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# Diffusivity of Al and Fe near the diffusion bonding interface of $Fe_3Al$ with low carbon steel

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**Abstract.** **The distribution of elements near the $Fe_3Al$/Q235 diffusion bonding interface was computed by the diffusion equation as well as measured by means of EPMA. The results indicated close agreement between the two for iron and aluminium. Diffusion coefficient in the interface transition zone is larger than that in the $Fe_3Al$ and Q235 steel at the same temperature, which is favourable to elemental diffusion. The diffusion distance near the $Fe_3Al$/Q235 interface increased with increasing heating temperature, *T*, and the holding time, *t*. The relation between the width of the interface transition zone, *x*, and the holding time, *t*, conformed to parabolic growth law: $x^2 = 4{\cdot}8 \times 10^4 \exp(-133/RT)(t - t_0)$. The width of the interface transition zone does not increase significantly for holding times beyond 60 min.**

**Keywords.** **$Fe_3Al$; intermetallic; diffusion bonding; interface; diffusion.**

## 1. Introduction

$Fe_3Al$ intermetallic has high resistance to high temperature, abrasion and corrosion. It is likely to be a new high temperature structural material and has attracted close attention of many researchers (David *et al* 1989, 1993; Mckamey *et al* 1991). It has wide prospects in application if $Fe_3Al$ and carbon steel could be welded firmly by advanced diffusion bonding technology. The full diffusion of elements near the interface is critical to realize diffusion bonding of the dissimilar materials. In recent years, researchers have made some studies on elemental diffusion behaviour during bonding and have set theoretical model for diffusion bonding (Derby *et al* 1982). On the basis of the model, elemental diffusion equation near the TiAl/40Cr diffusion bonding interface has been set (He *et al* 2002). But up to now, atom diffusion behaviour near the $Fe_3Al$/Q235 interface is not reported.

The element diffusion coefficient in the interface transition zone is a dynamic value during diffusion bonding. Different microstructures in the interface transition zone for $Fe_3Al$/Q235 dissimilar materials are formed because of the difference in element concentration. In the present paper, based on Fick's second Law related to non-steady state diffusion, the interface initial and boundary conditions are determined to study the element diffusion behaviour near the $Fe_3Al$/Q235 interface by numerical analysis method. The computed result is compared with the element distribution measured by means of EPMA to understand the effect of technology parameters. The paper provides theoretical and experimental basis for studying diffusion behaviour near the interface.

## 2. Method

The materials used in the test are $Fe_3Al$ intermetallic and Q235 low carbon steel. $Fe_3Al$ was melted by the vacuum induction furnace and then fabricated into plate by the hot rolled technology, whose chemical compositions and the properties are shown in table 1. The chemical compositions and the properties of Q235 steel are (%): C 0·17, Mn 0·48, Si 0·28, S 0·018, P 0·020, yield strength, 225 MPa, elongation, 20%.

A mathematical model of element diffusion is set up for the case of diffusion bonding. A program is formulated to calculate the element distribution near the $Fe_3Al$/Q235 interface. The $Fe_3Al$/Q235 diffusion joints are obtained by vacuum diffusion bonding employing different technological parameters. Some specimens, including $Fe_3Al$/Q235 diffusion interface, are cut out by means of a line-cutting machine for metallographic observation. The distribution of Al and Fe near $Fe_3Al$/Q235 interface is measured by means of EPMA. The calculated value is compared with the measured value to analyse the effect of technological parameters on element diffusion behaviour near the $Fe_3Al$/Q235 interface.

