Experimental and numerical simulation study of Zr-based BMG/Al composites manufactured by underwater explosive welding

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ABSTRACT

Using the underwater explosive welding technique, the Zr50Ti27Cu12Ni11 bulk metallic glass (Zr-based BMG) and Aluminum 1060 plates were successfully welded. The interfacial microstructure characteristics was characterized using optical microscopy (OM), scanning electron microscopy (SEM) and high-resolution transmission electron microscopy (HRTEM). Meanwhile, the Johnson-Holmquist-Ceramics (JH-2) constitutive model was selected as the constitutive model of BMG to verify weldability of explosive welding experimental and reliability of interface structure formation using the Smoothed Particle Hydrodynamics (SPH) method. The experimental results indicated that the Zr-based BMG and Al plates were successfully welded with a slightly wave structure and without visible defects. The numerical simulation results showed that the validity of JH-2 constitutive model for BMG material selection is verified, meanwhile, the weldability of Zr-based BMG and Al was verified, which are in good agreement with experimental results.

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1. Introduction

Recently, bulk metallic glasses (BMGs) have attracted many attentions due to their unique amorphous atomic structure and excellent properties, such as corrosion resistance, superior strength and high hardness as compared with conventional crystalline metals [1,2]. To extend the applications of BMGs, various welding techniques have been studied. Wang et al. [3] successfully welded two Ti46Zr15Ni3Cu12Be20 BMG plates by the laser welding process. Kim et al. [4] succeed in welding Zr41Be23Ti14Cu12Ni10 BMG plates to Ti metal by electron beam welding.Shin et al. [5] welded tubular Zr-based BMGs to BMGs and crystalline metals by friction welding. How-
ever, in these studies, the areas of joints were limited by welding methods.

Compared with the various other welding methods mentioned above, the explosive welding technique can fabricate large-sized composite materials comparing to conventional welding methods which are difficult to produce that [6–9]. Up to now, Somerseliers have studied the joining of BMGs with dissimilar metals by explosive welding technique. Liu et al. [10] welded Ti40Zr25Cu12Ni9Be20 BMG with 1060 Al and found that the plates are welded together at an atomic scale. Jiang et al. [11] welded Zr41.2Ti13.8Cu21.5Ni10.0Be12.5 with Cu-based crystalline alloy by thick-walled cylinder explosion and achieved a strong metallurgical bonding. Feng et al. [12] welded Zr53Cu35Al13 bulk metallic glass with Cu by explosive welding technique. After welding, they found that the BMG was successfully welded with Cu without visible defects, and a diffusion layer formed at the interface. All of the results confirmed that the explosive welding technique is an effective method to realize the joining of BMGs with dissimilar metals. Otherwise, there were a few studies on the SPH numerical simulation of explosive welding of BMGs.

In this paper, an aluminum plate was welded with a Zr-based BMG plate by underwater explosive welding technique. After welding, the interfacial microstructure characterization of the obtained composites were investigated using OM, SEM and HRTEM. Meanwhile, in order to further reveal the bonding interface structure, the JH-2 constitutive model was selected and used as the constitutive model of BMG to simulate the explosive welding of Zr-based BMG and Al using the SPH method.

2. Experimental procedure

Fig. 1 presents the sketch of initial configuration of the underwater explosive welding technique. As shown in Fig. 1, the Zr60Ti17Cu12Ni11 (at.%) BMG plate, with the dimension of 160 mm × 140 mm × 5 mm, was used as the base plate. The pure aluminum 1060, with the dimension of 160 mm × 140 mm × 3 mm, was used as the flyer plate. The base plate and the flyer plate were set above a stainless steel anvil with a fixed stand-off distance at 5 mm using aluminum spacers placed at the four corners. The air gap between the bonded plates was sealed against water. The water depth from the flyer plate to the explosive was set to 30 mm using spacers palced. A special mixed ANFO explosive was employed. The density of ANFO explosive is about 0.6–0.8 g/cm³ and the detonation velocity is about 2400–2600 m/s. A tailored high-wall open box was used to place explosive. The thickness of the explosive was 20 mm, 30 mm and 40 mm, respectively. To obtain the detonation velocity, two probes were set in the explosive with a fixed distance to record the time interval. By triggering the electric detonator, the explosive was detonated and the underwater shock wave pushed the flyer plate to the base plate and made two plates welded together.

