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# Dynamic simulation of solid-state diffusion bonding

G.Q. Wu*, Z.F. Li, G.X. Luo, H.Y. Li, Z. Huang

*School of Material Science and Engineering, Beijing University of Aeronautics and Astronautics,*
*37 Xueyuan Road, Haidian District, Beijing 100083, PR China*

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## Abstract

By using the real information of the intended bonding surface and considering the effect of the diffusion distance in a definite time, a new theoretical model for diffusion bonding was proposed. The effects of different operating mechanisms, bonding parameters and microstructures on bonding were investigated. The simulation results indicate that, it is vital to consider the real information of the intended bonding surfaces and the effect of diffusion distance in a definite time; the metastable microstructure and the stable ultrafine microstructure exhibit better bonding characteristic than that of the original stable microstructure, which is in agreement with experimental results.

*Keywords:* Diffusion bonding; Modeling; Diffusion; Surface; Microstructure

## 1. Introduction

Diffusion bonding process has an important influence on the design and manufacture of workpieces, since it is of great advantage to bond similar or dissimilar materials. However, process conditions are often chosen by trial and error for there are so many control factors. Therefore, the simulation of the bonding process, to predict the extent of bonding when bonding different materials at given bonding temperatures, bonding pressures and bonding times, has been a focus of researches [1–6]. Derby and Hill [4–6] proposed a fully comprehensive quantitative model, in which seven mechanisms that operate in pressure sintering were considered in diffusion bonding. To predict the bonding process precisely, the actual information of roughness of the intended bonding surfaces and the kinetic conditions of operating mechanisms in diffusion bonding should be considered.

In this paper, basing on Derby and Hill's model, a new theoretical model containing the information of actual roughness of the intended bonding surfaces and the effect of the diffusion distance in a definite time was proposed. According to the characteristics of different microstructures, the effects of different microstructures, i.e. the original stable microstructure, the metastable microstructure formed by laser surface melting and the stable ultrafine microstructure formed by laser surface melting and pre-bond heat treatment, on bonding were investigated primarily.

## 2. Modeling of voids shrinkage

This new model considers the operating mechanisms during bonding as well as Derby and Hill's models [4–6], the differences between the present method and Derby and Hill's methods are described below.

### 2.1. Application of the real rough surface in diffusion bonding

The representative surface topography of the intended bonding surface used in this paper is shown in Fig. 1. The attended bonding samples were ground with SiC-paper down to 1200, 800, 320 grits, respectively, and finally cleaned by degreasing in acetone in an ultrasonic bath for 10 min. The surface roughness information was measured and collected by a surface topography measuring system in which a Talysurf 5P-120 surface topographyer was used. The least uprightness-distinguishing rate is 10 nm.

Because a real rough surface is used, it can be assumed that a linear relationship lies between the real contacting area and the

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* Corresponding author. Tel.: +86 10 82313240; fax: +86 10 82313240.
*E-mail address:* guoqingwu@buaa.edu.cn (G.Q. Wu).

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**Nomenclature**

| | |
|---|---|
| $c$ | major semi-axis of ellipse |
| $d$ | radius of curvature of the point of the longest length of surface diffusion in a definite time $t$ |
| $D_s$ | surface activation energy |
| $h$ | height of unit cell, equivalent to minor semi-axis of ellipse |
| $k$ | Boltzmann's constant |
| $P_{\text{eff}}$ | contacting pressure in the stage of plastic yielding deformation |
| $r_c$ | radius of curvature on major semi-axis |
| $t$ | bonding time |
| $T$ | bonding temperature |
| $\dot{V}_1$ | rate of change of a volume with respect to time contributed by surface diffusion mechanism |
| $W$ | the longest length of spread of surface diffusion in a definite time of $t$ |

*Greek symbols*

| | |
|---|---|
| $\beta$ | coefficient |
| $\gamma_s$ | surface energy |
| $\delta$ | diffusion layer thickness |
| $\delta_s$ | surface layer thickness |
| $\theta$ | equivalent circle angle |
| $\sigma_y$ | the yield strength of the material at bonding temperatures |
| $\Omega$ | atomic volume |

load according to the principle of solid tribology [7], and so the plastic flow occurs [8,9] when

$$P_{\text{eff}} > \beta\sigma_y \tag{1}$$

where $\sigma_y$ is the yield strength of the material at bonding temperature, and β is a coefficient. The plastic yielding deformation occurs instantaneously, and thus not allowing the time-dependent diffusion or creep to take place. At a given bonding temperature and bonding pressure, after plastic contact, irregular bonding voids and discontinuous bonding lines are formed at the bonding interface (Fig. 2). To be convenient for simulation, the irregular voids are transformed into elliptical voids by keeping the volumes of voids constant (Fig. 3).

