IOP Conf. Series: Materials Science and Engineering **416** (2018) 012021 doi:10.1088/1757-899X/416/1/012021

Simulation of Thermal Field in Bulk Amorphous Steels

C Codrean, B Radu, D Buzdugan* and C Opriş

Politehnica University Timişoara, Piaţa Victoriei, No.2, 300006, Timişoara, Romania

*Corresponding author: dragos.buzdugan@upt.ro

Abstract. Bulk amorphous steels (BASs) have shown great potential for some structural applications due to very attractive physical, thermal and mechanical properties. This paper presents some results for numerical simulation of the thermal field developed during rapid cooling of Fe-Cr-Co-Mo-Y-C-B alloy, to obtain bulk amorphous steels. Rapid cooling technology gives the possibility to obtain bulk metallic alloys with an amorphous structure under conventional industrial conditions, using, for example, commercial-grade raw materials, low vacuum, conventional casting techniques, etc. Once the model being validate, it can be used to optimize the rapid cooling process and casting mold geometry to be able to investigate the possibility to obtain larger bulk amorphous steel components.

1. Introduction

The increasing use of amorphous alloys is due to the combinations of excellent properties: hardness, mechanical strength and ductility superior to metallic crystalline materials, high magnetic permeability and low coercive field, electrical resistivity almost independent of temperature and very high corrosion resistance. Therefore, in the last decades, the research has been focused on producing amorphous alloys with thicknesses greater than 1 mm, also called bulk amorphous alloys.

Compared to most other bulk amorphous alloys, such as Zr or Pd based alloys, Fe-based bulk amorphous alloys offer several important advantages: much lower raw material costs, higher mechanical strength, better corrosion resistance, and greater thermal stability [1, 2, 3]. A major obstacle to the development of Fe-based bulk amorphous alloys is their low glass forming ability (GFA) [1, 4, 5]. Also, another disadvantage of the Fe-based bulk amorphous alloys is their relatively high fragility.

The first bulk Fe-based amorphous alloy with the chemical composition $Fe_{73}Al_5Ga_2P_{11}C_5B_4$ was developed in 1995 by a group of Inoue-led researchers [6, 7] using high purity components. Recent research has shown the possibility of obtaining so-called bulk amorphous steels (BAS), which are actually C containing bulk amorphous Fe-based alloys, by melting pure components in a vacuum electric arc furnace and casting in the form of cylindrical rods in a copper mold in a protective atmosphere of argon [8, 9, 10, 11]. These BASs are very attractive materials for making, lighter automobiles, tall buildings, corrosion-resistant coatings, ship hulls and surgical instruments, in the future [8].

The GFA increase of Fe-based alloys was achieved by adding to their chemical composition yttrium and / or rare earths [1, 9, 10, 11]. Therefore, the aim of this work is to evaluate the cooling rate by thermal field analysis of Fe-Cr-Co-Mo-Y-C-B alloy in form of disc quenched in a water cooled copper mold.

IOP Conf. Series: Materials Science and Engineering **416** (2018) 012021 doi:10.1088/1757-899X/416/1/012021

2. Simulation

Multicomponent $Fe_{48}Mo_{14}Cr_{11}Co_4B_6P_8Si_7Y_2$ BAS in disk form were elaborated by water cooled copper mold casting using mostly ferroalloys and pure elements. The elaborated samples were structurally analyzed by X-ray diffraction using an X'Pert³ Powder diffraction system with a Cu anode. Finite Element Analysis method was used to investigate the thermal field evolution during copper mold casting in order to estimate the cooling rate needed to obtain an amorphous structure. A 3D geometric model of the Cu mold and disk were used for the transient analysis. The Cu mold, having a diameter of 120 mm and 60 mm in length, is made up of two symmetrical parts which are screwed together, thus resulting the cavity with a diameter of 10 mm and thickness of 2 mm. The boundary conditions are the following:

- the melt temperature is 1150 °C and the initial mold temperature is 22 °C
- the melt already fills the mold cavity at the initial moment
- all the surfaces separating the mold and the disk from the outside environment have been considered as surfaces through which the heat is transferred by convection into the external environment
- the contact surface between the cast alloy (disk) and the mold was considered a surface, through which heat is transferred by conduction, as a result of contact between the cast alloy and the copper mold.
- the mold is cooled with water flowing through the channels and the heat is transferred by the forced convection.