To inspect the welding quality, the weldment were cut parallel to the explosion direction. The cross-section of the weldment was processed by grit abrasive papers and micron diamond slurries. The interfacial microstructure characteristic of the weldment was observed by HNL 300TPL type optical microscope (OM) and FEI Quanta TM 250 scanning electron microscope (SEM). To obtain high-resolution phase and diffraction patterns of the weldment, the high-resolution transmission electron (HRTEM) specimen was prepared by focused ion beam (FIB) system (FEI Quanta 3D FEG) and were carried out using an FEI Tecnai G2 20 S-Twin transmission electron microscope.

Fig. 2 shows the Zr-based BMG plate before welding and the amorphous nature was confirmed by X-ray diffraction (XRD) in a Bruker D8 Advance diffractometer with Cu Kα radiation. The XRD pattern shows only broad diffraction maxima, and there are no visible peaks of crystalline phase, indicating an amorphous structure.

Explosive welding is known to be successful only when certain parameters, particularly collision angle β and horizontal collision velocity Vc are in the range as defined in the welding window. β is almost proportional to the vertical velocity Vp, and the kinetic energy lost ∆KE increases with the increase of Vp. The energy that the bonding interface achieved is a very significant factor contributing to the welded quality of explosive welding. In the process of collision, the kinetic energy of the flyer plate is converted into other forms of energy, which produce high pressure at the bonding interface. The metals flows in the impact region because of the very high pressure, and promote solid-state welding [13]. In the case of underwater explosive welding technique, because the thickness of the plates are very thin, so the kinetic energy is lower than the regular cases. The upper limit may not be considered during the design process of welding parameters [14].

In this work, three different thickness of explosive were adjusted to the underwater explosive welding of Zr-based
BMG and Al. Using the underwater explosive welding window theory, the collision point velocity $V_C$ and the collision angle $\beta$ were calculated and the values were found to be 2300 m/s, 2350 m/s, 2400 m/s and 22.6°, 23.0°, 23.3°. The kinetic energy loss under three different explosive thickness were 2.55 MJ/m², 2.76 MJ/m² and 2.96 MJ/m², respectively [15]. With the increased of the kinetic energy loss, the welded interface shows different characteristics. To further study the weldability of Zr-based BMG and Al, the SPH numerical simulation was carried out.

3. Numerical simulation model

3.1. SPH method

Smoothed Particle Hydrodynamics (SPH) is a relatively new meshless method. The particles are used instead of classical elements to avoid the distortion of Lagrangian grids. Comparing with the conventional Lagrangian method, the SPH method allows large deformation and can realize complex constitutive behavior. At present, it has been applied to various fields, such as detonation, penetration, high-speed impact and fluid dynamics [16,17].

The SPH method mainly contains two key steps, that is the kernel approximation and the particle approximation. The kernel approximation standard expression is given as bellow,

$$f(r) = \int f(r')w(r - r', h)dr'$$

where $r$ is the location of the particles, $h$ is the smooth length, $W$ is the kernel function. As shown in Fig. 3, the kernel function $W$ depends on the distance between two points $|r_i - r|$ and the smooth length $h$.

The particle approximation is the core of the SPH method, which transforms the continuous integration of functions and their derivatives into discrete summation on arbitrarily arranged particles. The formula of particle approximation is as followed,

$$\langle f(r_i) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(r_j) w(r_i - r_j, h)$$

where $m_j$ and $\rho_j$ are the associated mass and density of the particles respectively.