## 3. Results and analysis

### 3.1 *Diffusion bonding technology of $Fe_3Al$/Q235 dissimilar materials*

The $Fe_3Al$ and Q235 steel plate are overlapped to be joined by the vacuum diffusion bonding. Oxide film on the sur-

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face of workpiece is removed by mechanical and chemical methods. Workhorse-II vacuum diffusion bonding equipment is used with a heat power, 45 kW. Other parameters of diffusion bonding are: temperature, $T = 960 \sim 1080$°C, holding time, $t = 15 \sim 60$ min, pressure, $P = 10 \sim 17{\cdot}5$ MPa and vacuum, $5 \times 10^{-4}$ Pa. The assemblage and location of diffusion bonding samples in the vacuum chamber are shown in figure 1.

A good diffusion interface cannot be formed if the heating temperature is too low, since extent of diffusion is not sufficient even though the holding time is longer and the pressure is larger. But if the heating temperature is too high, the grains will grow up seriously and the diffusion transition zone can become wider, which will adversely affect the performance of the diffusion bonding joint. The test results indicated that the heating temperature should not be lower than 1000°C in order to ensure the interface combination. A schematic of the relationship between different variables during the $Fe_3Al$/Q235 diffusion bonding is shown in figure 2.

The diffusion of Al atom near the $Fe_3Al$/Q235 interface is determined by the heating temperature and holding time. When the holding time is short, the atoms do not have enough time to diffuse and the bonding is weak. Satisfactory $Fe_3Al$/Q235 diffusion bonding joint can be obtained even for a holding time of 30 min if the temperature, $T = 1040$°C. But the grains become coarser if the holding time is too long. The test results indicated that the holding time should be < 60 min to obtain an excellent diffusion bonding joint.

Since $Fe_3Al$ and Q235 steel differ greatly in physical performance, too large a pressure will lead to the deformation of $Fe_3Al$ base material. The test results indicated that the pressure should be < 17·5 MPa during diffusion bonding of $Fe_3Al$/Q235 dissimilar materials in order to prevent the deformation of weldment.

**Table 1.** Chemical composition and thermo-physical properties of $Fe_3Al$ intermetallic.

| Chemical compositions (%) | | | | | | |
|---|---|---|---|---|---|---|
| Fe | Al | Cr | Nb | Zr | B | Ce |
| 80·2 | 15·71 | 0·92 | 1·93 | 0·28 | 0·09 | 0·15 |

Some properties of $Fe_3Al$

| Structure | Order critical temperature (°C) | Young's modulus (GPa) | Melting point (°C) | Coefficient of thermal expansion ($10^{-6}\cdot K^{-1}$) | Density ($g\cdot cm^{-3}$) | Tensile strength (MPa) | Elongation (%) | Hardness (HRC) |
|---|---|---|---|---|---|---|---|---|
| $DO_3$ | 540 | 140 | 1540 | 11·5 | 6·72 | 455 | 2 | 29 |