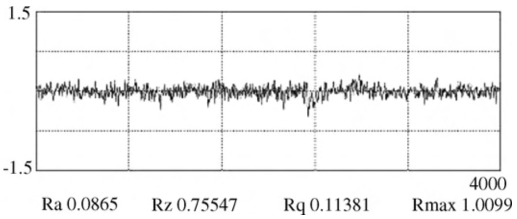


Fig. 1. Representative surface topography of the intended bonding surface ground with SiC-paper down to 1200 grit.

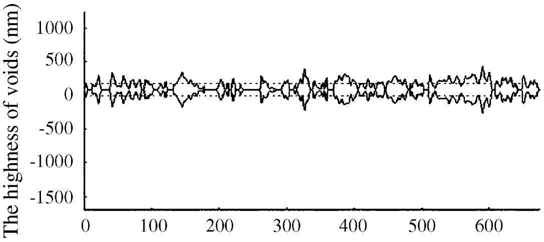


Fig. 2. Simulation result of contacting surface with irregular voids and discontinuous bonding lines after plastic yielding deformation.

### 2.2. *Effect of the time limit of diffusion distance during diffusion bonding*

The driving force of surface diffusion comes from the differences in surface free energy. Once there is a difference in surface curvature, mass is transferred along the surface to make the surface curvature consistent. Hill et al. assumed the driving force to be the difference in maximum and minimum radii of curvature of the ellipse, which overestimates the effect of the surface source mechanisms. The simulation results show that most voids cease in a very short time and the voids left are too large compared to the original voids, which is inconsistent with the experimental results (Fig. 4(a)) [1–3,10]. In fact, the surface diffusion (mass transference) should have a distance limit in a definite time. Mullins gives an equation to calculate the length of spread of surface diffusion in a definite time of $t$ [11]:

$$W = 0.46\left(\frac{D_s\delta\gamma_s\Omega}{kT}t\right)^{1/4} \tag{2}$$

The term $W$ becomes smaller and smaller with reduction of the time of $t$, and hence it can be assumed that the length of the curve from point B of minimum radii of curvature to point A of the longest length of surface diffusion in a definite time of $t$ is approximately equal to $W/2$, and the radii of curvature of the point A can be calculated (Fig. 5):

$$d = \frac{(c^2\sin^2\theta + h^2\cos^2\theta)^{3/2}}{ch} \tag{3}$$

Therefore, the driving force should be the difference in the radii of curvature of points B and A, and a new reduction factor $(1/r_c - 1/d)$ is given. Hence the equation for surface diffusion

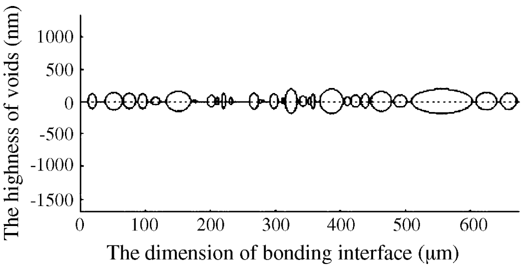
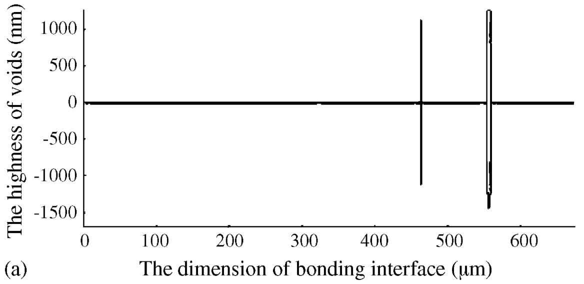


Fig. 3. Simulation result of contacting surface with elliptical voids.