3. Results and discussion

The BAS disk obtained by water cooled copper mold casting is presented in Figure 1. Figure 2 shows the diffraction pattern of the elaborated disk in which can be observed only a broad peak specific to the amorphous structure.

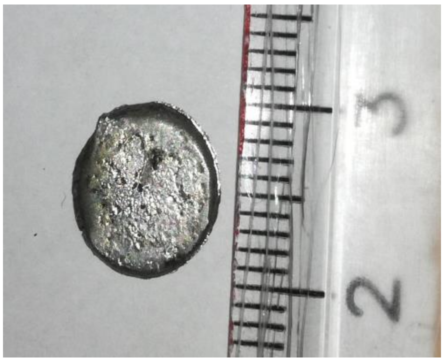

Figure 1 $Fe_{48}Mo_{14}Cr_{11}Co_4B_6P_8Si_7Y_2$ BAS disc.

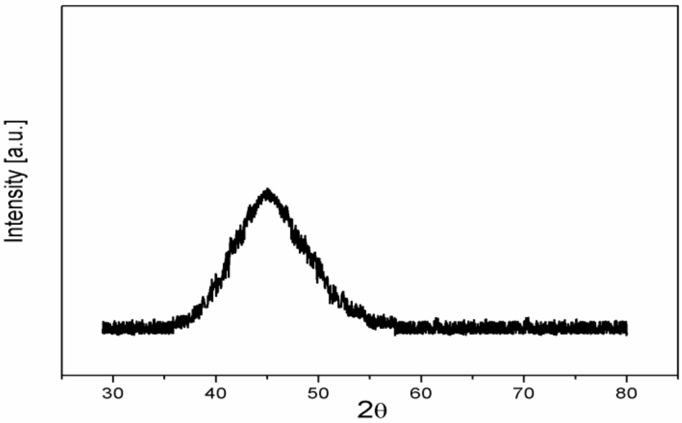

Figure 2 XRD pattern of the $Fe_{48}Mo_{14}Cr_{11}Co_4B_6P_8Si_7Y_2$ BAS disc.

The BAS disk obtained by water cooled copper mold casting is presented in Figure 1. Figure 2 shows the diffraction pattern of the elaborated disk in which can be observed only a broad peak specific to the amorphous structure. The accuracy of the finite element results were assured by using a fine tetrahedral mesh with higher number of nodes in areas where the temperature gradient was estimated to be the highest. The mesh contains 169171 elements and 247836 nodes and is presented in Figure 3.

Transient analyze performed on the entire assembly cast disk – mold provided data for temperature evolution during cooling time, allowing to estimate the cooling rate to obtain a bulk amorphous disk. Figure 4 shows the temperature evolution in cross section of the mold and disk until cooling at room temperature.

IOP Conf. Series: Materials Science and Engineering **416** (2018) 012021 doi:10.1088/1757-899X/416/1/012021

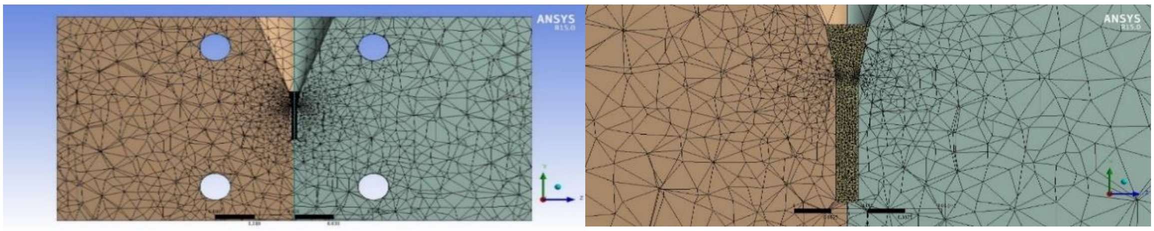

Figure 3. Mesh of the mold and detail in the disc area.

