Finite element simulation of micro-imprinting in Mg–Cu–Y amorphous alloy


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Abstract
Mg–Cu–Y-based metallic glasses have exhibited superior glass-forming ability, and can be cast into bulk metallic glasses (BMGs). At temperatures above the glass transition temperature, the BMGs become supercooled viscous materials that can be formed into complicated shapes or patterns on micro- or even nano-scales. This paper presents the simulated forming evolution, using a finite element simulation software DEFORM 3D, and the experimental observations for the micro-imprinting of the Mg58Cu31Y11 BMGs for making hexagonal micro-lens arrays. The results demonstrate that the imprinting is feasible and promising.

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1. Introduction

Metallic glassy alloys exhibit some unique physical properties such as excellent elasticity and strength as compared to their corresponding crystalline alloys. Meanwhile, significant plasticity occurs in the supercooled liquid region, \( \Delta T_x = T_x - T_g \) (where \( T_x \) is the crystallization temperature and \( T_g \) is the glass transition temperature), due to a drastic drop in viscosity at temperatures above \( T_g \) upon heating [1]. Accordingly, it is possible to form products by means of the superplastic deformation capability over this temperature region [2,3]. And such excellent workability and surface printability in the supercooled liquid state has been considered to be one of the most attractive properties of bulk metallic glasses (BMGs). The homogeneous flow nature of amorphous metals with a low viscosity allows us to form easily into complicated shapes and surface patterns [4]. In general, the low viscosity and high thermal stability (against crystallization) of the supercooled liquid are the two main prerequisites of BMGs required for superplastic micro-forming or micro-imprinting.

The temperature dependence of viscosity of the Zr-, Mg-, La-, and Pd-based BMGs has been measured using various techniques, and was assessed on the basis of the fragility concept proposed by Angell in some papers [1,5–9]. Compared with the Zr-, La- and Pd-based BMGs, the Mg amorphous glasses possess much lower \( T_g \) temperatures in the range of 140–160 °C, enabling favorably low working temperatures for micro-forming or micro-imprinting [10]. In addition, the Mg-based BMGs exhibit sufficiently high glass-forming ability (GFA) [11], a sufficiently wide supercooled liquid region before crystallization [12], and high specific strength [13]. Thus it is necessary to study the flow behavior around and above \( T_g \) in metallic glasses. In our previous work, it is confirmed that the Mg58Cu31Y11 amorphous alloy exhibited reasonably good GFA with a wide supercooled liquid region before crystallization [10]. In this report, the comparison of the experimental observations and finite element simulations on the micro-imprinting behavior of this alloy is presented.

2. Experimental details

The Mg58Cu31Y11 BMGs in the rod form with a diameter of 4 mm were prepared by a copper mold injection casting technique, through the induction melting of pure Mg and pre-alloyed Cu–Y ingots in an argon atmosphere. The basic thermal properties were first measured in a continuous heating mode by differential scanning calorimetry (DSC, TA Instruments DSC 2920) and a thermomechanical analyzer (TMA, PerkinElmer Diamond). The applied heating rate was 10 K/min. The \( T_g, T_x \) and \( T_m \) (solidus temperature) measured by DSC are 140, 206, and 438 °C, respectively.

The new process is used to fabricate a BMG mold to replicate micro-lens array on PMMA sheets by hot embossing. The original convex mold is the Ni–Co die made by the electroplating and lithography processes, as shown in Fig. 1. The patterns in the Ni–Co
mold are the half-spherical and hexagonal micro-lens arrays, each side of the hexagonal is around 185 μm. These patterns are formed into the secondary Mg58Cu31Y11 BMG mold by hot pressing into the pattern shown in Fig. 1(b). Finally, the concave pattern in the secondary Mg58Cu31Y11 mold is further transformed to the PMMA sheets.

In this study, relationship between the load and strain during its initial imprinting stage is simulated by the commercial software DEFORM 3D for the load prediction. The Ni-Co lens mold has a diameter of 330 μm and height of 14 μm, and the projected area of the hexagonal micro-lens array pattern is about 6.238 × 10⁻⁷ m².

3. Results and discussion

The temperature dependence of the relative displacement of the bulk amorphous Mg58Cu31Y11 alloys is obtained by TMA operated in the compression mode at various stress levels and a fixed heating rate of 10 K/min [1]. The maximum displacement (∆Lmax) occurred in the supercooled liquid region reaches 60.9, 162.6, 265.3, 748.8, and 923.3 μm under the applied compressive load of 0.8, 2.4, 7.1, 117.8, and 318.5 kPa, respectively. Such displacements correspond to engineering strains ∆Lmax/L0 (where L0 is the original specimen height 4 mm) of 1.52%, 4.07%, 6.63%, 18.72%, and 23.08%. The relative displacements become pronounced at temperatures greater than Tg, indicating the high deformability of the glassy alloy in the supercooled liquid region. We have defined T onset for the onset temperature for the viscous flow, T c for the semi-steady-state viscous flow temperature, and T finish for the finish temperature for the viscous flow. Under a higher loading stress, crystallization tends to start at a lower temperature, and brings viscous flow to the end sooner. The measured stress and strain curves for this amorphous alloy at these three characteristic temperatures are shown in Fig. 2.