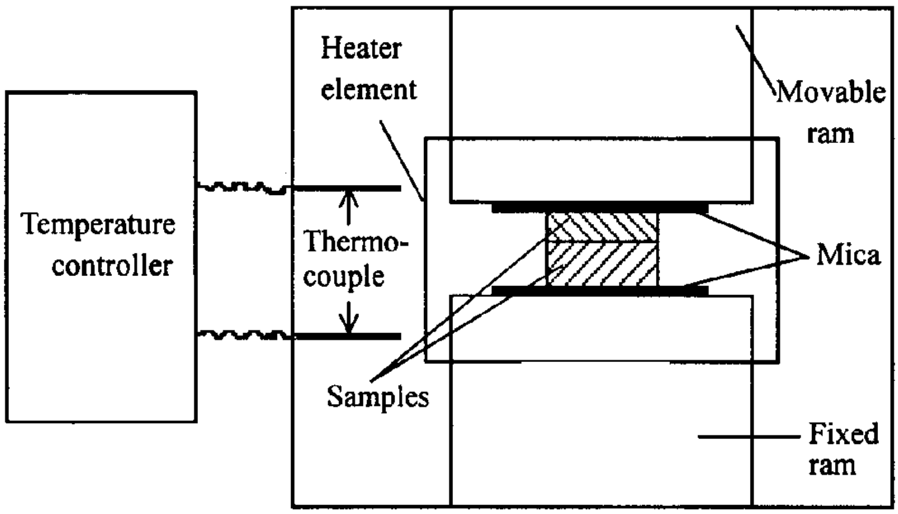


**Figure 1.** Assemblage and location of diffusion bonding samples in the vacuum chamber.

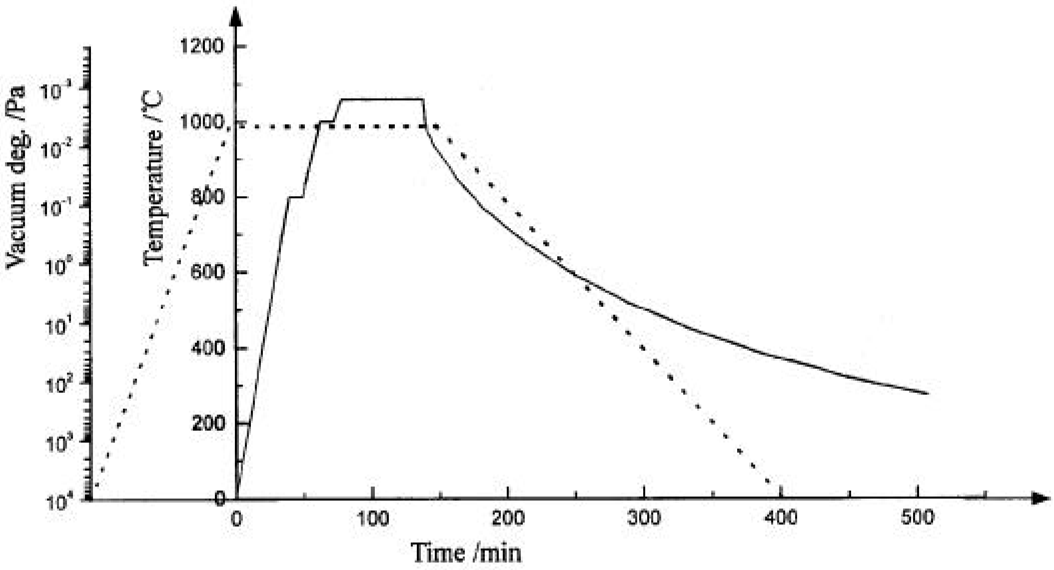


**Figure 2.** The technological parameter during the diffusion bonding of $Fe_3Al$/Q235 dissimilar materials.

**Table 2.** Diffusion factor ($D_0$) and activity energy ($Q$) of elements in $Fe_3Al$ and Q235 steel.

| | $Fe_3Al$ alloy | | Q235 steel | |
|---|---|---|---|---|
| Parameters | Al | Fe | Al | Fe |
| $D_0$ ($10^6$ $\mu m^2 \cdot s^{-1}$) | 1·7 | 4 | 170 | 200 |
| $Q$ ($kJ \cdot mol^{-1}$) | 211·1 | 166·4 | 142 | 239 |

### 3.2 *Numerical analysis of diffusion of element near the interface*

The elements diffuse across $Fe_3Al$/Q235 interface which can be calculated by the diffusion equation. Suppose an element has an initial concentration in $Fe_3Al$ intermetallic and Q235 steel of $C_1$ and $C_2$, respectively, the element distribution near the $Fe_3Al$/Q235 interface obeys non-steady state diffusion equation of Fick's second Law (Huang 1996):

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}. \quad (1)$$

The element concentration equation near the $Fe_3Al$/Q235 interface is obtained according to the initial condition, $C(x, 0) = C_1(x < 0)$, $C_2(x > 0)$; and boundary condition, $C(x, t) = C_1(x = -\infty)$, $C_2(x = +\infty)$. Owing to the larger difference of element diffusion coefficient in the $Fe_3Al$ and Q235 steel, boundary condition is set up as

$$D_1\frac{\partial C_A(x=0,t)}{\partial x} = D_2\frac{\partial C_B(x=0,t)}{\partial x}. \quad (2)$$