3.2. Model set-up of explosive welding

Numerical modeling of the explosive welding process was carried out using ANSYS/LS-DYNA 15.0 (the related program runs on the High-Performance Computer Shuguang 5000A). The
3.3. Material constitutive model

The core of the numerical simulation was the constitutive model of Zr-based BMG. In the past, there were few studies on the dynamics simulation of metallic glasses. In previous studies on the dynamic loading of metallic glasses, researchers usually selected the Johnson-Cook constitutive model as the constitutive model of BMGs [19,20]. The JH-2 constitutive model is a well-defined material model which considers strain-rate effect, material damage and also confinement effect [21]. It has been popularly used in simulating glass and ceramic materials responses to shock and impact loads [22–25]. In this paper, due to the similarity with ceramic materials, the JH-2 constitutive model was innovatively used in this work.

As shown in Fig. 5, JH-2 strength model divides materials strength into three states: intact state, damage state and fracture state. The values of damage factor \(D\) (range from 0 to 1) are used to determine the strength between different states. Different states have different strength equations, which are expressed as the relationship between the standard equivalent stress and the standard hydrostatic pressure. The standard form is expressed as,

\[
\sigma^* = \sigma_i^* - D(\sigma_i^* - \sigma_f^*)
\]  \(3\)

Where \(\sigma^* = \sigma/\sigma_{\text{HEL}}\), \(\sigma\) is the actual equivalent stress and \(\sigma_{\text{HEL}}\) is the equivalent stress at Hugoniot Elastic Limit (HEL), \(\sigma_i^*\) is the normalized intact equivalent stress, \(\sigma_f^*\) is the normalized fracture stress.

The normalized intact strength is defined as,

\[
\sigma_i^* = A(P^* + T^*)^M[1 + C \ln\left(\frac{\dot{\varepsilon}}{\varepsilon_0}\right)]
\]  \(4\)

and the normalized fractured strength as,

\[
\sigma_f^* = B(P^*)^M[1 + C \ln\left(\frac{\dot{\varepsilon}}{\varepsilon_0}\right)]
\]  \(5\)

Where \(A, B, C, M, \text{and } N\) are material constant, the normalized pressure is \(P^* = P/P_{\text{HEL}}\), where \(P\) is the actual pressure and

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**Fig. 5** – JH-2 strength model.

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particle size has a great influence on the simulation process, especially in computational time and stability. At the same time, the particle size also plays a significant role in visualizing the metal jet and welded interface. In this case, the explosive welding process was simplified to 2D oblique collision model. As shown in Fig. 4, the model sizes of both base plate and flyer plate are both 5 mm in length, and the thickness was set to 5 mm and 3 mm respectively. The particle size was set to 5 \(\mu\)m and the total number of particles was 1,600,000 in the model. The impact angle between the flyer and base plate was fixed as 23° and the impact velocity \(V_p\) of the flyer plate was set to 937 m/s [15]. The boundary condition was set to a free boundary to ensure that the stress wave can reflect back [18].

To ensure accuracy and stability of the simulation, the time steps were automatically computed. The pressure, velocity, stresses and strains of each particle were recorded at the end of every time step. JOHNSON_HOLMQUIST_CERAMICS constitutive model was used to simulate the behavior of the base plate (Zr-based BMG). JOHNSON_COOK constitutive model and MIE_GRÜNEISEN equation of state were used to simulate the behavior of the flyer plate (Al).
Fig. 6 – The welded interface of Zr-based BMG/Al under different resolution. (a) The specimen of composite plate parallel to detonation. (b) Optical micrograph of the welded interface. (c) SEM image of the welded interface.

Table 1 – The JH-2 constitutive model parameters for Zr-based BMG.

