PROCEDURE FOR PREDICTING THE DISTRIBUTION OF IMPURITY IN HEAT-TREATED METALS

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Impurity concentration profiles in metals are predicted using a simple one dimensional model for unsteady state diffusion in a temperature gradient. Good agreement with the experimental data of Darken and Oriani is obtained, both for diffusion of carbon in ferrite and for nitrogen in ferrite. This calculation method has promise not only for prediction of the effects of existing heating processes on interior and surface compositions of metals but also for the design of specific new heating processes to achieve desirable properties.

Presented herein is a simple calculation method for predicting impurity concentration profiles in metals subjected to heating. The mass flux equation for coupled concentration and thermal diffusion in one dimension is simplified by assuming that the temperature gradient approaches steady state much faster than does the concentration gradient, and, hence, the unsteady state temperature gradient can be approximated by the known steady state gradient. This simplification allows integration of the mass transfer equation to determine the space- and time-dependence of impurity concentration. Predicted concentration profiles are compared with the experimental data of Darken and Oriani (1) to show the accuracy of the simplified calculation method.

SIMPLIFIED MODEL AND SOLUTION

The model used here for impurity diffusion is a flat metal plate, sufficiently large and thin to permit ignoring edge effects (Fig. 1). The initial concentration of impurities within the plate, $C(X, 0) = C_t$, is uniform from surface, $X = 0$, to surface, $X = a$. At time $t = 0$, a temperature difference τ is applied across the two faces. This temperature difference is maintained at a constant, and $\tau = T(a,t) - T(0,t)$.

Imposition of the temperature difference τ across the flat plate causes redistribution of impurity in the plate by thermal diffusion; the mass flux initially is a function only of temperature gradient. Immediately following the first incremental redistribution, the diffusion process becomes a function of both temperature and concentration gradients. The coupling of these two gradients is discussed elsewhere (2, 3). The mass flux of impurity, J, in the one-dimensional model can be expressed in terms of the concentration gradient, $\frac{dC}{dx}$, and the temperature gradient, $\frac{dT}{dx}$, by the equation

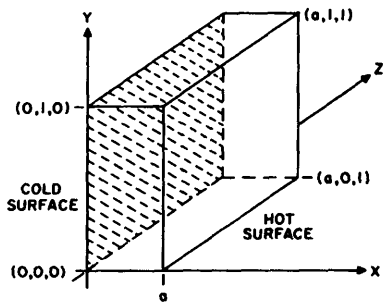

FIGURE 1. Bulk diffusion model.

$$J = -D' \frac{dC}{dx} - D'' \frac{dT}{dx} \qquad \text{Eq. 1}$$

where D′ is the concentration diffusion coefficient and D″ is the thermal diffusion coefficient. Even for the simple case of a flat plate with initially homogeneous concentration subjected to a constant linear temperature gradient across the plate faces, the solution of equation 1 is complicated by the fact that both unsteady state con-

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centration and temperature profiles must be described. Thus, in principle, the equation 1 conjugate for energy flux must be solved simultaneously with equation 1. However, an approximate solution for the impurity concentration profile can be obtained by using the following simplification.

The approximation introduced is to assume that the temperature profile in the flat plate is established in a very short time compared to the time required for appreciable redistribution of impurity. Thus, the simplified model is a flat plate with initially homogeneous impurity concentration, $C(x,0) = C_0$, and a linear temperature gradient, $\frac{dT}{dx} = \tau/a$ (for all x), which is invariant with time. In addition, the boundary conditions of zero mass flux at each face of the plate are imposed.

To solve for the concentration profile in the simplified model, equation 1 is differentiated with respect to the space coordinate x; note that $\frac{dJ}{dx} = -\frac{dC}{dt}$, to give

$$\frac{dC}{dt} = D'\frac{d^2C}{dx^2} + \frac{\tau}{a}\frac{dD''}{dx} \qquad \text{Eq. 2}$$

The thermal diffusion coefficient, D'', is related to the so-called heat of transport, Q*, and is described in numerous references (2) as

$$D'' = \frac{D'Q^*C}{RT^2} \qquad \text{Eq. 3}$$

Considering Q* to be constant, substitution of equation 3 in equation 2 yields

$$\frac{dC}{dt} = D'\frac{d^2C}{dx^2} + \frac{D'Q^*}{RT^2}\frac{\tau}{a}\frac{dC}{dx} \qquad \text{Eq. 4}$$

The Fourier series solution[15] of equation 4 yields the following expression for the space- and time-dependence of the impurity concentration,

$$C(x,t=0) = C_0,\ \frac{\partial C}{\partial t} = 0 \text{ at } t=0$$

$$C(x,t) = C_0\left\{\alpha \exp(-\alpha x/a)/[1-\exp(-\alpha)] + \sum_{k=1}^{\infty} 16\alpha k^2[1-(-1)^k\exp(-\alpha/2)]/(\alpha^2+4\pi^2k^2)^2 \cdot[\alpha\sin(k\pi x/a) - (2\pi k/\alpha)\cos(k\pi x/a)] \cdot\exp[-\alpha z/2a - (k^2\pi^2+\alpha^2/4)D't/a^2]\right\} \qquad \text{Eq. 5}$$

where $\alpha = \tau D''/D'$ Eq. 6

COMPARISON WITH EXPERIMENTAL DATA

To evaluate the impurity concentration profile expression given in equation 5, predicted profiles were compared with the experimental data of Darken and Oriani (1). These investigators utilized experimental systems which are compatible with the model and boundary conditions considered in the derivation of equation 5. Darken and Oriani employed thin plate systems and controlled face temperatures with large heat sinks. Two systems were studied, nitrogen impurity in a ferrite plate 1.0 cm thick and carbon impurity in a ferrite plate 1.2 cm thick. Concentrations were determined at four interior cross sections in the plates at 24, 48, or 96 hr after application of fixed temperature differences across the faces of the plates. Predictions of impurity concentration profiles were made using equation 5 with values of the heat of transport of −23.0 kcal/mole for carbon in ferrite and carbon, and −42.3 kcal/mole for nitrogen in ferrite and nitrogen.

