A Solution for Diffusion Equations and the Distribution of Alloying Elements in Sintered Alloys

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Abstract

The error function can be calculated based on the Simpson method through a subroutine program. An integration program by FORTRAN language was made for diffusion equations of extended source with infinite extent and limited extent. The results on some alloying elements such as C, Co, Cr, Mn, Mo, Ni and V's diffusion in iron, showed the diffusion distance for Ni and Mo can only be 1~3 μm and more distance for Co at common sintering temperature of 1120 ℃. To refine the particle size of the added elements down to a scale of micrometers is an effective way to get homogeneous distribution.

Keywords: Diffusion, Sintered alloy, error fuction

1. Introduction

In powder metallurgy materials it should always introduce alloying elements in order to improve its mechanical properties. However, sometimes it could not diffuse entirely to get a homogeneous microstructure and it can definitely affect its properties especially on its fatigue limit [1-3]. On the other hand in the materials science the diffusion theory has been investigated and sufficient data in binary alloy systems were published [4, 5]. If these data can be used for calculation on the diffusion process very easily and quickly, it is may be a suitable method to establish process parameter. The aim of the work is to explore calculation method by computer and to analyze distribution in iron-based alloys in order to get suitable materials.

2. Diffusion Equations and its Solution

In the diffusion of extended source of infinite extent with the initial concentration C_0 and diffusion coefficient D in a plane as shown in Fig.1, the concentration distribution equation after diffusion for time t as in Fig.2 is

$$C(x,t)=\frac{C_0}{\pi^{1/2}}\int_{x/(2\sqrt{Dt})}^{\infty} e^{-\eta^2}d\eta \qquad (1)$$

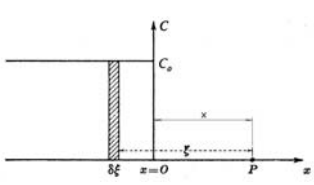
Taking $\eta=\xi/(2\sqrt{Dt})$ and the integration $erf(z)$ is named the error function

$$erf(z)=\frac{2}{\pi^{1/2}}\int_0^z e^{-\eta^2}d\eta \qquad (2)$$

In the cases of extended source of limited extent initially confined in the region $-h<x<+h$ as in Fig.3, the equation after diffusion for time t should be

$$C(x,t)=\frac{1}{2}C_0\left\{erf\frac{h-x}{2\sqrt{Dt}}+erf\frac{h+x}{2\sqrt{Dt}}\right\} \qquad (3)$$

The equation (1) can be used for calculation of distribution along the boundary of two particles and the equation (3) can predict whether or not the added alloying particle is diffused sufficiently.



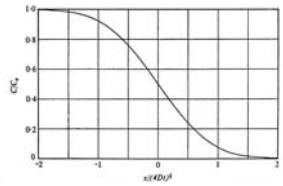


Fig. 1. Extended initial distribution **Fig.2. Distribution curve**

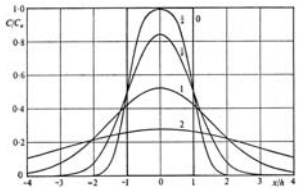


Fig. 3. Distribution curve for an extended source

A definite integral, $I=\int_a^b f(x)dx$, can be expressed as a polynomial by Simpson method. If the distance of (a, b) can be divided by m and then it has $h=(b-a)/2m$ and

$$I\approx\frac{h}{3}\left\{\begin{array}{l}f(a)+4\left[f(a+h)+f(a+3h)+\cdots+f(a+(2m-1)h)\right]+\\2\left[f(a+2h)+f(a+4h+\cdots+f(a+(2m-2)h)\right]+f(b)\end{array}\right\} \qquad (4)$$

According to Simpson method the error function can be calculated through a subroutine program by computer and

the alloying elements distribution curves could be driven from equation (1) or (3). Schematic programming by FORTRAN is illustrated in Fig.4