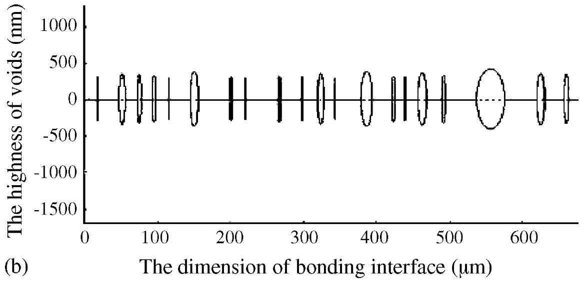


Fig. 4. Simulation result of diffusion bonding at the same conditions: (a) Hill's model and (b) model in this paper.

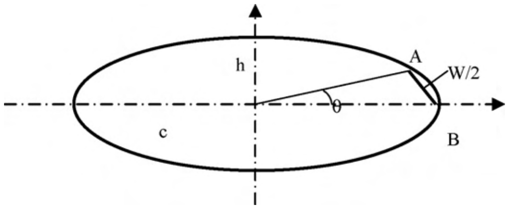


Fig. 5. Schematic diagram of the mass transference along the surface.

mechanism from a surface source to a neck now becomes:

$$\dot{V}_1 = \frac{2\Omega\delta_s D_s \gamma_s}{r_c kT}\left(\frac{1}{r_c} - \frac{1}{d}\right) \quad (4)$$

where

$$r_c = \frac{h^2}{c} \quad (5)$$

The equations of mechanism of volume diffusion from a surface source to a neck should also be changed correspondingly. Fig. 4(b) shows the simulation result of diffusion bonding in this model at the same conditions as in Hill's model, it can be seen that it shows more agreement to the experimental results from the phenomena of voids closure.

## 3. Results and discussion

### 3.1. Effects of bonding conditions

The bonding conditions, including the bonding surface roughness, bonding time, bonding temperature and bonding pressure, act as four important control factors in influencing the bonding characteristic in diffusion bonding, and the effects of these four parameters on the bonding quality are discussed, respectively, below.

The effect of actual surface roughness on the rate of bonding process gives in Fig. 6. The result shows that, the time needed for voids closure increases with the increasing degree of surface roughness, and represents a trend of accelerated growth in curve (Fig. 6(a)). From the function of operating mechanisms, it can be seen that, there is a gradual increase in the contribution to voids closure from creep deformation mechanisms with the increase of the degree of surface roughness. In this case, the contribution from the surface source mechanisms is gradually decreasing and the interface source mechanisms shows relatively smaller contribution increases first and decreases afterwards, to the voids closure, as shown in Fig. 6(b). The analysis of above simulation results reveal that a rough surface can severely decrease the rate of voids closure, and the heights of the voids formed after contacting will be lower as less rough surfaces are used, which is of great contributive to realizing the diffusion bonding.

Fig. 7 displays the contributions from the operating mechanisms to voids closure with the variations in bonding time. The result shows that, the contribution from surface source mechanisms is dominant in the initial stage of bonding, which hence tends to change the voids from elliptical to circular cross-section.

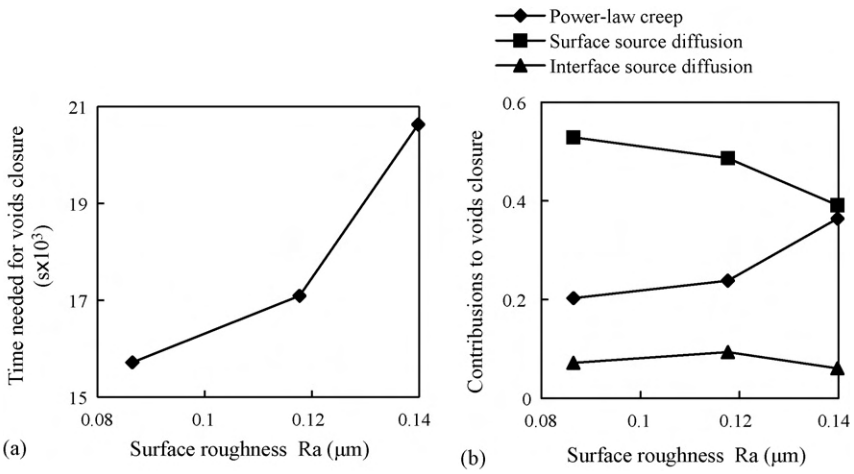


Fig. 6. Prediction of the model showing (a) effects of surface roughness on the voids closure and (b) contributions from each operating mechanisms to the voids closure with the variations in surface roughness (bonding at 900 °C under a pressure of 30 MPa).

