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Modelling and simulation of twin-roll casting of bulk metallic glasses

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1. Abstract

As an economic and direct route to continuous thin strip production from the melt, twin roll casting (TRC) has been established as an effective process for aluminium alloys. Its adaptation to casting of bulk amorphous alloy strip necessitates matching of the thermal and mechanical behaviour of the cooling multi-component melt to the requirements (especially cooling rate, and strip exit temperature and thermal gradient) of vitrification. Using a dedicated control volume numerical model of TRC, simulation of the casting of 2 mm thick Vit 1 ($Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$) alloy strip shows that the acceptable casting speeds are in the range 2.5 to 3.5 cm/s. The effects of varying strip thickness and strip-roll heat transfer coefficient (HTC) on this casting window are assessed. The differences between modelling of conventional alloy solidification and metallic glass formation are presented.

Keywords: Twin Roll Casting, Bulk Metallic Glass, Vit 1

2. Introduction

2.1. Twin Roll Casting (TRC)

TRC is a continuous combined solidification-deformation process whereby liquid metal is fed into the gap between two counter-rotating water cooled rolls. The alloy solidifies through the contact length and is then plastically deformed through the roll bite (the narrowest point between the rolls). The intimate contact due to the separation forces increases the heat transfer coefficient significantly which helps to speed up solidification. In the case of a binary alloy the deformation also refines the microstructure giving finer grain sizes.

TRC is a proven technology for the continuous production of aluminium sheet. It produces sheets to near net shape requiring little further rolling in comparison to conventional casting and rolling techniques.

Some of the key process variables involved include: roll speed, melt-roll heat transfer coefficient, application of lubrication/cooling, roll gap and liquid feed-tip set back.

2.2. Bulk Metallic Glass

Glass (also referred to as amorphous or vitrified) is a non crystalline solid. It has no long range specific atomic arrangement which is repeated like in conventional pure metals or alloys.

Metallic Glass (MG) is an amorphous metal alloy; it combines the characteristics of both glass and metal. Some metallic glass alloys display strengths up to twice that of steel, greater wear and corrosion resistance, greater elasticity and may be tougher than some ceramics.

Bulk Metallic Glass (BMG) is defined as a section for which the critical diameter exceeds 1 cm where the critical diameter commonly refers to the maximum diameter of a cylinder which can be cast into a fully amorphous form.

The size and shape of commercially producible components is still quite limited. Flat rolled sheets/ plates represent more than 80% of the market for the production of general metal/ alloy products [1]. If BMG was readily available in this form its value would be greatly increased. This will require a continuous process to produce the sheet or plate which as of yet remains to be developed and implemented commercially.

2.3. TRC of BMG

TRC, which can achieve high cooling rates (10^2 - 10^3 K/s) has been examined as a possible method to continuously produce BMG strips [1-3]. Various problems were encountered such as: achieving the cooling rates required, selecting an optimum casting speed taking into account the low conductivity of metallic glass and determining the HTC between rolls and the strip. However, the research did conclude that TRC is a viable method for continuous production of BMG strip. This project seeks to identify the optimum range of casting speeds to produce a fully amorphous strip. The effects of varying key parameters such as HTC and strip thickness are examined.

3. Materials and Methods

3.1. Metallic Glass Alloy

The alloy chosen to model was $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10.0}Be_{22.5}$ i.e. Vitreloy 1 (Vit 1). This choice was based on fact that Vit 1 is the most extensively characterised metallic glass which has been produced to date. It also has a very low critical cooling rate (R_c) of 1 K/s and so should be one of the easiest to produce in its fully amorphous state.

3.2. Description of model

The model, originally developed by Browne [4] to simulate TRC of binary alloys, in particular those of aluminium, was adapted in order to model TRC of a BMG.

The steady state model uses the finite difference method to solve the partial differential equations of heat transfer from the strip to the rolls, taking enthalpy as the dependent variable. The equations are discretised via the control volume formulation method.