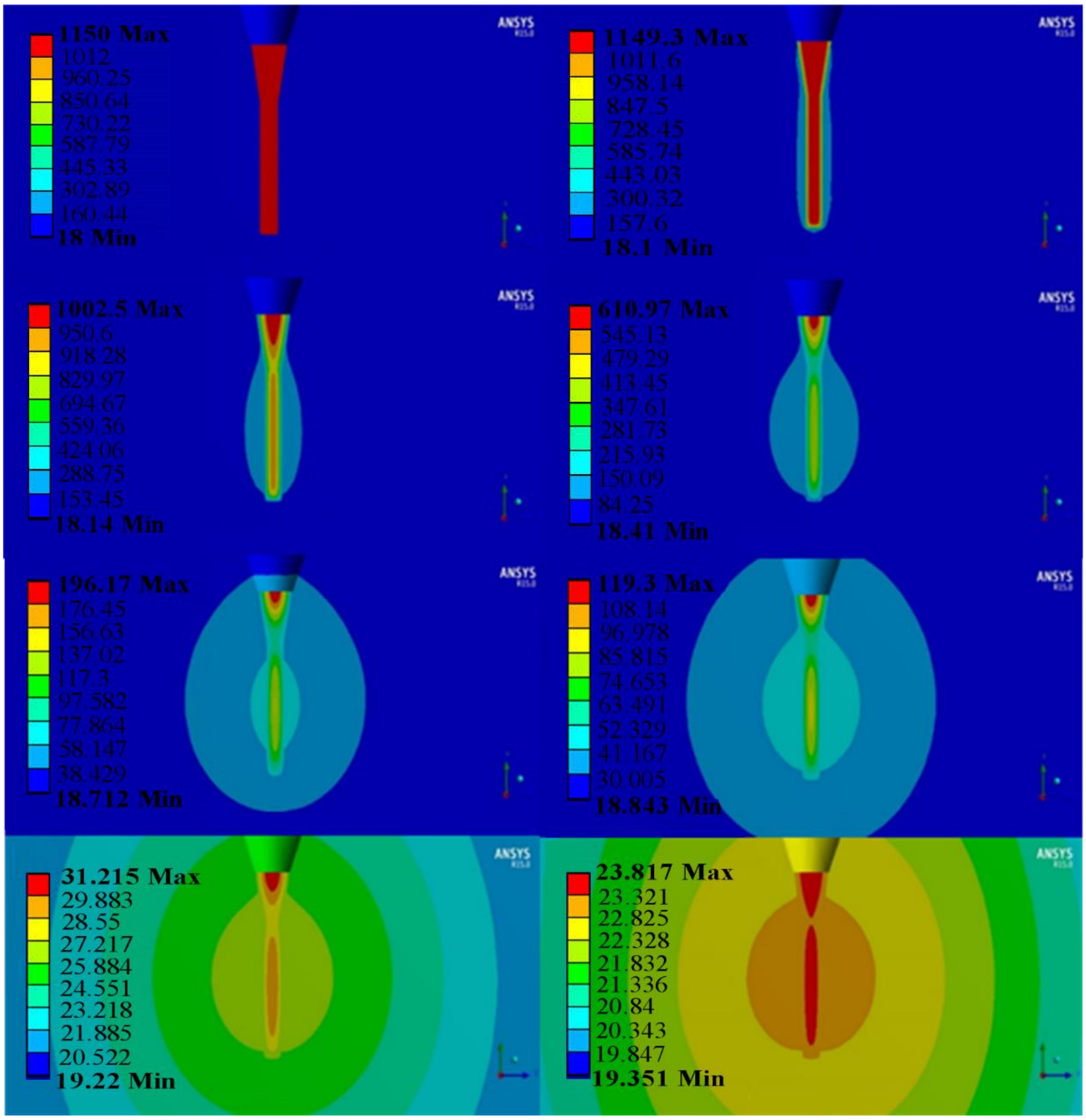

Figure 4. Thermal field distribution in cast alloy at 0s; 0.02s; 0.1s; 0.3s; 0.5s; 0.8s; 1s; 1.5s.

Figures 5 and 6 present the temperature evolution and cooling rates in disk cross section at different distances from the center of the disk. It can be noted that the cooling rate decreases from 3739 K/s in the surface to 1872 K/s in the core. The values of cooling rate are higher than the values reported in the literature, approximately 100 K/s [7] for Fe-based bulk metallic glasses.