<table>
<thead>
<tr>
<th>G (kg/m²)</th>
<th>G (GPa)</th>
<th>A (GPa)</th>
<th>B (GPa)</th>
<th>C</th>
<th>M</th>
<th>N</th>
<th>EPSI</th>
<th>T (GPa)</th>
</tr>
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<tr>
<td>5640</td>
<td>38.9</td>
<td>8.887</td>
<td>0.088</td>
<td>0.0054</td>
<td>0.35</td>
<td>2.304</td>
<td>1.0</td>
<td>1.8</td>
</tr>
<tr>
<td>2</td>
<td>HEL (GPa)</td>
<td>PH (GPa)</td>
<td>6.2</td>
<td>4.33</td>
<td>1.0</td>
<td>0.21</td>
<td>1.75</td>
<td>116.7</td>
</tr>
</tbody>
</table>

Table 2 – The Johnson-Cook parameters for Al-1060.

<table>
<thead>
<tr>
<th>G (kg/m²)</th>
<th>G (GPa)</th>
<th>A (MPa)</th>
<th>B (MPa)</th>
<th>C</th>
<th>m</th>
<th>n</th>
<th>C ′ (J/kg⁻¹K⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2700</td>
<td>27.6</td>
<td>324</td>
<td>114</td>
<td>0.002</td>
<td>1.34</td>
<td>0.42</td>
<td>885</td>
</tr>
<tr>
<td>300</td>
<td>T₀ (K)</td>
<td>Tₘ (K)</td>
<td>D₁</td>
<td>D₂</td>
<td>D₃</td>
<td>D₄</td>
<td>D₅</td>
</tr>
</tbody>
</table>

\( P_{\text{HEL}} \) is the pressure at HEL. The normalized maximum tensile hydrostatic pressure is \( T^* = T/P_{\text{HEL}} \), where \( T \) is the maximum tensile hydrostatic pressure the material can withstand. \( \dot{\varepsilon} \) is the actual strain state and \( \dot{\varepsilon}_0 = 1.0 \text{s}^{-1} \) is the reference strain state.

The cumulative form of the JH-2 damage model is similar to the Johnson-Cook fracture model, which can be expressed as,

\[
\sum_{i=0}^{N} \varepsilon_f^i = D_1 (P^* + T^*) D_2 \]

The plastic strain to fracture under constant pressure is defined as;

\[
\varepsilon_f = D_1 (P^* + T^*) D_2 
\]

Where \( \Delta \varepsilon_p \) is the plastic strain produced in each time step cycle, \( \varepsilon_f \) is the plastic strain to fracture under a constant pressure \( P \), \( D_1 \) and \( D_2 \) are damage factor.

Equations of state are generally used to describe the relationship between hydrostatic pressure and volumetric strain of materials. JH-2 model adopts the state equation of cubic polynomial. The equation of state for the material is as follows:

\[
P = K_1 \mu + K_2 \mu^2 + K_3 \mu^3 + \Delta P, \mu = \frac{\rho}{\rho_0} - 1
\]
Where $K_1$, $K_2$, and $K_3$ are model constants ($K_1$ is the bulk modulus of material), $\mu$ is the bulk strain, $\rho$ is the current density of the material and $\rho_0$ is the initial density of the material. $\Delta P$ is the additional pressure, which is related to the value of damage factor $D$.

To apply the JH-2 constitutive model in numerical simulation of Zr-based BMG, the strength model, equation of state (EOS), and damage model parameters first need to be determined. The transverse strain and longitudinal strain are measured directly by static compression experiment, and the elastic modulus and poisson ratio of Zr-based BMG are obtained at the same time. The bulk modulus and the shear modulus are as follows.

$$K_1 = \frac{E}{3(1-2v)} \quad G = \frac{E}{2(1+v)}$$  \quad (9)$$

The EOS parameters are provided by plate impact experiment and fitted by using the linear interpolation method. The JH-2 constitutive model parameters of Zr-based BMG are given in Table 1 [26–31].

