The Computer Simulation of Concentration Field for Be/00Cr17Ni14Mo2 Stainless Steel by Hot Pressing

Hui LI, Ying-kun GONG, Yi-lin CHEN, Fei DUAN and Xuan WANG
Chongqing Academy of Metrology and Quality Inspection, Chongqing 401123, China

Keywords: Concentration field, Computer simulation, Hot pressing, Be, 00Cr17Ni14Mo2.

Abstract. In order to provide the best technic parameter for hot pressing, the distributions of Fe and Be near the Be and 00Cr17Ni14Mo2 stainless steel (Be/SS) diffusion bonding interface under different technic parameter were simulated by the finite element method and measured by means of scanning auger microspectrotry (AES). The simulated results were compared with experimental value, The distributions of Fe and Be near the Be/SS diffusion bonding interface and the relationships between the width of diffusion layer, the heating temperature, the holding time and the pressure were also discussed. The results indicate that under the condition of heating temperature 1323K and 1023K with diffusion pressure 60MPa and holding time 7200s, respectively, the simulated distributions of Fe and Be near the Be/SS diffusion bonding interface fit with the experiment values, and the width of diffusion layer at 1323K is about 2.5 times the one at 1023K. Under the condition of heating temperature 1023K with holding time 7200s, the width of diffusion layer measured at 30MPa, 40MPa, 50MPa and 60MPa is fit well with the simulated results and the relationship between the width of diffusion layer (x/µm) and the diffusion pressure (p/MPa) follows the equation 

\[ x = -1.5 \times 10^{-2}p^2 + 2.8275p - 0.1575 \]

Under the condition of heating temperature 1023K with diffusion pressure 60MPa, the simulation curve between the width of diffusion layer (x/µm) and the holding time (t/s) follows the equation

\[ x = 10t^3 - 60.571t^2 + 135.64t + 0.2143 \]

Introduction

At present, scholars have carried on a lot of research on diffusion bonding of dissimilar metals, which involved the elements diffusion, phase transitions, interfacial reaction and joint stress-strain etc. Computer simulation is using reasonable mathematical model to get useful information at less cost and shorter time, which will provide the basis for optimization process. In recent years, the literatures reported computer simulation in diffusion bonding\(^{[1-8]}\), but the literatures were less which reported the effects of heating temperature, holding time and diffusion pressure on the diffusion bonding that were analyzed at the same time. This paper based on physical processe of the diffusion bonding established the mathematical model of concentration field of Be/00Cr17Ni14Mo2 stainless steel (Be/SS) by diffusion bonding. Finite element method with Matlab software system was used as numerical analysis and carried on the simulation distributions of Fe and Be near the Be/SS diffusion bonding interface under different technic parameter, and the simulated results were compared with values measured by AES, so guiding the choice of the best technic parameter for diffusion bonding.

Experiments

Specimens and Experiments

Beryllium specimens are made of hot-pressed beryllium, which contains 0.61% BeO, 0.027% Be2C and 0.08% Fe. 00Cr17Ni14Mo2 stainless steel (SS) is the austenite anti-hydrogen stainless steel, which contains 17.2% Cr, 14.27% Ni, 2.19% Mo and 1.05% Mn, and its impurity total contents is less than 0.17%. Bars of Be and SS are 10 mm in diameter and 12 mm in height. The diffusion bonding was achieved by hot pressing under the condition of heating temperature 1323K and holding time 7200s with diffusion pressure 60 MPa (1323K/60MPa/7200s) and heating temperature
1023K and holding time 7200s with diffusion pressure 30MPa, 40MPa, 50MPa and 60MPa, respectively, and cooled was in furnace and vacuum degree was $10^{-3}$ Pa.

**Principle and Model**

Based on the actual diffusion bonding situation, we established a mathematical model of elements diffusion, determined the reasonable boundary conditions and initial conditions, and carried on the simulation of concentration field by finite element method with Matlab software system. The distributions of Fe and Be near the Be/SS bonding interface were measured along the axial direction of diffusion bonding by AES, whose values were compared with the simulation results, and the relationship between the technological parameters and the elements diffusion near the Be/SS bonding interface was analyzed.

Diffusion bonding can be summed up as solutions of certain differential equations, but the boundary conditions are very complex. It is very difficult to solve these differential equation, so must make many simplifying assumptions to find analytic solution. To simplify the analysis, only the diffusion of Fe and Be are discussed in diffusion couple of Be and SS (shown in Figure 1); the assumption of stainless steel and beryllium are ideal solid solution; and diffusion coefficient is isotropic and independent of concentration.