The element concentration equation near the diffusion bonding interface is obtained as

$$C(x,t) = \begin{cases} C_A(x,t) = \dfrac{C_1+C_2}{2} + \dfrac{\sqrt{D_2}(C_1-C_2)}{\sqrt{p}(\sqrt{D_1}+\sqrt{D_2})} \left[\displaystyle\int_0^{n_1} \exp(-h_1^2)\,dh_1\right] (x<0) \\ C_B(x,t) = \dfrac{C_1+C_2}{2} + \dfrac{\sqrt{D_1 D_2}(C_1-C_2)}{\sqrt{p}(D_2+\sqrt{D_1 D_2})} \left[\displaystyle\int_0^{n_2} \exp(-h_2^2)\,dh_2\right] (x>0). \end{cases} \quad (3)$$

According to the error function,

$$erf(Z) = \frac{2}{\sqrt{p}}\int_0^Z \exp(-h^2)\,dh,$$

the error function solution of (3) is

$$C(x,t) = \begin{cases} C_A(x,t) = \dfrac{C_1+C_2}{2} + \dfrac{\sqrt{D_2}(C_1-C_2)}{\sqrt{p}(\sqrt{D_1}+\sqrt{D_2})}\, erf\left(\dfrac{x}{4D_1 t}\right) (x<0). \\ C_B(x,t) = \dfrac{C_1+C_2}{2} + \dfrac{\sqrt{D_1 D_2}(C_1-C_2)}{\sqrt{p}(D_2+\sqrt{D_1 D_2})}\, erf\left(\dfrac{x}{4D_2 t}\right) (x>0). \end{cases} \quad (4)$$

Equation (4) is the relation between element concentration, diffusion distance, *x*, and holding time, *t*, near the $Fe_3Al$/Q235 interface. The most important parameter in the calculation is diffusion coefficient, *D* (including diffusion factor, $D_0$ and activity energy, *Q*). The element concentration on two besides the interface was measured by means of EPMA. The element diffusion coefficient was calculated by diffusion factor, $D_0$ and activity energy, *Q*, measured by means of radioactive isotope tracer method. The values of $D_0$ and *Q* of the elements in $Fe_3Al$ alloy and Q235 steel are shown in table 2.

According to the Arrhenius equation, $D = D_0 \exp(-Q/RT)$, the program is edited to calculate the diffusion coefficient, *D*, of Al, Fe elements at different temperatures in $Fe_3Al$ alloy, and the results are shown in figure 3.

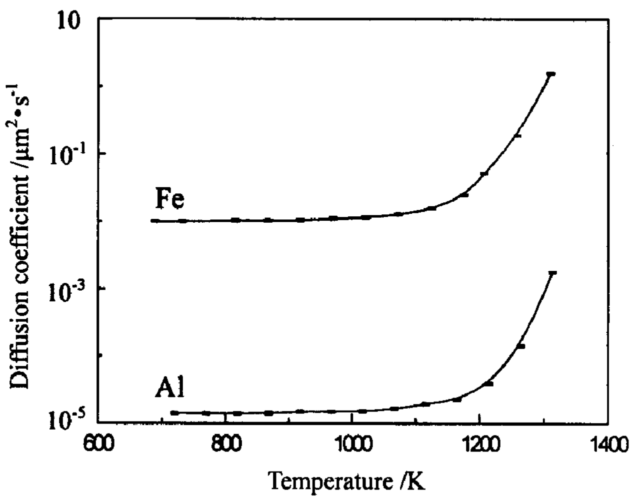


**Figure 3.** Variation of diffusion coefficient with temperature in $Fe_3Al$ alloy.

For a heating temperature, $T = 1060°C$ and holding time, $t = 45$ min, concentration distribution of Al and Fe near the $Fe_3Al$/Q235 interface is shown in figure 4. The calculated values of concentration agree with the measured values. However, the calculated values cannot reflect fluctuations in element concentration. There was element segregation near the interface. The relation between the diffusion distance and square root of holding time near the $Fe_3Al$/Q235 interface at different temperatures is shown in figure 5.