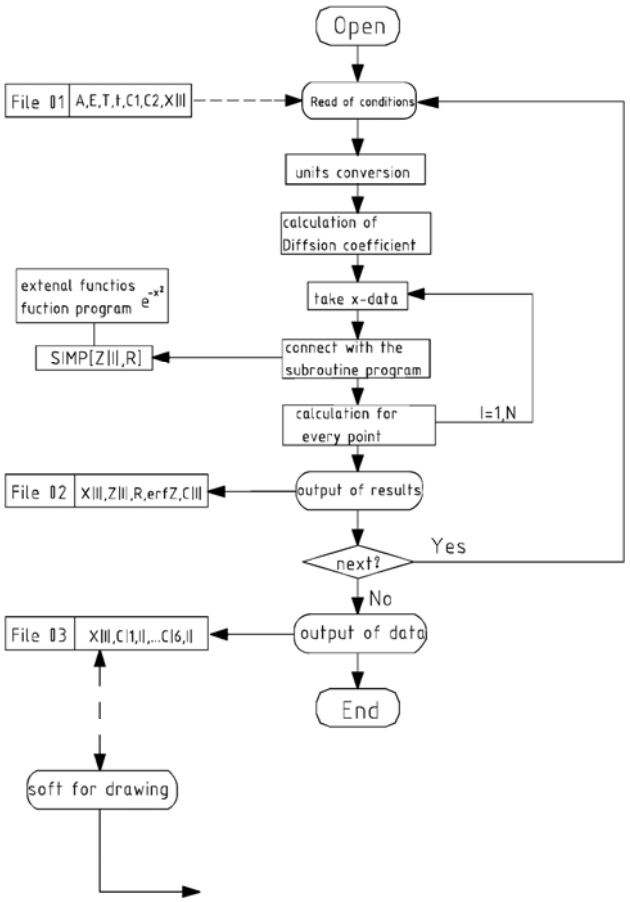


Fig. 4. Schematic programming for calculation of diffusion

Diffusion of some alloying elements such as C, Co, Cr, Mn, Mo, Ni and V in iron-based alloys, the frequency constant A and activated energy E could found in the literature [5]. Calculation results are shown in Fig.5 both for extended source with infinite extent and limited extent at the temperature of 1120℃ and 1300℃. It can be seen that the diffusion distance for Ni and Mo can only be 1~3 μm and more distance for Co. Increasing the sintering temperature up to 1300℃ the curve could be improved so that distance can increase to 3~6 μm. In the case of Mo's diffusion in Fe at the temperature of 1120℃, the effect of different particle size can be calculated using the model of extended source limited extent and equation (3). Calculation result is shown in Fig.6, from which it should be realized that adapting fine Mo powder of 0.2~0.5μm would be binifit for better performance. In the case of 6μm carbon's diffusion in Fe, the calculation result is shown in Fig.7. It is very easy to diffuse to the distance of 40~60μm at the temperature above 900℃.

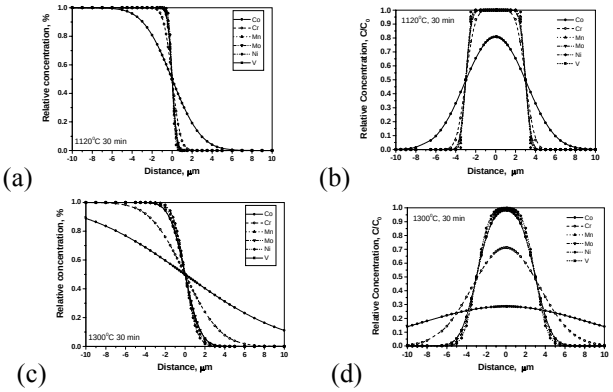


Fig. 5. Distribution curve of alloying elements in iron

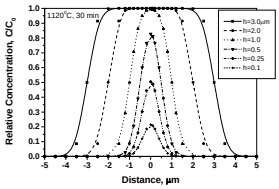


Fig. 6. Mo Distribution curve

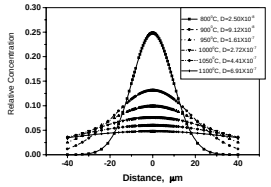


Fig. 7. C Distribution curve

3. Summary

The error function can be calculated based on the Simpson method. A program was made for diffusion equations of extended source with infinite extent and limited extent. At the temperature of 1120℃, the diffusion distance for Ni and Mo in iron can only be 1~3 μm and more distance for Co. Increasing the temperature up to 1300℃, distribution curve could be improved. To refine the particle size of the added elements down to a scale of micrometers is an effective way to get homogeneous distribution.

4. References

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