Elements diffusion from one side to the other side on the Be/SS bonding interface can be used for solving the unsteady equation in one-dimensional infinite medium. The elements initial concentration are respectively $C_1$ and $C_2$ in Be and SS, and the elements of both sides on the bonding interface do not occur in diffusion before hot pressing, and the concentration distribution near the bonding interface follows the unsteady diffusion equation in the second Fick’s law.

Control equation,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \tag{1}$$

Initial conditions is while $t = 0$,

$$\begin{cases} C = C_1, x > 0 \\ C = C_2, x < 0 \end{cases}$$

Boundary conditions is while $t \geq 0$,

$$\begin{cases} C = C_1, x = \infty \\ C = C_2, x = -\infty \end{cases}$$

There $C$ is the concentration, $D$ is the diffusion coefficient, $t$ is the holding time. According to the error function, the solution of diffusion equation 1 is the following equation 2.

$$C_1 = \frac{C_0}{1+K(D_1/D_2)^{1/2}} \cdot [1 + K(D_1/D_2)^{1/2} \cdot \text{erf}(\frac{x}{2\sqrt{D_1}t})]$$

$$C_2 = \frac{KC_0}{1+K(D_1/D_2)^{1/2}} \cdot [1 - \text{erf}(\frac{|x|}{2\sqrt{D_1}t})]$$

There

$$C_0 = \frac{C_2 + C_1}{2}, \quad K = \frac{C_2}{C_1} \tag{2}$$

Table 1. The diffusion coefficients under 1323K/60MPa/7200s (cm²/s).

<table>
<thead>
<tr>
<th></th>
<th>Be</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>3.10×10⁻¹²</td>
<td>1.21×10⁻¹²</td>
</tr>
<tr>
<td>SS</td>
<td>8.09×10⁻¹³</td>
<td>3.88×10⁻¹⁵</td>
</tr>
</tbody>
</table>
Table 2. The diffusion coefficients under 1023K and 7200s with different pressure (cm²/s).

<table>
<thead>
<tr>
<th></th>
<th>30 MPa</th>
<th>40 MPa</th>
<th>50 MPa</th>
<th>60 MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be in SS</td>
<td>8.25×10⁻¹⁴</td>
<td>1.24×10⁻¹³</td>
<td>1.80×10⁻¹³</td>
<td>3.58×10⁻¹³</td>
</tr>
<tr>
<td>Be in Be</td>
<td>4.80×10⁻¹²</td>
<td>7.31×10⁻¹²</td>
<td>9.61×10⁻¹²</td>
<td>1.06×10⁻¹¹</td>
</tr>
<tr>
<td>Fe in Be</td>
<td>5.72×10⁻¹³</td>
<td>9.92×10⁻¹²</td>
<td>2.35×10⁻¹²</td>
<td>3.29×10⁻¹²</td>
</tr>
<tr>
<td>Fe in SS</td>
<td>9.93×10⁻¹⁶</td>
<td>2.16×10⁻¹⁵</td>
<td>2.58×10⁻¹⁵</td>
<td>3.73×10⁻¹⁵</td>
</tr>
</tbody>
</table>

Introduced respectively the distributions of Be and Fe measured by AES under 1323K/60MPa/7200s, 1023K/30MPa/7200s, 1023K/40MPa/7200s, 1023K/50MPa/7200s and 1023K/60MPa/7200s into equation 2, and the diffusion coefficients obtained by the error function in Be and SS are shown in Table 1 and Table 2, respectively.

In a few hours, the diffusion distance is about hundreds of micrometers, therefore, divided only finite element in very small zone near the Be/SS bonding interface (shown in Figure 2). Introduced the diffusion coefficients in Table 1 and Table 2 into equation 1, and obtained the simulation distribution curves of Be and Fe near the Be/SS bonding interface under 1323K/60MPa/7200s, 1023K/30MPa/7200s, 1023K/40MPa/7200s, 1023K/50MPa/7200s and 1023K/60MPa/7200s.

Results and Discussion

The Simulated Results Fit with the Experimental Data

The simulation results and the experimental values of the Be and Fe distribution near the Be/SS bonding interface are shown in Figure 3 and Figure 4 under 1323K/60MPa/7200s and 1023K/60MPa/7200s, respectively, which the simulation results are basically consistent with the values measured by AES. This paper is regardless of the thermodynamic process and the reaction diffusion, can not simulate whether or not formed intermediate phases and segregation. In addition, due to regardless of alloying elements mutual influence caused the change of diffusion coefficient and induced diffusion by the temperature gradient in cooling process, the simulation data further away from the Be/SS bonding interface are larger differences with the experimental results.
Effect of Heating Temperature on the Diffusion Bonding

Based on the effect of instrument error and different elements mutual interference, the distance of diffusing spread to the other side with 10% concentration is used as the width of diffusion layer in the diffusion couple of Be and SS. The experimental curves and simulation curves of Be and Fe near the Be/SS bonding interface are shown in Figure 3 and Figure 4 under 1323K/60MPa/7200s and 1023K/60MPa/7200s, respectively, which the simulated and measured width of diffusion layer are respectively 280µm and 260µm at 1323K, and they are respectively 109µm and 115µm at 1023K, so the width of diffusion layer at 1323K is about 2.5 times the one at 1023K. The higher the heating temperature, the faster the diffusion and the better the bonding joint strength, but recrystallization and phase transformation may take place at high heating temperature, which leads grain growth and composition segregation and strength decline in the bonding joint.