According to figure 5, the relation between the diffusion distance, *x* and holding time, *t*, near the $Fe_3Al$/Q235 interface during the diffusion bonding satisfies following parabolic law

$$x^2 = K_p(t - t_0), \tag{5}$$

in which *x*, diffusion distance, μm; $K_p$, diffusion rate, $\mu m^2/s$; *t*, holding time, s; $t_0$, latent time, s.

Element diffusion rate is accelerated with increasing temperature, as seen from increase in the slope plots in figure 5 with temperature.

### 3.3 *Width of $Fe_3Al$/Q235 interface transition zone*

There is an obvious interface transition zone near the $Fe_3Al$/Q235 interface. The width of this interface transition zone increases with holding time. The calculated diffusion coefficients of Al and Fe in the $Fe_3Al$/Q235 diffusion transition zone for different heating tempera-

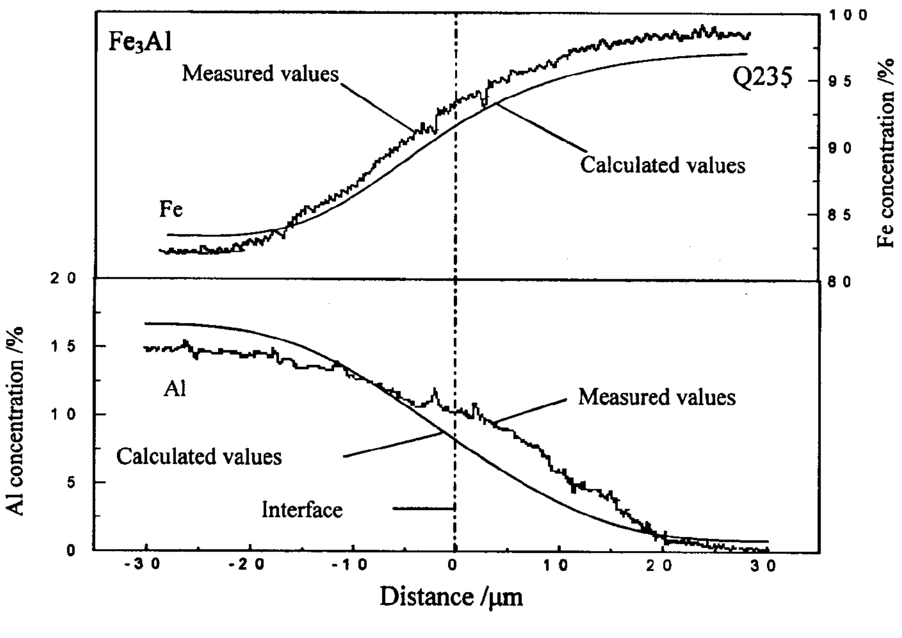


**Figure 4.** Element concentration distribution near the $Fe_3Al$/Q235 diffusion interface.

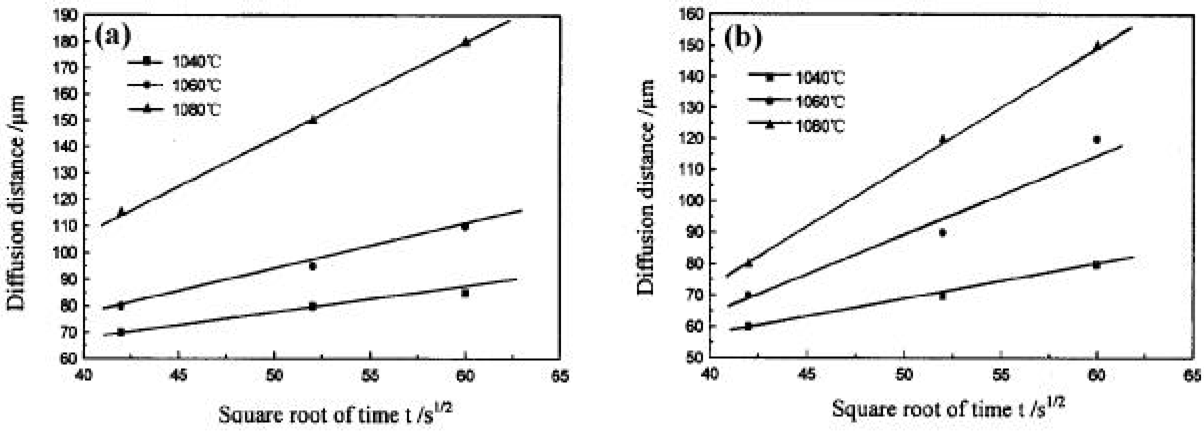


**Figure 5.** Relation between diffusion distance and square root of holding time near the $Fe_3Al$/Q235 interface: (**a**) Al and (**b**) Fe.

**Table 3.** Diffusion coefficients of Al and Fe in the $Fe_3Al$/Q235 diffusion transition zone.

| Temperature (°C) | | 1040 (1313 K) | 1060 (1333 K) | 1080 (1353 K) |
|---|---|---|---|---|
| $D$ ($\mu m^2 \cdot s^{-1}$) | Al | 0·51 | 1·91 | 3·80 |
| | Fe | 0·72 | 1·15 | 2·05 |
| ln ($D$ $\mu m^2 \cdot s^{-1}$) | Al | – 0·67 | 0·69 | 1·29 |
| | Fe | – 0·27 | 0·14 | 0·72 |

