distribution in austenite were expressed on the CRT display of the color image processor, NEXUS 6400 conected with the mini-computer.

Figure 3 shows the dissolving distance d in Fig. 1 with time elapsed after the cementite starts to dissolve at various heating rate. The ferrite is transformed into austenite by a diffusionless massive transformation at about 1373K on rapid heating[7], therefore the calculation was stopped in this study when the temperature reaches at 1373K, even if cementite did not dissolved completely. It is clear that the time required for the pearlite to be transformed into austenite becomes shorter as the heating rate increases. When the heating rate is 10^5K per second, the pearlite dissolution requires about 3 ms at most.

Figure 4 shows the calculated results of the carbon concentration changes with time, when the heating rate is 10^4K per second. Carbon content distribution during the pearlite dissolution is shown in the pseudo-color image on the display. The pearlite and ferrite are shown by white and black, respectively. The color codes to show austenite are based on brown, yellow, green and blue, which correspond to the carbon concentration. The nearly eutectic content of carbon is shown by red in order to draw attention. The interfaces of prior cementite and ferrite are shown by two black lines, and the width of cementite $2c$ is enlarged with a magnification of x 1.05. The α/γ interface is a little bowed. In this case, complete dissolution of cementite is found in 10.6 ms, as shown in Fig. 4 (d).

The differences in carbon content distribution at the same time under the different heating rate are shown in **Fig. 5**. The distribution of carbon content in the austenite expands more widely as the heating rate increases.

4. Discussion

Shown in **Fig. 6** is a sketch of the pearlite dissolution and austenitization of the surrounding ferrite by carbon diffusion from the prior pearlite colony in hypo-eutectoid steel, where v_A means the dissolving velocity of the pearlite which corresponds to the proceeding velocity of the position A in Fig. 1, and v_B means the proceeding velocity of interface B at which the carbon atoms start to diffuse, that is, the carbon content starts to decrease from 0.77 wt. pct. in the prior pearlite colony.

Figure 7 shows the changes of the velocity v_A with time at verious heating rate, which is obtained from Fig. 3.

In order to calculate the velocity v_B, it is assumed that the prior pearlite colony is a sphere with radius r_0 (= $b/2$), and is inside the infinite ferrite matrix. If v_B is greater than v_A, the point B coincides with the point A in Fig. 6. The carbon diffusion equation is mathematically defined in the following way:

$$\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{D}\frac{\partial}{\partial t}\right)C(r,t)=0 \qquad (21)$$