The material behavior of the flyer plate was modeled using the Johnson-Cook constitutive model, which can be expressed as,

$$\sigma_Y = \left[ A + B \left( \dot{\varepsilon}^p \right)^n \right] \left[ 1 + C \ln \left( \dot{\varepsilon}^p \right) \right] \left[ 1 - T^m \right]$$  \quad (10)$$

Where $A$, $B$, $C$, $m$, $n$ are the model constants, $\sigma_Y$ is the flow stress, $\dot{\varepsilon}^p$ is the equivalent plastic strain, $\dot{\varepsilon}^p$ is the plastic strain rate, $T^* = (T - T_0) / (T_m - T_0)$, $T_m$ and $T_0$ are the melt temperature of the solid material and the room temperature respectively. The Johnson-Cook parameters for aluminum 1060 are given in Table 2.

The Mie-Grüneisen equation of state is used for the flyer plate, which can be expressed as,

$$p = \left\{ \begin{array}{ll}
\frac{\rho c_0^2}{\gamma_0} \left[ 1 + \left( 1 - \frac{\gamma_0}{\gamma} \right) \frac{\mu - \frac{\rho}{2} \dot{\varepsilon}^2}{\mu + \frac{1}{2}} \right] \left[ 1 - \frac{s_1 - 1}{s_2} \frac{\mu - s_2}{\mu + s_2} \frac{\rho}{\rho_0} \right] \dot{\varepsilon}^{\gamma_0 + a_0} & \gamma_0 \geq 0 \\
\frac{\rho c_0^2}{\gamma_0} \left[ 1 + \left( 1 - \frac{\gamma_0}{\gamma} \right) \frac{\mu - \frac{\rho}{2} \dot{\varepsilon}^2}{\mu + \frac{1}{2}} \right] \dot{\varepsilon}^{\gamma_0 + a_0} & \gamma_0 < 0 
\end{array} \right.$$  \quad (11)$$

Where $\mu = \frac{\gamma_0}{\gamma} - 1$, $\rho$ in which and $\rho_0$ are the current density and the initial density, respectively, $\dot{\varepsilon}$ is the internal energy density, $a$ is the first order volume correction to Grüneisen parameter $\gamma_0$, $s_1$, $s_2$, $s_3$ are solid materials parameters determined from shock wave measurements, and $c_0$ is the bulk sound speed of material. The Mie-Grüneisen equation of state parameters for aluminum 1060 is given in Table 3.

### 4. Results and discussion

**Table 3 – The Mie-Grüneisen equation of state parameters for Al-1060.**

<table>
<thead>
<tr>
<th>$\gamma_0$</th>
<th>$c_0$ (m/s)</th>
<th>$s_1$</th>
<th>$s_2$</th>
<th>$s_3$</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.97</td>
<td>5240</td>
<td>1.4</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Fig. 6a features the photograph of the successfully specimen welded using underwater explosive welding. The surface of the welded specimen shows no obvious cracks. To further study the microstructure characteristic of the welded interface, the OM and SEM were employed. As shown in Fig. 6b and c, the welded interface of Zr-based BMG and Al presents an almost flat structure without obvious defects or pores appeared at or near the joining interface. In Feng et al.’s [12] study, an almost flat interface without obvious defects has also been formed between the Zr-based BMG and Cu plates, which is similar to our experimental results.

To further study the microstructure of joining interface and phase nature of the welded material, the weldment containing the joining interface was prepared by FIB for HRTEM observation. Fig. 7 shows the interface between bright contrast Al phase and the dark contrast Zr-based BMG phase, from which a slightly wavy structure appeared in the interface. The diffraction pattern shown in Fig. 8b was taken from the grain marked “B” in Fig. 8a. Interestingly, between grain “B” and the thin region “C” there is a boundary marked by two arrows. While, the diffraction pattern of region “C” was taken without any further tilting, the difference between Fig. 8b and c indicates that there is a small misorientation angle between grain “B” and thin region “C”. Thus, the boundary between grain “B” and thin region “C” is in fact is low angle grain boundary. The shape of the region “C” is different from the normal grains of aluminum, which may be related to the intense plastic deformation during the explosive welding process. The intense plastic deformation causes the deformation of grains and formed deformation zone in the bonding interface.