tures are shown in table 3. The variation of diffusion coefficients with temperature near the $Fe_3Al$/Q235 interface is shown in figure 6.

From the plots in figure 6, the following are estimated: $Q_{Al}$ = 133 kJ/mol, $Q_{Fe}$ = 103·9 kJ/mol, $D_{0(Al)} = 10^6 \times 23{\cdot}2\ \mu m^2/s$, $D_{0(Fe)} = 10^6 \times 8{\cdot}4\ \mu m^2/s$.

For the same heating temperature, the diffusion coefficient in the interface transition zone is larger than that in $Fe_3Al$ alloy and Q235 steel, and increases rapidly with the heating temperature, which is favourable to element diffusion near the $Fe_3Al$/Q235 interface.

The width of the diffusion transition zone is represented using the maximum diffusion distance of Al element near the interface. The calculation indicated that the approximate width of $Fe_3Al$/Q235 diffusion transition is given by:

$$x^2 = 4{\cdot}8 \times 10^4 \exp\left(-\frac{133}{RT}\right)(t - t_0)\,. \qquad (6)$$

The measured values of the width of the diffusion transition zone, for different heating temperatures ($T$ = 1020 ~ 1080°C) and holding times ($t$ = 30 ~ 80 min), are shown in figure 7.

As noted earlier, the width of the diffusion transition zone, $x$, increases gradually with increasing heating temperature, $T$ and holding time, $t$. However, the increase is small beyond 60 min. The calculated value ($x$ = 30·1 μm) of the width of $Fe_3Al$/Q235 diffusion transition zone from (6) is compared with the EPMA measured value ($x$ = 28·6 μm) under the condition of 1060°C × 60 min diffusion bonding. There is a good agreement between the two values.