The calculation domain for the model is assumed to be flat and rectangular in shape. Treating the domain in this manner is quite reasonable as the roll shell thickness is small in comparison to the diameter of the roll. Using the fact that there is central symmetry about the centre of the strip being cast, only one half the strip and one roll need be simulated.

The contact length is split into a series of control volumes, specified by the user. The remainder of the roll is represented as a

coarser mesh in order to save computing time - justified by the much lower thermal gradients and heat transfer there.

End effects are negligible so the process may be assumed to be two dimensional. The thermal conductivity of the material is assumed to be independent of temperature.

The explicit scheme is employed which means the only unknowns required to solve the equations, are the values of the thermal gradients and the enthalpies at each wall of any control volume [4].

$$\left(\frac{\delta T}{\delta x}\right)_e, \left(\frac{\delta T}{\delta x}\right)_w, \left(\frac{\delta T}{\delta y}\right)_n, \left(\frac{\delta T}{\delta y}\right)_s, H_w, H_e$$

For the conductive terms the central difference scheme is used.

For the convective terms the upwind scheme is used.

A number of important assumptions are made in order to simulate the behaviour of a BMG during TRC:

- The flow is laminar i.e. no mixing of the melt occurs as it flows through the path
- Vitrification of the alloy is regarded as a continuous transformation i.e. there is a continuous increase in viscosity as temperature decreases from the liquid phase.
- The value of specific heat is taken as a constant based on values obtained from literature. The value chosen was assumed to be a reasonable estimate as the specific heat doesn't vary widely over the temperature range involved for TRC [6]
- The value of viscosity which is also a function of temperature is taken to vary according to the Vogel-Fulcher-Tammann (VFT) equation [7,8]

$$\eta = \eta_0 \exp\left(\frac{DT_0}{T-T_0}\right)$$

Where:

T_0 = The VFT temperature, 390 K for Vit 1

η_0 = The high temperature limit of viscosity 0.001 mPa s for Vit 1

D = The fragility parameter 23.8 for Vit 1

This equation is only valid above the glass transition temperature (T_g). As the temperature of the melt approaches T_g the viscosity rises sharply. The viscosity is employed as a means to choose a value for the HTC. Thus, once the temperature of the melt decreases to within a set distance of T_g the model simply selects the highest heat transfer coefficient.

- Three assumed values, increasing for three distinct stages of the process, where chosen based on the range of HTC specified by literature [1,3]
 - 0.15 (Wcm⁻² K)
 - 0.25 (Wcm⁻² K)
 - 0.40 (Wcm⁻² K)
- The diameter of the rolls chosen for the model was 20 cm and the strip thickness was initially chosen as 2mm.

4. Results

Having developed a working model, capable of simulating the thermal behaviour of both a binary alloy and an amorphous alloy, a number of simulations were performed.

Using the specified alloy-roll contact length, the diameter of the rolls and the number of nodes across the calculation domain it is possible to work out the distance each node is from the start of the contact length. Using these values of distance and the casting speed it is a simple matter to calculate the time taken for the melt to be processed through the rolls. Using the temperature and time readings it is also possible to calculate the cooling rate at the different locations within the strip.

4.1. BMG - Vit 1

The material properties and process parameter for Vit 1 which were required to run the model were obtained from the literature [1,3]

Over the same range of casting speeds as used in the binary alloy model (1–5cm/s), it was found that the Vit 1 strip exits at sufficient low temperatures to remain strong enough to ensure continuous casting. The matter of interest is then whether the strip is fully amorphous throughout or if it contains some crystalline particles. The research carried out by Lee et al [1,3] set two criteria for the successful casting of a fully amorphous strip.

- The strip surface temperature must be above T_g at the roll bite
- The strip mid temp. must be below CCT nose at the roll bite

The first criterion is necessary as if the surface of the strip is below T_g upstream of the roll bite, the surface will have transformed to a metallic glass. The rolls will not be capable of deforming the strong metallic glass and thus they will be damaged, or the process will be stopped, or both.