Figures 2-7 graphically illustrate the agreement obtained between predicted and experimental impurity concentration profiles. The agreement is particularly good for nitrogen impurity in ferrite ($C_0 = 0.021$ wt %) (Fig. 2-4). In Figures 2 and 3 a minimum can be noted in both the predicted and experimental impurity concen-

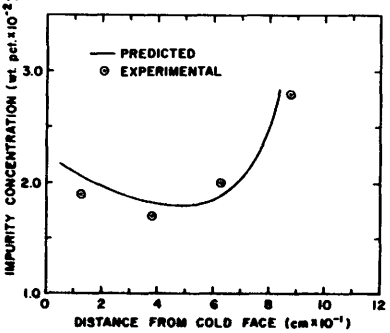

FIGURE 2. Concentration of nitrogen in ferrite versus distance from cold face. Plate thickness = 1.0 cm; hot face temp. = 766 C; cold face temp. = 418 C; run length = 24 hr.

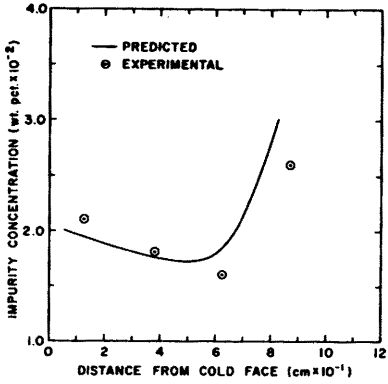

FIGURE 3. Concentration of nitrogen in ferrite versus distance from cold face. Plate thickness = 1.0 cm; hot face temp. = 803 C; cold face temp. = 510 C; run length = 24 hr.

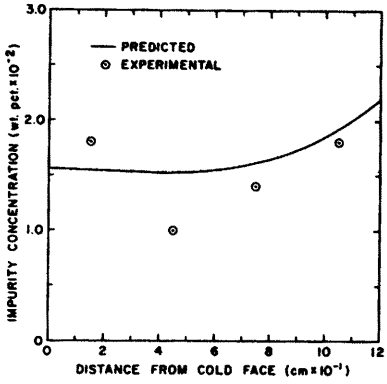

FIGURE 5. Concentration of carbon in ferrite versus distance from cold face. Plate thickness = 1.2 cm; hot face temp. = 677 C; cold face temp. = 525 C; run length = 24 hr.

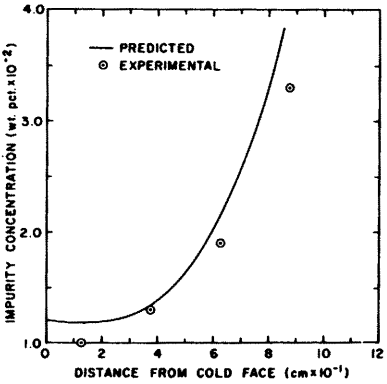

FIGURE 4. Concentration of nitrogen in ferrite versus distance from cold face. Plate thickness = 1.0 cm; hot face temp. = 756 C; cold face temp. = 622 C; run length = 96 hr.

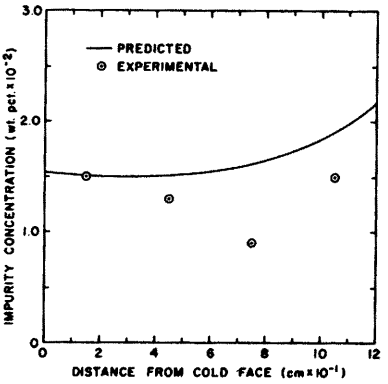

FIGURE 6. Concentration of carbon in ferrite versus distance from cold face. Plate thickness = 1.2 cm; hot face temp. = 696 C; cold face temp. = 537 C; run length = 48 hr.

tration profiles. Such minima would be expected experimentally whenever the temperature difference across the faces of the plate is large enough to make an appreciable difference in the mass flux across the sample. Thus a variation in the diffusion coefficient is created. Consequently, the temperature of the cold end is low enough to "freeze" the diffusion in the cold region. For carbon impurity in ferrite (C_o = 0.016 wt %), the agreement between predicted and experimental concentration profiles (Fig. 5-7) is not as good as that for nitrogen in ferrite (Fig. 2-4). However, considering the scatter in the data, which can be noted in Figures 5-7, and possible uncertainty in the heat of transport data used, the predicted concentration profiles are in sufficiently good agreement with the experimental data to conclude that the model is valuable for practical heat-treating calculations.

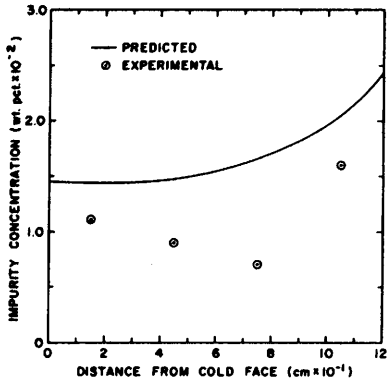

FIGURE 7. Concentration of carbon in ferrite versus distance from cold face. Plate thickness = 1.2 cm; hot face temp. = 690 C; cold face temp. = 554 C; run length = 96 hr.

CONCLUSIONS

A simple model of the process of impurity diffusion during the heating of metals has been formulated. The successful applications of this model for predicing impurity concentration profiles indicates the potential for using comparable models for the design of specific heat-treating processes.

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