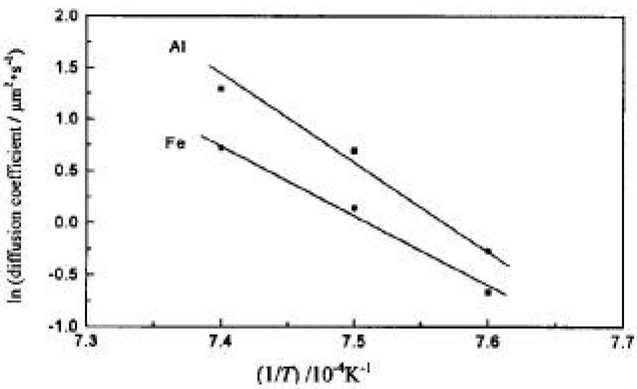


**Figure 6.** Relation of diffusion coefficients and temperature near the $Fe_3Al$/Q235 diffusion interface.

Diffusion transition zone with a certain width is required for best performance of the $Fe_3Al$/Q235 joints. There exists a certain latent time, $t_0$, for the formation of $Fe_3Al$/Q235 diffusion transition zone. This time, $t_0$, becomes shorter with increasing heating temperature, $T$. Therefore, holding time, $t$, should be controlled properly

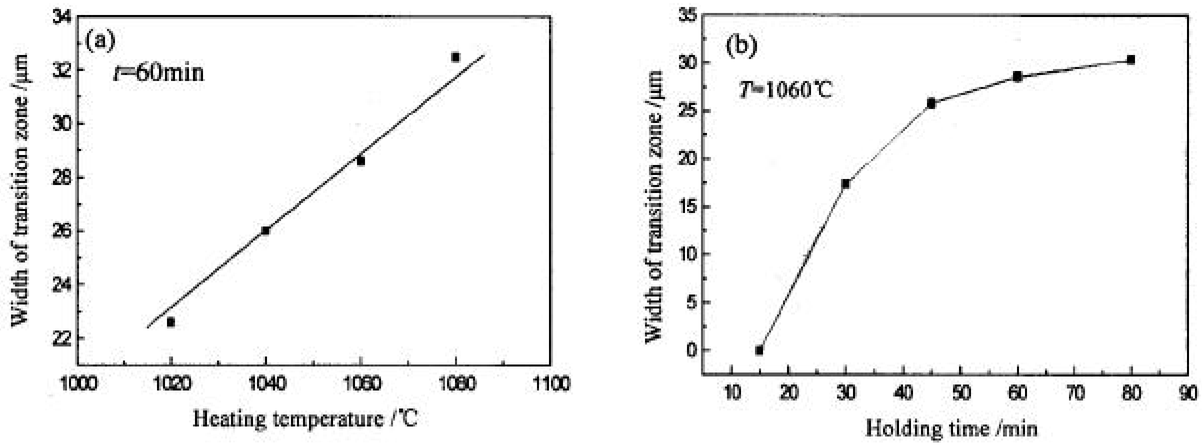


**Figure 7.** Effect of (**a**) heating temperature and (**b**) holding time on width of the diffusion transition zone.

at a given heating temperature, *T*, to obtain the desired optimum width of the transition zone.

## 4. Conclusions

(I) The calculated values of concentration of Al, Fe near the $Fe_3Al$/Q235 interface conform to the experimental values obtained by EPMA. With increasing heating temperature, *T* and holding time, *t*, diffusion distance of the elements in the diffusion transition zone for $Fe_3Al$/Q235 dissimilar materials increases.

(II) Diffusion coefficient of Fe and Al in the $Fe_3Al$/Q235 interface transition zone is larger than that in $Fe_3Al$ and Q235 base materials at the same temperature. The microstructure near the $Fe_3Al$/Q235 interface is favourable for diffusion.

(III) There exists a latent time, $t_0$, for the formation of diffusion transition zone near the $Fe_3Al$/Q235 interface. The relation between the width of transition zone, *x*, and holding time, *t*, follows a parabolic growth law.

(IV) Activation energy for diffusion of Fe and Al has been estimated.

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