The second criterion ensures crystallisation does not occur at the centre of the strip. An estimate of the Continuous Cooling Transformation curve for Vit 1 is shown in Fig. 1. Also plotted here is the predicted temperature of the strip with time.

If the strip is not cooled fast enough its temperature will fall within the CCT curve where crystallisation will occur. The centre is the hottest part of the strip thus the criterion specifies this temperature needs to be below the CCT nose (≈ 860 K) i.e. the crystallisation temperature (T_x). If the temperature is too close to 860 K crystallisation will more than likely occur to some degree, given that the cooling rate will drop significantly once the strip exits the roll gap.

Both these criteria must be upheld in order to ensure a successful and fully amorphous casting.

4.2. Casting Speed

Examining the predicted strip surface temperature verses time, and the strip mid thickness temperature verses time, with respect to the two criteria described above, the range of allowable casting speeds may be identified as 2.5-3.5 cm/s.

The results of the model may be compared to that of the literature, for the allowable speeds predicted.

Only the mid thickness temperature for the 3 casting speeds has been plotted as this will be the area of concern in relation to the CCT curve.

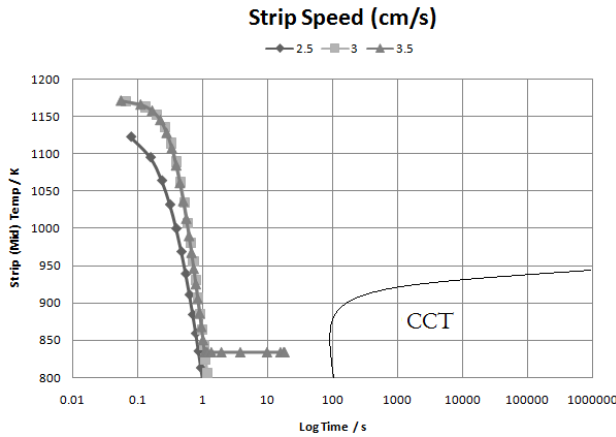


Fig. 1, Predicted mid-strip cooling curves for allowable casting speeds, after [3].

An estimate of the CCT curve has also been included in Fig. 1 in order to show the relative position of the cooling curves for the strip.

For a casting speed of 3.5 cm/s the exit point can be identified where the temperature plateaus i.e. the section of negligible air cooling. This area is below the range of the graph for both 2.5 and 3 cm/s.

The air cooling has been modelled as negligible whereas in a real situation there would be some small but finite amount of cooling based on the surroundings. The thermodynamics for crystallisation, as discussed earlier, are quite sluggish to take effect at this temperature but if the strip is maintained at a temperature close to 860 K for a long period of time it will eventually cross into the region bounded by the CCT curve as may well be the case for the 3.5 cm/s casting. Both the 2 and 3 cm/s casting will have low enough exit temperatures that crystallisation will be hindered.

4.3. Critical cooling rate

The critical cooling rate for Vit 1 is 1 K/s. The cooling rate achieved at the strip mid thickness for a 2mm strip, during casting is far higher than this ($\approx 700-1000$ K/s).

At the slowest casting speed (1cm/s) modelled for a 2mm strip, the rolls reach a temperature of approx. 90 °C.

4.4. Effects of strip thickness

Increasing the thickness from 2 to 4 mm and examining the temperature variation with time for both the strip surface and strip mid thickness, a new casting range is identified between 1 and 1.5 cm/s. Similarly for the case of a 1mm strip the casting speed needs to be within 6-9 cm/s to uphold the criteria discussed previously.