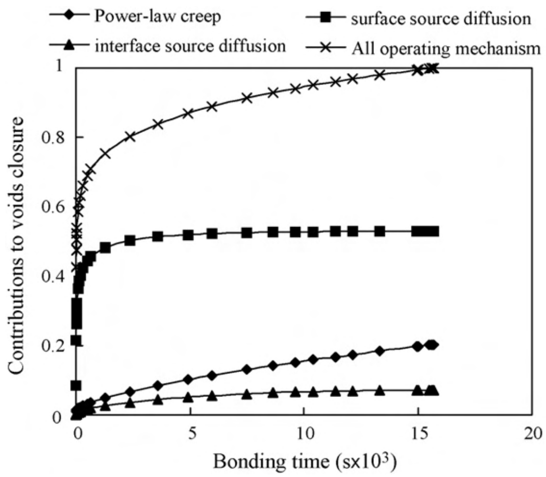


Fig. 7. Variations in the contributions from each operating mechanisms with the change of the bonding time.

After unity of the aspect ratios of the voids, the creep deformation mechanisms and interface source mechanisms act as two dominant manners to the voids elimination.

When bonding in the conditions of given bonding pressure of 30 MPa and initially actual surface roughness ground with SiC-paper down to 1200 grit, a detailed investigation of the effects of bonding temperatures on bonding quality are shown in Fig. 8. The results illustrate that the bonding time lasted for the voids elimination can be apparently shorten with the elevation of bonding temperature. At the bonding temperature of 700 °C, it takes 20 h to attain less than 80% of the rate of voids closure. However, compared to the previous bonding temperature, only 40 min is needed to achieve 80% of the rate of voids closure at the bonding temperature of 900 °C, and the voids are completely closed in 4 h, as indicated in Fig. 8(a). It also can be seen from Fig. 8(b) that, with the increase of bonding temperature, there is an increase contribution to the voids closure from the plastic deformation mechanisms, and the contribution from the creep deformation mechanisms and surface source mechanisms decrease relatively. By contrast with above three mechanisms, the contribution to the voids closure, which increases slightly with the elevation of bonding temperature, from interface source mechanisms is relatively low.

Besides the bonding temperature, the bonding pressure is considered as another key parameter in diffusion bonding. Fig. 9 graphically shows the influence of different bonding pressures on the bonding quality when bonding in the case of a fixed initial actual surface roughness and bonding temperature of 900 °C. The results show that the bonding time needed for the voids elimination is obviously shorten with the increase of bonding pressure. In the case of a bonding pressure of 20 MPa, more than 20 h is allowed to complete the voids closure, but the use of higher bonding pressure of 30 MPa allows to decrease bonding time to only a few more than 4 h for voids elimination. With the enhancement of bonding pressure, there is an increasing contribution to the voids closure from both the plastic deformation mechanisms and the creep deformation mechanisms, but slight decrease in the contribution from surface source mechanisms.

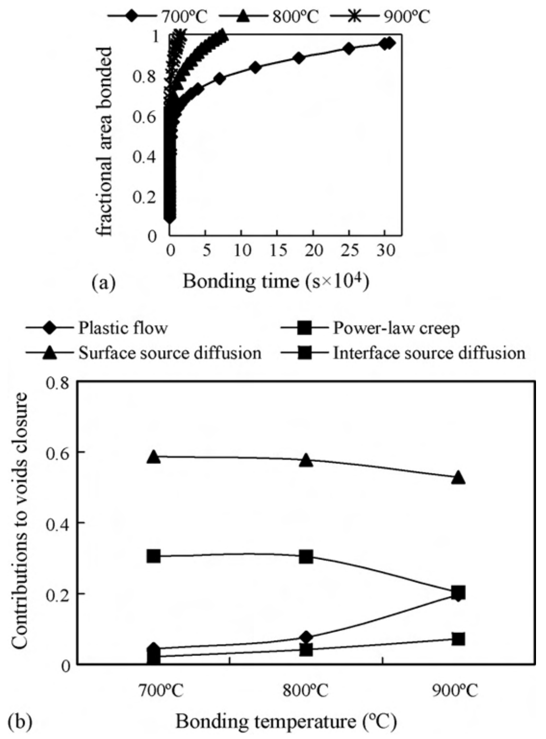


Fig. 8. Prediction of the model illustrating (a) effects of the bonding temperature on the voids closure and (b) contributions from all operating mechanisms to the voids closure with different bonding temperatures (bonding under a pressure of 30 MPa using a surface ground with SiC-paper down to 1200 grit).