The finite element simulation was started from the beginning stage of the micro-imprinting stage. The glass transition temperature of Mg58Cu31Y11 BMG is about 140 °C. Therefore, temperature of 150 °C is chosen for the hot embossing experiment and simulation. For simulation, the forming velocity of top die is first set to be low, i.e., 0.0005 mm/s, in order to explore the minimum applied load for the micro-imprinting. Based on the input stress and strain curves at various temperatures, the calculated pressure versus imprinting time is obtained, for example, at 150 °C, as shown in Fig. 3. In the beginning stage within 120 s, the BMG can be formed at low pressures, in the neighborhood of 0.05–2 kPa. The residual material becomes thinner, resulting in sudden load increase over 180–360 s. The simulated results suggest that the Mg58Cu31Y11 BMG can be formed from the first minute, with a low pressure less than 50 Pa. Nevertheless, the achieved strain is rather low, and the imprinted patterns are not well defined. With increasing time to over 360 s and pressure to ~2 kPa, the imprinting proceeds continuously. The current simulation is only for the initial stage of the micro-imprinting. To complete the imprinting into well-defined hexagonal micro-lens arrays, much longer time and much higher load are necessary.

In reality, the forming speed of 0.0005 mm/s appears to be much lower than acceptable, thus a higher load is applied. The actual applied pressure needed for satisfactory forming is found to be above 100 kPa, for the practically acceptable forming time of a few minutes.

Experimentally, the deforming evolution of the micro-lens array on the BMG material with different forming times is shown in Fig. 4, with parameters of embossing temperature at 150 °C, time duration of 4 min, and two different applied loads of 100 and 300 kPa. It was found that the applied pressure of 400 kPa is the optimum. Fig. 5 shows the forming extent of the BMG upon subject to an applied pressure of 400 kPa and forming time of 1 and 4 min by the spring plates. It will usually take about 4 min to complete the embossing process. When the embossing time is too long, the BMG material may be crystallized. Thus, the forming time of 4 min appears to be an optimum and acceptable time duration for the micro-imprinting.

Before the embossing process, it is obvious that there are some defects on the surface of a BMG raw material, which is created during its manufacturing process. Fig. 6 shows the SEM micrograph of the typical surface morphology. To improve this, the surface was polished with abrasive papers.
The simulated imprinting evolution and the corresponding load prediction: (a) 150 °C, 60 s, pressure 31 Pa and (b) 150 °C, 240 s, pressure 1176 Pa.

The forming extent of the BMG under an applied pressure of (a) 100 kPa and (b) 300 kPa for 4 min.

The surface profiles of micro-lens in its original convex Ni/Co mold, imprinted concave Mg-based BMG, and the final imprinted convex PMMA are shown in Fig. 7. Note that the profile of the concave BMG has been reversed its sign for the sake of comparison.

The original convex Ni/Co mold is 184.68 μm in width. This concave BMG mold is 183.56 μm in width and the roughness is less than 30 nm. Finally, the convex PMMA micro-lens is 183.44 μm in width and the roughness is also less than 30 nm. The shrinkage rate...
Fig. 6. SEM micrograph of the formed BMG, operated at 150 °C for 4 min under a pressure of 400 kPa.

Fig. 7. Comparison of the surface profiles of the original Ni–Co mold, Mg₅₈Cu₃₁Y₁₁ mold, and the PMMA. The result reveals that pressure level of 400 kPa and forming time of 4 min are good combinations to replicate a micro-lens array. The simulated results of the applied pressure and the resulting forming extent are in reasonable agreement with the experimental observation. The surface profiles of the original convex Ni/Co mold, imprinted concave Mg-based BMG, and the final imprinted convex PMMA are closely matched, suggesting that the application of BMGs for micro-forming or micro-imprinting is feasible.

4. Summary

This study presents a new process to fabricate micro-lens array, utilizing the viscous flow behavior of the metallic glassed and polymer PMMA at temperatures slightly above their glass transition temperature. The working temperature for embossing is selected to be 150 °C, based on the DSC and TMA data. The Ni–Co mold with an inscribed circle 330 μm in diameter has been successfully fabricated out using the electroplating process. Excellent replicated patterns can be obtained using a larger applied pressure level. The simulated results of the applied pressure and the resulting forming extent are in reasonable agreement with the experimental observation. The surface profiles of the original convex Ni/Co mold, imprinted concave Mg-based BMG, and the final imprinted convex PMMA are closely matched, suggesting that the application of BMGs for micro-forming or micro-imprinting is feasible.

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