Effect of Holding Time on the Diffusion Bonding

The simulation distribution curves of Be and Fe near the Be/SS bonding interface are shown in Figure 5 and Figure 4, which the widths of diffusion layer are 55µm, 84µm, 102µm and 109µm under 1023K/60MPa/1800s, 1023K/60MPa/3600s, 1023K/60MPa/5400s and 1023K/60MPa/7200s, respectively. The simulation curve between the width of diffusion layer and the holding time is shown in Figure 6, which as the extension of holding time, the width of diffusion layer initially increase in a high speed and then it increase in a low speed. The simulation curve between the width of diffusion layer of Be and Fe (x/µm) and holding time (t/s) follows equation 3 under 1023K/60MPa. Appropriate to extend holding time is benefit to the microstructure and composition uniformity and improve performance in the bonding joint. But diffusion bonding temperature is
generally above recrystallization temperature, and may lead grain growth in longer holding time, especially the holding time should be controlled for the joints on possible forming brittle intermetallic compounds which reduce the joint performance.

\[ x = 10t^3 - 60.571t^2 + 135.64t + 0.2143 \quad 0 \leq t \leq 7200s \]  

\[ x = 1.5 \times 10^{-2} p^2 + 2.8275p - 0.1575 \quad 0 \leq p \leq 60 \text{ Mpa} \]

**Effect of Diffusion Pressure on the Diffusion Bonding**

Determination of Be and Fe distribution curves near the Be/SS bonding interface by AES are shown in Figure 7 and Figure 4, which the widths of diffusion layer are 70µm, 90µm, 104µm and 115µm under 1023K/30MPa/7200s, 1023K/40MPa/7200s, 1023K/50MPa/7200s and 1023K/60MPa/7200K, respectively. The simulation curve and the experimental curve between the width of diffusion layer and the diffusion pressure are shown in Figure 8, which the experimental values are similar to the simulation results, and as the extension of diffusion pressure, the width of diffusion layer initially increases in a high speed and then it increases in a low speed. The relationship between the width of diffusion layer of Be and Fe(x/µm) and the diffusion pressure(p/MPa) follows equation 4 under1023/7200s. The pressure increasing can reduce the vacancy formed between the diffusion bonding interface, increase the bonding zone and improve diffusion speed. Base on the theory of metal physics, as the pressure further increasing, the vacancy may be closed or move to the surface, so the vacancy concentration decrease and the dislocation pile up, which reduce diffusion speed.

In fact, heating temperature, diffusion pressure and holding time mutually affect on the diffusion process. In order to achieve the same width of diffusion layer, increased diffusion pressure may decrease heating temperature or holding time, such as the width of diffusion layer under 1023K/60MPa/5400s(See Figure 6) and 1023K/50MPa/7200s(See Figure 8) are respectively 102µm and 104µm.
Figure 8. The relationship between diffusion distance and diffusion pressure (1023K/7200s).

**Conclusion**

1) The simulation distributions of Be and Fe near the Be/SS bonding interface are basically consistent with the values measured by AES under 1323K/60MPa/7200s and 1023K/60MPa/7200s, and the widths of simulation diffusion layer fit well with the experimental values. The width of diffusion layer at 1323K is about 2.5 times the one at 1023K.

2) The widths of simulation diffusion layer are similar to the test data under 1023K/30MPa/7200s, 1023K/40MPa/7200s, 1023K/50MPa/7200s and 1023K/60MPa/7200s, and the relationship between the width of diffusion layer of Be and Fe (x/µm) and the diffusion pressure (p/MPa) is the following equation.

\[ x = 1.5 \times 10^{-2} p^2 + 2.8275p - 0.1575 \quad 0 \leq p \leq 60 \text{ MPa} \]

3) The simulation curve between the width of diffusion layer of Be and Fe (x/µm) and the holding time (t/s) is following equation under 1023K/7200s.

\[ x = 10t^3 - 60.571t^2 + 135.64t + 0.2143 \quad 0 \leq t \leq 7200\text{s} \]

**References**