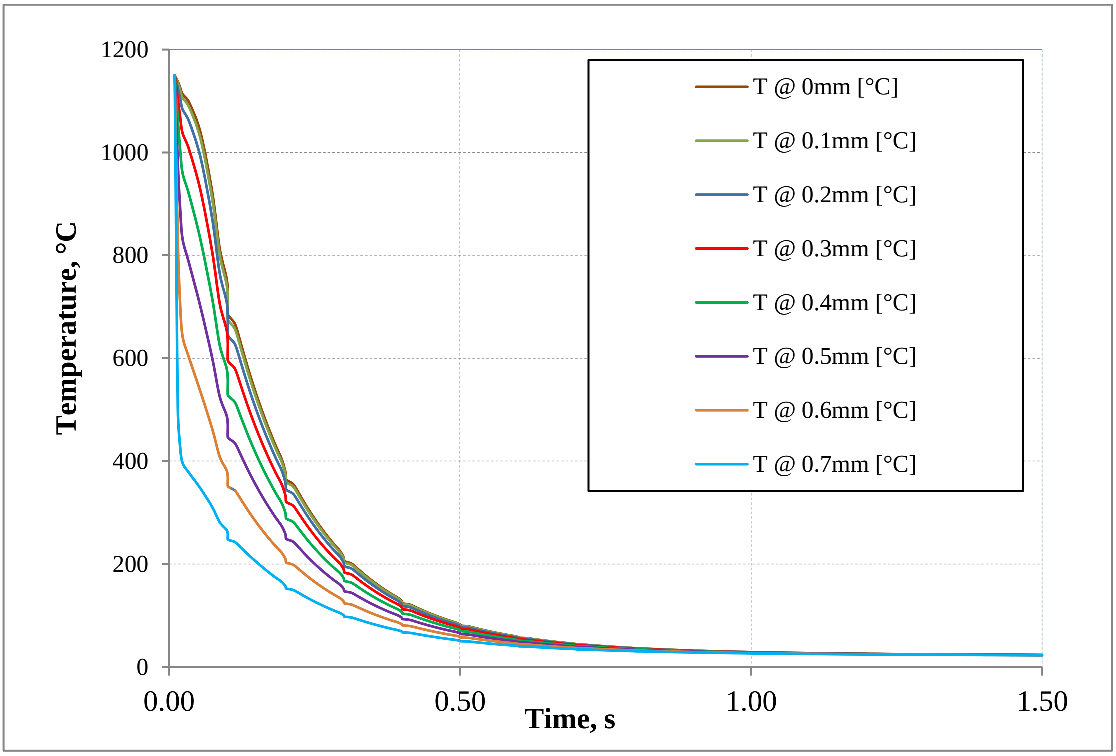

Figure 5 Temperature evaluation in disk cross section at 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6 and 0.7 mm from the center of the disk.