4.5. Effects of Heat Transfer Coefficient

Without changing the pattern of heat transfer i.e. the three distinct stages, the HTC values were doubled. The increased heat transfer significantly lowered the 2mm strip exit temperature and thus narrowed the range of allowable casting speeds (4.5-5 cm/s) based on the first criterion. Similarly by halving the initial HTC values, the strip exit temperature is increased. This has a much greater effect on the range of allowable casting speeds ($\approx 1.4-1.3$ cm/s) based on the second criterion.

5. Discussion

Combining the allowable casting speeds for both criteria results in the optimum range of 2.5 to 3.5 cm/s for a 2mm thick fully amorphous strip.

At casting speeds below 2.5 cm/s it can be seen that the strip surface temperature will be below T_g as shown in Fig. 2, which will halt casting / damage the rolls. At casting speeds above 3.5 cm/s the strip mid thickness temperature will be above 860 K which will result in crystallisation as shown in Fig. 3 [1].

As found in the literature [1,3] the microstructure of the cast strip will contain a small amount of crystalline particles which are present prior to casting. A melting procedure including a period designed to completely melt all particles followed by stabilising at a temperature low enough to ensure crystallization will not occur may be employed to eliminate any crystalline particles present prior to casting.

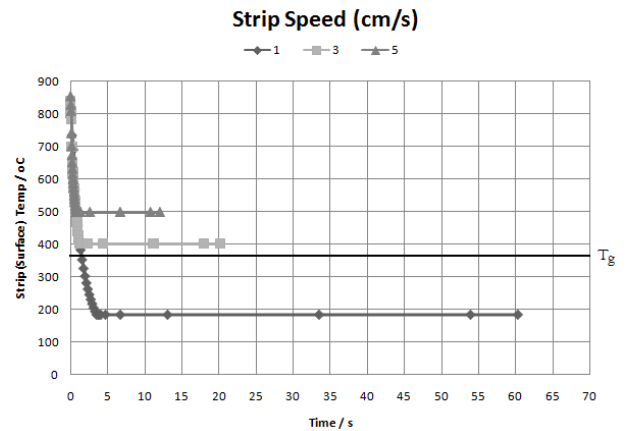


Fig. 2, Predicted Strip surface temperature v. time for 2mm BMG

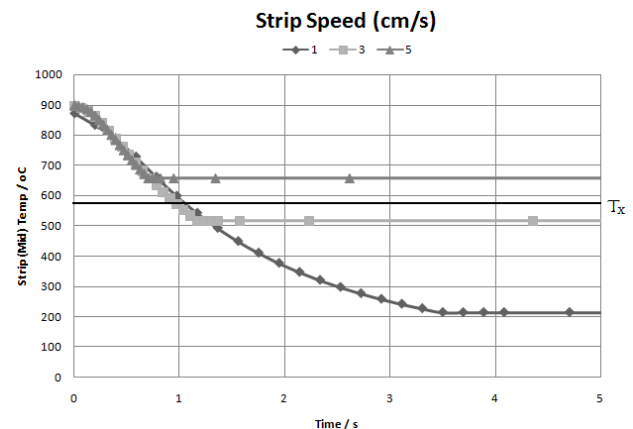


Fig. 3, Predicted mid-strip temperature v. time for 2mm BMG

The cooling rates observed (Fig. 4) give a good indication of the possible applications of TRC. The research carried out by Lee *et al* [3] confirmed LM2 alloy ($Zr_{56.2}Ti_{13.8}Cu_{6.9}Ni_{5.6}Nb_{5.0}Be_{12.5}$) with a critical cooling rate of 250 K/s could be successfully cast using TRC.

