Investigation of Methods for Calculation of Interdiffusion Coefficients of Iron and Nickel Powder Mixtures

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Abstract. In this research, new methods were devised and investigated for calculation of interdiffusion of iron and nickel powder mixtures in porous media. We consider that two particles is like thin film in diffusion couples and we use SEM and EDAX analysis and two mathematical methods to calculating “Interdiffusion Coefficient”. In these samples after metallography the observation with SEM show that microstructure consists of ferrite and nickel-rich regions. Diffusion profile was established by EDAX analysis from center of grain rich of nickel up to the out of its boundary and with an experimental method and spherical equation of second Fick’s law of diffusion, we obtain acceptable results for interdiffusion coefficient. We did not use other additional element to produce samples and our sample have 4% nickel and 0.8% Microwax in pure iron powder (WPL200) and after mixing and compaction sintering was carried out in a mesh-belt conveyor furnace in 1120 ºC and 30 min in control endogas atmosphere. The green density of our sample is 6.8 g/cm³.

Keywords: Interdiffusion Coefficients, Powder, Nickel, Iron

1 Introduction
Alloys based on mixture of Fe and Ni powders are common throughout powder metallurgy (P/M). This alloys may seem simple, considering that the two elements are close together in periodic table and are similar chemically, and in terms of electronic structure and atomic radius. However, the behavior of these alloys is complex. As shown in the Fe-Ni phase diagram in Figure 1, the liquidus and solidus temperatures are high, with a narrow solidification range. The face-centered cubic crystal structure of iron (γ or austenite) is stabilized by alloying with nickel (the γ region expands with increasing nickel concentration). Sintering techniques have been exploited for several years in the production of Fe-Ni alloys. In mixed elemental powder sintering, there are fundamentally three events- particle adhesion, densification, and homogenization. Adhesion occurs by surface diffusion, typically during heating. Concomitant bonding without densification provides handling strength in the powder mass. At higher temperatures, densification processes become active, leading to pore elimination via grain boundary diffusion. However, as high sintered densities are achieved the microstructure is not homogeneous, but consists of Ni-rich islands in the Fe-C steel matrix. During the sintering
of mixed Fe-Ni powders, the adhesion, densification and homogenization events are factors. In the early stage of sintering, chemical gradients associated with mixed Ni and Fe powders improve diffusion fluxes over those associated with surface energy which normally drives single-phase sintering. Thus initial sintering can be improved significantly by the addition of Ni. However, this chemical gradient enhancement decreases with increasing temperature as the concentration gradients are eliminated.

Also, Ni enlarges the austenite zone and lowers the ferrite-to-austenite transformation temperature. Since lattice diffusivity in face-centered cubic Fe is much lower than that the body-centered cubic Fe, the phase transformation lowers the sintering rate. The concentration of Ni in Fe increases during sintering, inducing Ni-rich areas to transform into austenite earlier than would occur with a low Ni content. The result is slower high temperature densification due to the reduced diffusion rate. Also, when Fe goes through the alpha-to-gamma transformation, there is a significant increase in grain size. This result in a decrease in annihilation sites for vacancies and substantial decrease in the sintering rate, which is sensitive to grain boundary area. Thus the addition of Ni powder to Fe powder enhances early stage sintering but retards later stage sintering. The coefficient of diffusion Fe is much higher than those of Ni, leading to possible pore creation during interdiffusion. For example, raising the sintering temperature from 1100 °C to 1250 °C increases the interdiffusion coefficient of Fe into Ni by a factor of four, while that of Ni diffusion into Fe increases by only two and half times. The difference in diffusivity is another factor that influences densification and homogenization in mixed Fe-Ni powder sintering. Thus, it is difficult and costly to obtain a fully homogenized Fe-Ni alloy based on the sintering of mixed elemental powder if the Ni content is high.  

This study measures the interdiffusion coefficient of mixture of Fe-Ni powders that sinter in 1120°C and 30 min time, in this study we assume that the particles of given type are spherical and of the same size, we can drive a simple model that particle of Ni surrounded by Fe and during sintering gradient of concentration causes the interdiffusion of these particles so after sintering we have grains Ni-rich areas. By using SEM and EDAX analysis and two mathematical methods a considerable good result near solid particle obtained.