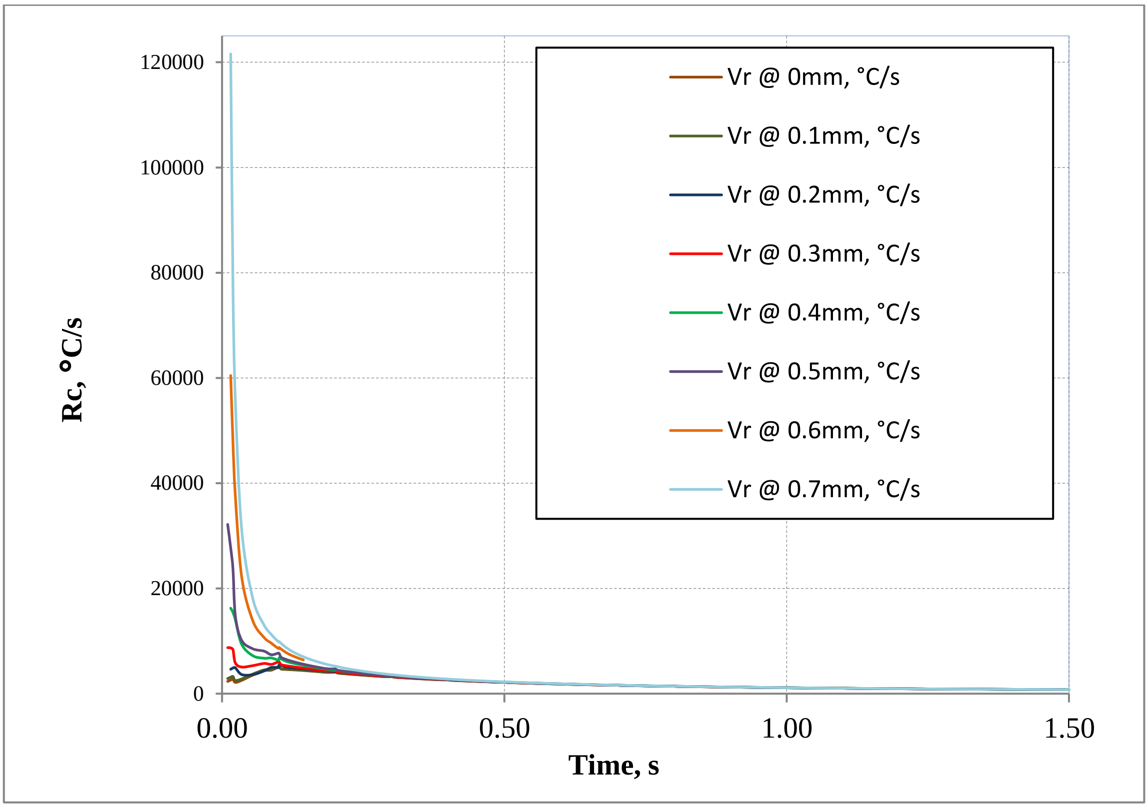

Figure 6 Cooling rate in disk cross section at 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6 and 0.7 mm from the center of the disk.

4. Conclusions

Multicomponent $Fe_{48}Mo_{14}Cr_{11}Co_4B_6P_8Si_7Y_2$ BAS in disk form was elaborated by copper mold casting using mostly ferroalloys and pure elements. The finite element analysis model is verified since it was obtained a minimum cooling rate of 1872 K/s which has led to an amorphous structure. This model helps to estimate the critical cooling rate in processing the bulk metallic glasses by copper mold casting since it is difficult to determine it by experimental analysis.

5. References

[1] Babilas R., Nowosielski R. 2010 Iron - based bulk amorphous alloys, *Archives of Materials Science and Engineering* **44** 5-27.
[2] Rao B.R. 2009 Bulk Metallic Glasses: Materials of Future, *DRDO Science Spectrum*. 212-8.
[3] Wang W H, Dong C and Shek C H 2004 Bulk metallic glasses *Materials Science and Engineering: R: Reports* **44** 45–89
[4] Inoue A., Takeuchi A. 2002 Recent progress in bulk glassy alloys, *Materials Transactions* **43** 1892–06.
[5] Kui H W, Greer A L and Turnbull D 1984 Formation of bulk metallic glass by fluxing *Applied Physics Letters* **45** 615–6
[6] Basu J., Ranganathan S. 2003 Bulk metallic glasses: A new class of engineering materials, *Sadhana*- **28** 783-798.
[7] Suryanarayana C and Inoue A 2011 *Bulk metallic glasses* (Boca Raton, FL: CRC Press)
[8] Fang H, Hui X and Chen G 2008 Effects of Mn addition on the magnetic property and corrosion resistance of bulk amorphous steels *Journal of Alloys and Compounds* **464** 292–5
[9] Iqbal M, Akhter J I, Zhang H F and Hu Z Q 2008 Synthesis and characterization of bulk amorphous steels *Journal of Non-Crystalline Solids* **354** 3284–90
[10] Gostin P F, Gebert A and Schultz L 2010 Comparison of the corrosion of bulk amorphous steel with conventional steel *Corrosion Science* **52** 273–81
[11] Tsai P H, Xiao A C, Li J B, Jang J S C, Chu J P and Huang J C 2014 Prominent Fe-based bulk amorphous steel alloy with large supercooled liquid region and superior corrosion resistance *Journal of Alloys and Compounds* **586** 94–8

Acknowledgements

This work was supported by research grants PCD-TC-2017 No. 16179/21.11.2017.