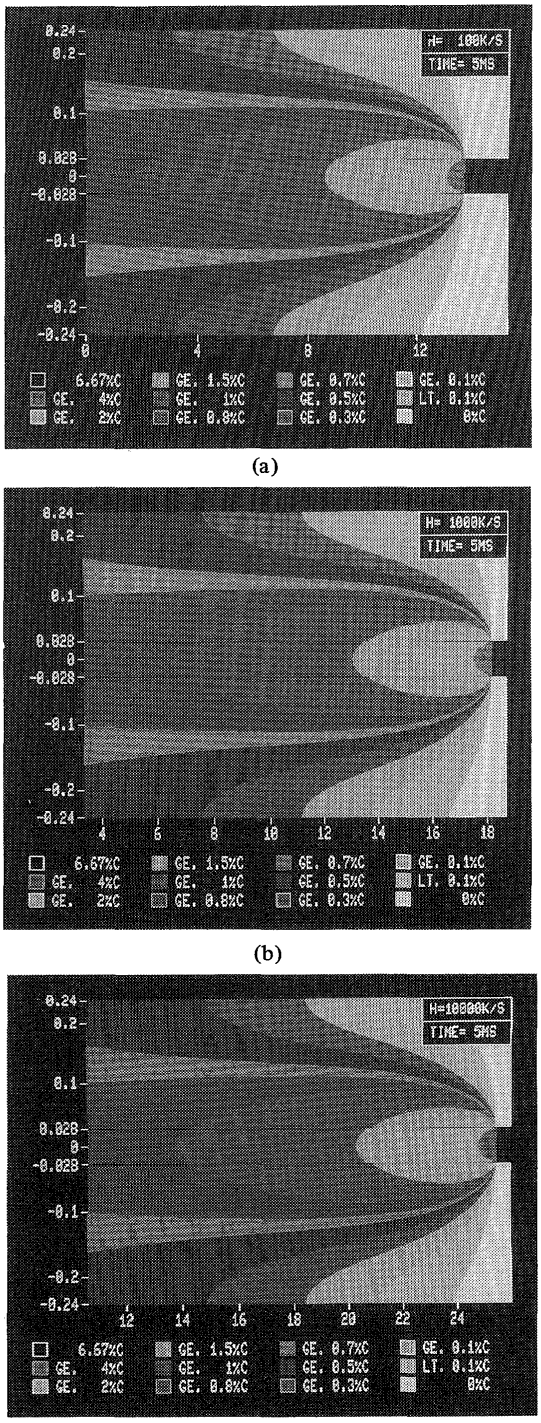


Fig. 5 Comparison of the carbon content distribution at the same time under the different heating rate: (a) 10^2K/s; (b) 10^3K/s; and (c) 10^4K/s.

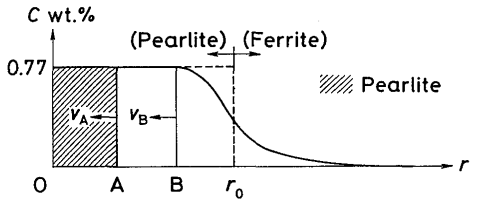


Fig. 6 A schematic sketch of the pearlite dissolution and austenitization of surrounding ferrite by carbon diffusion from prior pearlite colony in hypo-eutectoid steel.

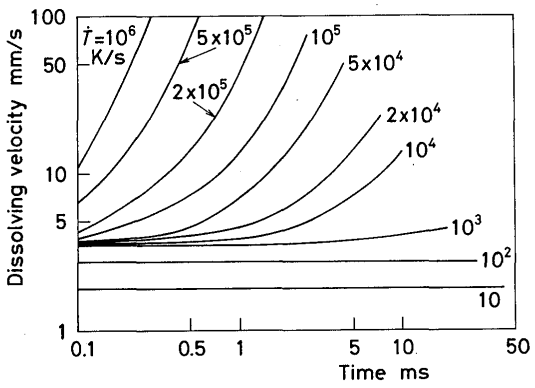


Fig. 7 Dissolving velocity v_A in Fig. 6 with time at various heating rate.

The boundary conditions and initial condition can be summarized as:

$$\frac{\partial}{\partial r} C(0, t) = 0 \tag{22}$$

$$C(\infty, t) = C_\alpha \tag{23}$$

$$C(r, 0) = \begin{cases} C_P , & 0 \leqslant r \leqslant r_0 \\ C_\alpha , & r > r_0 \end{cases} \tag{24}$$

In order to consider the temperature dependence of the carbon diffusion coefficient, the explicit finite difference method is used to solve Eqs. (21) ~ (24).

The calculated results of the changes of the velocity v_B with time at various heating rate are shown in **Fig. 8**. At the early state of the carbon diffusion, the carbon content varies in only a few grids in the finite difference model, then the velocity v_B is not calculated correctly. Therefore, the results at the early state are not shown in Fig. 8. It is clear that the dissolving velocity v_A is much greater than the diffusing velocity v_B, comparing Fig. 7 with Fig. 8.

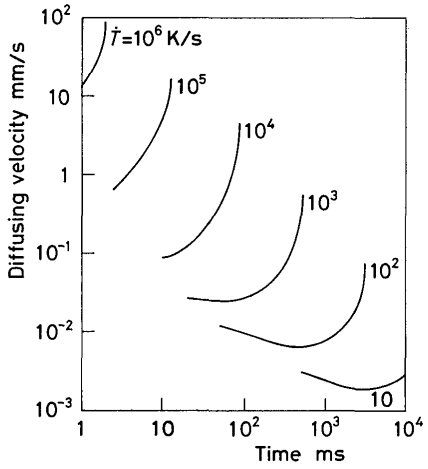


Fig. 8 Diffusing velocity v_B in Fig. 6 with time at various heating rate.

These results suggest that, in Ac_3 transformation process of hypo-eutectoid steel on rapid heating, the pearlite colonies have been already transformed to austenite which can supply carbon attoms sufficiently to the surrounding ferrite matrix. Therefore, Ac_3 transformation process can be analyzed theoretically independent of the pearlite dissolution.

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