2 Experimental Procedure:
In this research, we use Ni and Fe powder to produce experimental samples after mixing, compaction and sintering, cylindrical samples prepared for metallurgy and this process was performed by optical and secondary electron microscope.

3 Result and Discussion:
Metallography indicates that these samples included of ferrite, ferrite rich of nickel, minor pearlite and porosity. Figure (2) show these regions. Also, EDAX analyses show us concentration gradient of Nickel from ferrite rich zone to Nickel poor zone.

Figure 2: Microstructure of Fe-4%Nickel by secondry electron microscope
Bright zone: Ferrite rich of Nickle, Gray zone: α-Iron, minor pearllite, Dark zone: porosity
The results of some other analysis from these samples around the grain Ni rich show the same variation, with mathematical Eq.1, Eq.2 and least square method and some linear condition we assume two particles like thin film so diffusion could perform in one dimension and two different negative and positive directions.

\[ c(x,t) = \frac{bc_0}{2\sqrt{\pi Dt}} \exp \left[ -\frac{x^2}{4Dt} \right]. \]  

(1)

\[ \ln c(x,t) = \ln \frac{bc}{2\sqrt{\pi Dt}} - \frac{x^2}{4Dt}. \]  

(2)

**Table 2: Result of the experimental data for first method**

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th>[ n(\sum x_i^2) - (\sum x_i)^2 ]</th>
<th>[ 4.5584*10^{-14} ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>[ \frac{1}{\Delta}[(n(\sum x_i y_i) - \sum x_i \sum y_i)] ]</td>
<td>[ -0.02808*10^8 ]</td>
</tr>
<tr>
<td>( b )</td>
<td>[ \frac{1}{\Delta} (\sum y_i \sum x_i^2 - \sum x_i \sum x_i y_i) ]</td>
<td>Not required</td>
</tr>
</tbody>
</table>

Fig. 4 shows the results of LnC(X,t) according X, by reactifying these data, the slope of this diagram is better show of \(-\frac{1}{4Dt}\). Rectifying take places by continuing the first line passing from first data until cutting the horizontal line at -35 (μm). By adding this content to all data, the line passing from second data intersect the horizontal line at zero. The
original era of diffusion can obtain according to this rectifying.

\[ c = c_i \neq 0, 0 < r < r_0, t = 0 \]
\[ c = c_f \neq 0, r = r_0, t > 0 \]

In this linear condition Ci, Cf, C are initial, final and average of concentration and \( r_0 \) is the average radius of Nickel particles and with forcing this linear condition the solution of Fick’s equation is as below: Eq. 4

\[ \frac{c - c_f}{c_i - c_f} \approx \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp \left[ -\frac{\pi^2 n^2 Dt}{r_0^2} \right]. \] (4)

In this equation if the experimental time is too long with assuming the first serial sentence, the result of calculation of equation is like below: Eq. 5 and we could calculate “D” with Eq.6

\[ \ln \frac{c - c_f}{c_i - c_f} \approx \ln \frac{6}{\pi^2} + \ln \left[ -\frac{\pi^2 Dt}{r_0^2} \right]. \] (6)

The result of D can obtain by putting data from EDAX analysis and assuming time equal 30 min and radius equal \( 10 \times 10^{-4} cm \) as follow:

\[ \ln(0.10139-0.02201)/(0.99-0.0220) \approx -0.4977 + \ln \left[ -\frac{\pi^2 D \times 30 \times 60}{100 \times 10^{-8}} \right] \]

\[ D = 11.334 \times 10^{-11} cm^2/sec \]

4 Summary

1- By using the method of calculation of interdiffusion coefficient Linear Diffusion at one coordination we can obtain \( D = 4.9458 \times 10^{-11} cm^2/sec \)

2- After rectifying data the interdiffusion coefficient obtain
$$D = 3.5992 \times 10^{-11} \, \frac{cm^2}{sec}$$

3- By using Calculation of interdiffusion coefficient at spherical coordination of mixture of Fe-4\%Ni powders that sinter in 1120\°C and 30 min we can obtain $D = 11.334 \times 10^{-11} \, \frac{cm^2}{sec}$

References