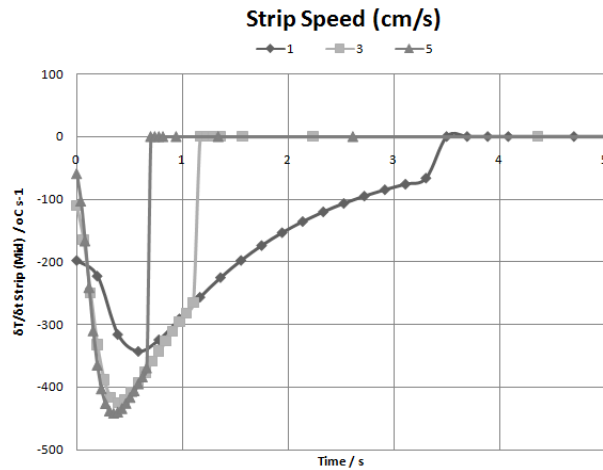


Fig. 4, Mid Strip cooling rate v time 2mm BMG

The point where the strip exits the roll bite is easily identified by the corresponding drop in temperature of the rolls.

Taking into account the 2 criteria for a successful casting, there is only a very narrow range in which to cast at a thickness of 4 mm i.e. between 1 and 1.5 cm/s. As the mid strip thickness temperature is likely to be very close to the nose of the CCT curve, a small amount of crystallisation will more than likely occur during the casting. The higher strip exit temperature relative to the 2 mm strip is due to the poor conductivity of Vit 1 when compared to a binary alloy such as aluminium. The thicker strip retains more heat as it takes longer to conduct the heat from the centre to the surface and away through the rolls. Of course the starting enthalpy also scales with strip thickness.

For the case of the 1 mm strip, there is now less distance through which heat has to be conducted, thus the temperature of the strip is reduced further along the contact length than is the case seen for the 2mm strip. Obviously at these lower temperatures there is no concern of the temperature at the strip mid thickness being too close to the CCT curve. This is an advantageous situation as the strip needs to be cast at higher speeds (6-9 cm/s) which, in turn means greater productivity.

The HTC is one of the hardest variables to define for the process. The literature [1,3] specifies a range of HTC between 0.3 to 0.4 $Wcm^{-2}K$ for a successful casting. For the model a range of 0.15-0.4 $Wcm^{-2}K$ was chosen. The low initial value accounts for the poor contact between the strip and the rolls which quickly proceeds to 0.25 $Wcm^{-2}K$ and then 0.4 $Wcm^{-2}K$, as viscosity and contact pressure increases.

By doubling the values used it may be seen that the increased amount of heat transfer significantly reduces the strip exit

temperature. Immediately obvious from this is the fact that the allowable casting will be reduced in order to stay with the limits specified by the two criteria.

If on the other hand the HTC values are halved, the strip will exit the rolls at higher temperatures which is acceptable based on the first criterion, but as for the case of increased thickness, the same problem will be encountered with the mid thickness temperature. This greatly limits the allowable casting range.

It can be seen that the model is quite sensitive to this variable. A lot of efforts should be applied to determining as accurate an estimate as possible for the casting conditions being used. This will ensure more realistic results which can subsequently be verified by casting trials.

6. Summary

The effects of changing the strip thickness were examined in relation to the range of casting speeds that would produce a fully amorphous strip. It was found that by doubling the strip thickness to 4 mm the range of possible casting speeds is greatly reduced, from 2.5 – 3.5 cm/s to 1 – 1.5 cm/s. With this in mind it is still possible to produce a fully amorphous strip but not at as productive a rate as thinner gauge strips.

Changing the heat transfer coefficient also has a significant effect on allowable range of casting speeds. This variable, being very hard to determine, is one of the primary limits on the accuracy of the model. Reasonable estimates may be made but if a more accurate figure could be obtained (e.g. by the methods used in [4]), the optimum casting conditions predicted by the model could be refined even more. This may become important as the possibility of twin roll casting more and more amorphous alloys are examined. If these alloys are on the borderline of success then accurate modelling will help reduce the cost and effort of further experimentation.

Bulk metallic glass is as Greer [5] says “on the threshold”. With the advances in understanding recently achieved the study of metallic glass will continue to be a hot topic for the foreseeable future. The applications of this material will be greatly increased with the breakthroughs expected from the ongoing research.

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