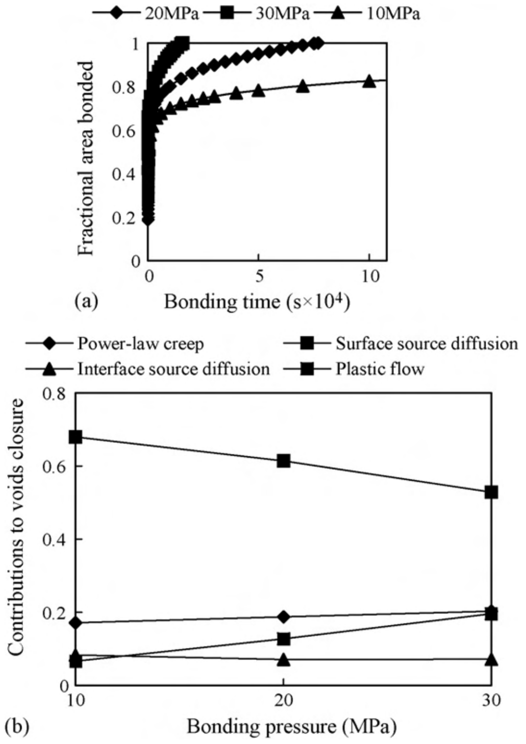


Fig. 9. Prediction of the model indicating (a) effects of the bonding pressure on the voids closure and (b) contributions from all operating mechanisms to the voids closure with different bonding pressures (bonding at 900 °C using a surface ground with SiC-paper down to 1200 grit).

### 3.2. Effects of different microstructures on diffusion bonding

Previous research [12] show that, the elevated temperature hardness of the microstructure formed by laser surface melting is lower than that of the stable microstructure after exceeding a particular value of bonding temperature which is consistent with the superplastic temperature of the microstructure formed by laser surface melting treatment. Therefore, in the condition of suitable bonding temperature, the elevated temperature hardness of the metastable microstructure obtained by laser surface melting treatment and the stable ultrafine microstructure formed by laser surface melting and pre-bond heat treatment will be lower than that of the original stable microstructure. To further investigate the effects of each individual operating mechanism on the voids closure by using prepared surfaces with above three typical microstructures, respectively, the materials data of Ti–6Al–4V alloy is adopted as fundamental materials parameters of the original stable microstructure in current model. According to the characteristic of the metastable microstructure and the stable ultrafine microstructure, the effects of above three typical microstructures on the voids closure are discussed by adjusting each relative materials parameter.

Fig. 10 shows the effect of diffusion ability of intended bonding materials on the voids closure. It can be seen from Fig. 10(a) that, in the case of a fixed initial surface roughness and bonding parameters, the rate of voids closure is accelerated as a result of the enhancement of diffusion ability within a particular range, and hence the bonding time for voids closure is apparently shorten. However, the diffusion ability, which is enhanced beyond a particular extent, shows slight contribution to the voids closure. Fig. 10(b) demonstrates the contribution from each operating mechanisms to the voids closure by using bonding materials with different diffusion ability. It can be seen that each individual mechanisms contributes slightly to the voids closure with the enhancement of diffusion ability. The results mentioned above show that, there is a significant contribution to the rate of voids closure from diffusion mechanisms, and the enhancement of diffusion ability, within a particular extent, will be helpful to accelerate the bonding process. In addition, although the creep deformation mechanisms show smaller contribution compared to that of diffusion mechanisms, its function in the diffusion bonding should not be ignored.

As the interfacial diffusion channels and the creep properties of bonding materials will change with the variations of grain size, the effect of grain size of intended bonding materials on the voids closure by using a fixed initial surface roughness and bonding process parameters is investigated, as shown in Fig. 11. The result reveals that, there is a significant increase in the contribution from grain boundary diffusion once the grain size is less than approximately 2 μm.