There is a clear interface between the Al phase and the Zr-based BMG phase marked by two red arrows. The diffraction pattern shown in Fig. 8d was taken at the location marked “D” in Fig. 8a. A clear diffraction ring in Fig. 8d indicates that the Zr-based BMG retains an amorphous structure, but nano-crystallites of intermetallic compounds are randomly scattered in the Zr-based BMG side as indicated by the diffraction spots in Fig. 8d. The light contrast

**Fig. 7 – The HRTEM image of Zr-based BMG/Al welded interface.**

**Fig. 8 – The selected area diffraction patterns of Zr-based BMG/Al welded interface.**
Fig. 8 – HRTEM image of Zr-based BMG/Al welded interface and corresponding SAED patterns (a) HRTEM image of Zr-based BMG/Al welded interface, (b) the SAED patterns of region “B” marked in Fig. 8a, (c) The SAED patterns of region “C” marked in Fig. 8a, (d) The SAED patterns of region “D” marked in Fig. 8a.
nano-crystallites submerged in the Zr-based BMG side are clearly observable in Fig. 8a. It is uncertain whether the nano-crystallites were formed during the explosive welding. The nano-crystallites are possibly formed during the preparation process of the bulk metallic glasses [32,33]. Therefore, for the formation reason of nano-crystallites, we will do further study in the future. Wang et al. [34] welded the Zr-based BMG and Al plates by Magnetic pulse welding technique and also formed the interlayer between the Zr-based BMG and Al plates. The SAED patterns of the BMG also retains the amorphous structure after welding. So our obtained results are consistent with their experimental ones.

Fig. 9a and b shows the characteristics of the welding interface at t = 1 \mu s and t = 2 \mu s in explosive welding process obtained by the SPH method, respectively. Fig. 10 provides a close-up of the interface at t = 2 \mu s, from which metal jet formed between the Zr-based BMG and Al plates. Most of the jets are from the flyer plate (Al), only a few jets from the base plate (Zr-based BMG). The interface presents an almost flat structure and there are no obvious wave structure was formed. Fig. 11 shows the change process of effective plastic strain. Four typical elements near the joining interface were selected, respectively. The effective plastic strain of two elements from Zr-based BMG shows an increasing trend with time, and which from Al plate increases firstly, then remain stable.

As a constitutive model of brittle materials, the JH-2 constitutive model has been widely used, especially in the impact response of ceramics. The accuracy of JH-2 constitutive model in simulating ballistic impact on ceramics has been proved acceptable. Chakraborty et al. [35] studied the damage in ceramic and ceramic-metal composite structures using the JH-2 model. Tian et al. [36] studied the anti-penetration performance of a ceramic-metal hybrid structure numerically. So in our work, the JH-2 model was selected as the constitutive model of BMGs. The SPH numerical simulation results show that the Zr-based BMG and Al plate were successfully welded together. An almost flat welded interface was formed, which is in consistent with the experimental results. All of these
prove the validity of JH-2 constitutive model for BMG material selection.

5. Conclusions

Using the underwater explosive welding technique, the Zr60Ti12Cu12Ni11 BMG and Aluminum 1060 plates were successfully welded with a slightly wave structure formed and without visible defects. The welding interlayer was formed between the Zr-based BMG and Al plates and the Zr-based BMG retains amorphous structure after underwater explosive welding. The numerical simulation results showed that it is feasible to select the JH-2 model as the constitutive model of BMG material, and the weldability of Zr-based BMG and Al was verified, which are in good agreement with experimental results. Although the JH-2 model is feasible for BMG materials, the model and parameters still need to be optimized in BMG dynamic simulations. To further study, the most suitable constitutive model and parameters of BMG materials will be developed in the future.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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