In the initial stage of bonding process, for the variations in quantity and size of voids will be induced as a result of the change of material hardness, the effect of variations in material hardness on the voids closure is shown in Fig. 12. The results indicate that, in the bonding conditions of given initial surface roughness and bonding process parameters, the process of voids closure is

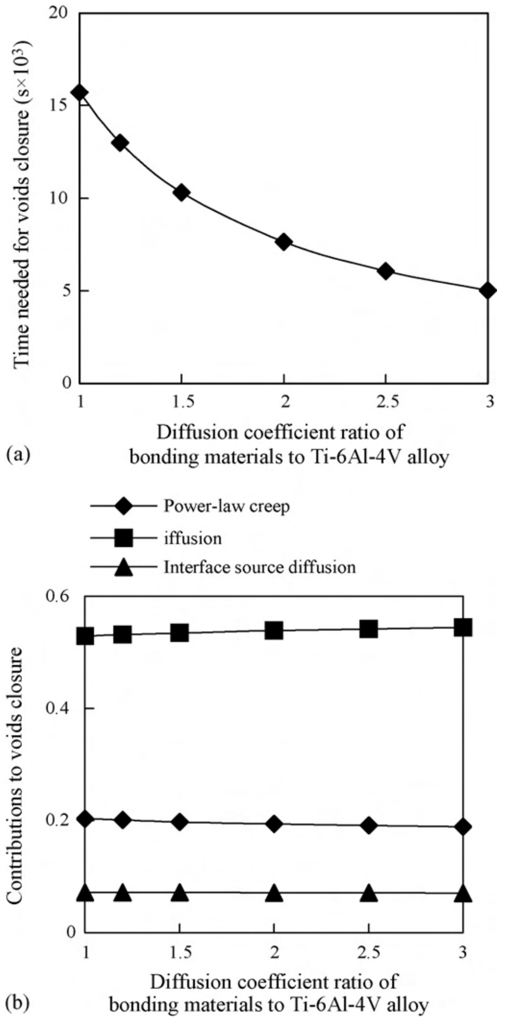


Fig. 10. Prediction of the model displaying (a) effects of the diffusion ability on the voids closure and (b) contributions from all operating mechanisms to the voids closure with different diffusion ability of the bonding materials (bonding at 900 °C under a pressure of 30 MPa using a surface ground with SiC-paper down to 1200 grit).

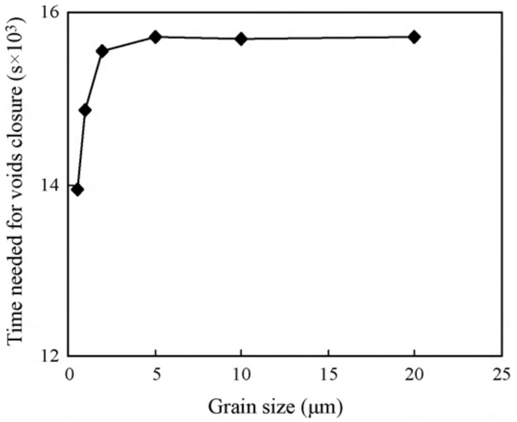


Fig. 11. Influences of the variations in grain size of the bonding materials on the voids closure (bonding at 900 °C under a pressure of 30 MPa using a surface roughness ground with SiC-paper down to 1200 grit).

Table 1
Data of three different microstructures presumed

| Control parameters | Microstructures | | |
|---|---|---|---|
| | Stable microstructure | Metastable microstructure | Stable ultrafine microstructure |
| Diffusion coefficient | Data of Ti–6Al–4V alloy | Two times of data of Ti–6Al–4V alloy | 1.5 times of data of Ti–6Al–4V alloy |
| Elevated temperature hardness | Data of Ti–6Al–4V alloy | 0.5 times of data of Ti–6Al–4V alloy | 0.5 times of data of Ti–6Al–4V alloy |
| Grain size | 20 μm | 5 μm | 0.5 μm |

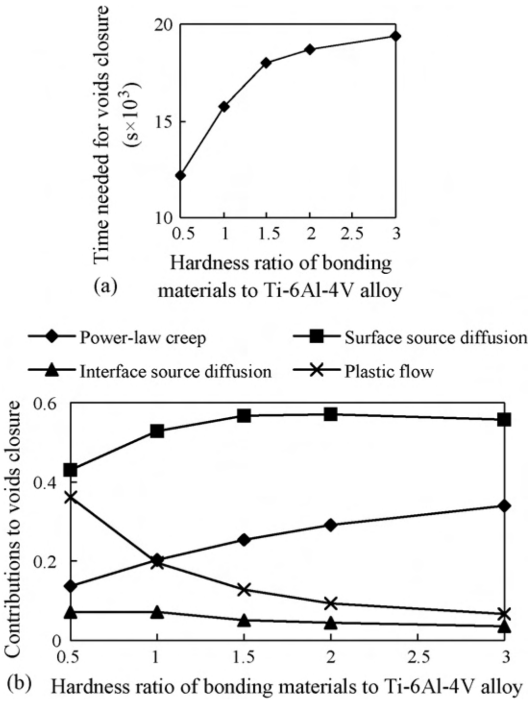


Fig. 12. Prediction of the model revealing (a) effects of material hardness on the voids closure and (b) contributions from each operating mechanisms to the voids closure with different hardness of the bonding materials (bonding at 900 °C under a pressure of 30 MPa using a surface *s* ground with SiC-paper down to 1200 grit).

slowed with the enhancement of materials hardness, and the contribution from each operating mechanisms is redistributed accordingly in the final stage of diffusion bonding.

According to the characteristics of different microstructures [12], the effect of different microstructures, i.e. the original stable microstructure, the metastable microstructure formed by laser surface melting and the stable ultrafine microstructure formed by laser surface melting and post-bond heat treatment, on bonding are investigated by presuming several control parameters (Table 1). The data of Ti–6Al–4V alloy [3] is used as the fundamental parameters of the stable microstructure of model material.

Table 2 gives the simulation result of bonding with different microstructures. For the samples with the metastable microstructure (e.g. the microstructure formed by laser surface melted treatment) and the stable ultrafine microstructure represent higher diffusion ability, smaller grain size and lower hardness at elevated temperature than the samples with the original stable microstructure [12], the former need less time of 5887 and 6990 s, respectively, to complete the voids closure than the later which needs a time of 15,711 s. The simulation result is in agreement with experimental results [13]. From the contribution of operating mechanisms to the voids closure, it can be seen that, the contribution from the plastic yielding deformation mechanisms increases greatly and those from the surface source mechanisms and the creep deformation mechanisms decrease relatively. Compared the effect of the metastable microstructure on the voids closure with that of the stable ultrafine microstructure, the samples with the metastable microstructure need a shorter time for the voids closure than that of the samples with the stable ultrafine microstructure, as shown in Fig. 13. In addition, due to the higher diffusion coefficient of the metastable microstructure than that of the stable ultrafine microstructure, surface source mechanisms play a key role for the voids closure in the initial stage of diffusion bonding, which accelerate the voids closure and hence shorten the bonding time.

Additionally, from the contributions of operating mechanisms of diffusion, it can be seen that, the interface source mechanisms operating in the samples with the stable ultrafine microstructure have larger contribution than that of the samples with the metastable microstructure for the former has a smaller grain-sized microstructure, which increase the channels for interface diffusion. The contributions from the surface source mechanisms and the creep deformation mechanisms are lower than those of the samples with the metastable microstructure correspondingly. The samples with metastable microstructure, though with a grain size which is an order of magnitude larger than that of the samples with stable ultrafine microstruc-

Table 2
Effects of different microstructures on times needed for the voids closure in bonding

| | Contributions from operating mechanisms on voids closure (%) | | | | Voids closure times (s) |
|---|---|---|---|---|---|
| | Creep | Surface diffusion | Interface diffusion | Plastic yielding deformation | |
| Stable microstructure | 20.3 | 52.9 | 7.2 | 19.6 | 15,711 |
| Metastable microstructure | 13.1 | 43.8 | 7.0 | 32 | 5,887 |
| Stable ultrafine microstructure | 11.6 | 42.9 | 9.5 | 32 | 6,990 |

Diffusion bonding at 900 °C under a pressure of 30 MPa, surface ground with SiC-paper down to 1200 grit.

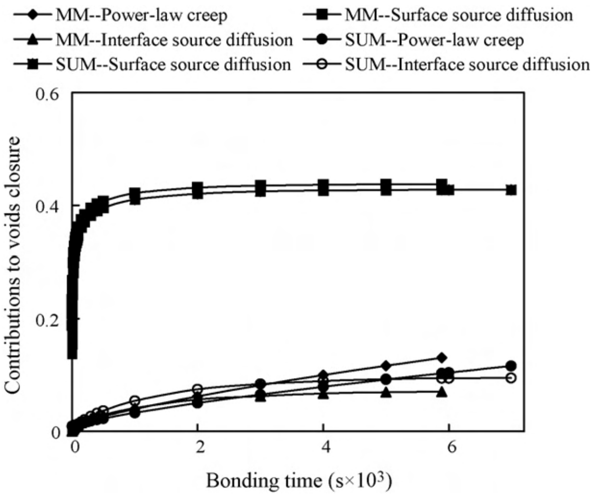


Fig. 13. Variations in the contribution from operating mechanisms to the voids closure with different bonding time by using the bonding samples with the metastable microstructure (MM) and the stable ultrafine microstructure (SUM) (bonding at 900 °C under a pressure of 30 MPa using a surface ground with SiC-paper down to 1200 grit).

ture, exhibit better bonds characteristic than the stable ultrafine microstructure for its higher diffusion ability.

## 4. Conclusions

By using the real information of the intended bonding surface and considering the effect of the diffusion distance in a definite time, a new theoretical model for diffusion bonding was proposed. The model, effectively reflecting the characteristics of the real bonding process, realizes the visualization and simulation of the bonding process in which many voids disappear dynamically.

The surface source mechanisms plays a key role in the voids closure in the initial stage of bonding, which leads to the change of voids from elliptical to circular cross-section, and after that, the power law creep mechanisms and the interface source mechanisms act as two dominant ways to the voids shrinkage and disappearance. With the increase of the surface roughness of the intended bonding materials, the time for bonding prolongs as expected and presents a trend of accelerated increase.

With the increase of bonding temperature or bonding pressure, the times for the voids elimination decrease greatly. With the elevation of bonding temperature, the contribution from the plastic yielding deformation mechanisms is larger than those from the creep deformation mechanisms and the surface source mechanisms. During the bonding process, the interface source mechanisms have a small contribution that increases lightly along with the elevation of bonding temperature. Compared with the contribution from the surface source mechanisms, there are lager contributions from both the plastic yielding deformation and the creep deformation mechanisms with the elevation of bonding pressures.

The metastable microstructure and the stable ultrafine microstructure could lead to the voids closure in much shorter bonding times than that of the original stable microstructure when bonding in the same bonding conditions, which is in agreement with experimental results. The samples with metastable microstructure, though with a grain size which is an order of magnitude larger than that of the samples with stable ultrafine microstructure, exhibit better bonds characteristic than that of the stable ultrafine microstructure for its higher diffusion ability.

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## References

[1] C.H. Hamilton, Titanium Science and Technology, vol. 1, Plenum, New York, 1973, p. 625.
[2] G. Garmong, N.E. Paton, A.S. Argon, et al., Metall. Trans. A6 (1975) 1269–1279.
[3] J. Pilling, Mater. Sci. Eng. 100 (1988) 137–144.
[4] B. Derby, E.R. Wallach, Metal Sci. 16 (1982) 49–56.
[5] B. Derby, E.R. Wallach, Metal Sci. 18 (1984) 427–431.
[6] A. Hill, E.R. Wallach, Acta Metall. 37 (1989) 2425–2437.
[7] S.Z. Wen, The Principle of Tribology, Publishing Company of Tsinghua University, Beijing, China, 1991, p. 364.
[8] D.S. Wilkinson, M.F. Ashby, Sci. Sinter. 10 (1978) 67–76.
[9] E. Arzt, M.F. Ashby, R.A. Verrall, Acta Metall. 31 (1983) 1977–1989.
[10] J.R.D. Williamson, Welding Technology for the Aerospace Industry, Proceedings of the Conference, AWS, Los Angeles, 1981, p. 55.
[11] W.W. Mullins, Metal surfaces, ASM (1963) p.17.
[12] G.Q. Wu, Z. Huang, Mater. Sci. Eng. A 345 (2003) 286–292.
[13] G.Q. Wu, Z. Huang, C.Q. Chen, Z.J. Ruan, Y. Zhang, Mater. Sci. Eng. A 380 (2004) 402–407.