Physical and Numerical Simulation Based Optimization in Continuous Casting of Cu SMA Alloys

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The continuous casting process is a widely used attractive technology in modern metal industry. Despite the widespread application due to the inherent complexity from the underlying physics, it is still not well understood. The objective of this paper is to model the thermo-mechanical behavior in continuous casting of Cu based SMA alloys. A coupled thermo-mechanical numerical simulation of solidifying rod is implemented in ProCAST software suite capable of modeling process under full non-equilibrium process conditions. The model is applied to calculate full time dependent temperature and stress distribution during continuous casting. Special focus has been identification of the solidification front sensitivity on the various process parameters: casting speed, thermal contact conductivity and water cooling system thermal efficiency. The stability of the solidification front profile is examined and typical process parameters are proposed. Results from the simulations compare favorably with experimental experience that one of the key parameters is casting speed full time dependent profile.

Keywords: Material Processing, Continuous Casting, Solidification, Thermo-mechanical, Multiphysics

Introduction

Shape memory alloys (SMAs) are advanced functional materials with special feature of being capable of memorizing and recovering original shape before deformation. Shape memory behavior comes from martensite-austenite reversible diffusionless phase transformation. Such a transformation is obtained by mechanical (loading) or thermal means (cooling/heating). SMA show superelasticity if deformed by critical stress value in the right temperature range (providing thermoelastic martensite formation – collective, diffusionless, movement of atoms that results in a crystal structure change). When the external stress is removed the deformation disappears and the material spontaneously returns to the original phase.

The SMA effect was first discovered in Au-47.5 at.% Cd alloy (in 1951.) and then in In-Ti alloy (1953.). Since then it has been found that numerous alloys [2-4] show shape memory effect (Ag-Cd, Au-Cd, Cu-Al-Ni, Cu-Sn, Cu-Zn, Cu-Zn-X, where X=Si, Sn, Al etc., In-Ti, Ni-Al, Ni-Ti, Fe-Pt, Mn-Cu, Fe-Mn-Si etc.). Among them the three most popular polycrystalline shape memory alloys are: Ni-Ti, Cu-based (Cu-Zn-Al, Cu-Al-Ni, Cu-Al-Mn, Cu-Al-Be etc.) and ferrous alloys (Fe-Pt, Fe-Mn-Si etc.) [4]. In this work we focus our attention to the Cu based SMAs.

Possibility for using the SMA in actual applications was first realized for Ni-Ti alloy in 1963 by its discoverer William Buehler. The Ni-Ti alloy are commonly referred as Nitinol (derived from Ni-Ti Naval Ordinance Laboratories, part of the US Department of Defence). After the discovery it was not quite clear what physical phenomena in these metals is responsible for "remembering" their original shapes. Dr. Frederick E. Wang, an expert in crystal physics, discovered the structural changes at the

atomic level we mentioned in the preceding paragraph [4]. Nitinol, as binary SMA, is very attractive for industrial and medical applications due to the important shape memory effect, pseudoelasticity, corrosion resistance and biocompatibility. Nitinol alloys dominate on the commercial market (biomedical, aerospace and automotive industries etc.). However most Ti-Ni-based alloys cannot be used at temperatures above 100 ^{o}C.
On the other hand Cu-based shape memory alloys were found to reveal the shape memory effect in 1964 [5]. The main advantages of Cu-based SMA are their low price compared to other SMAs. Many Cu-based SMAs have a better thermal and electrical stability and a higher operating temperatures. Their very high elastic anisotropy and large grain size cause brittle and poor mechanical properties owing to the high degree of order in the parent phase. Adding some alloying elements such as Mn, Fe, Ti, Zr, B etc. to the alloys can significantly improve their ductility and other properties modifying their operating temperatures.
Cu-based SMAs are considered as important functional materials for applications in to actuator or sensor technologies, and are termed as so-called smart or intelligent materials. The most important advantages of these alloys as an actuation mechanism are: simplicity (wear effects are rather small), high power/weight (power/volume) ratios, low price etc. The applications of Cu-based SMAs have limitations due to the poor ductility and workability that is result of the coarse-grained microstructure, the high elastic anisotropy, as well as precipitation of the brittle second-phase particles [6]. In order to overcome this problems the Cu-Al-Ni-Mn and Cu-Al-Mn-Ti(B) were investigated. The Cu-Al-Mn-based shape memory alloys have high potential for practical applications in medical, electrical devices, micromachines and energy-storage technologies [7].

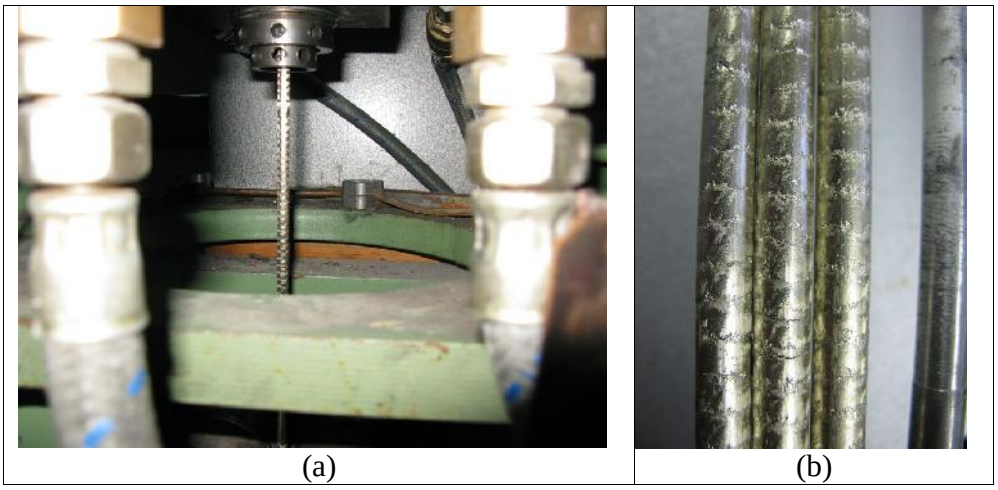
(a) (b)

Figure 1. Continuous casting: (a) rod exit from crystallizer and (b) alloy rods actually produced in experiment.

The production technologies of SMAs are induction melting, electro-arc melting, melt-spinning technique, powder metallurgy, combustion synthesis etc. [8,9]. Products can be hot worked (forgoing, rolling), cold working (wire drawing, rolling), etc. These techniques combined with heat treatments finally lead to the desired properties. Also, there are interesting microtechnology for production very thin shape memory alloys, such thin film production by vapour deposition, magnetron sputtering etc. But all these tecniques generally yield material/alloys in small quantities. It is well known that SMAs are very sensitive to the exact chemical composition and grain size (as a result of the heat treatment).

Coarse grains (25-100 μm) formed during solidification and after subsequent betatizing treatment of Cu-based SMAs make them brittle and highly prone for intergranular cracking during working. For example Cu-Al-Ni alloys have poor ductility due to the high degree of order and high elastic anisotropy in the parent β-phase. Generally, ternary Cu-based SMAs show generally a very large grain size. This problem can be solved by addition of adequate refining elements (Ti, B etc.) due to formation precipitates that limit the grain size and grain growth and/or by applying the technology of rapid solidification. In recent years the continuous casting technique is one of technology for production of SMAs, due to the special competitive growth mechanism of crystal and formation of cast product with a favorable texture [10, 11]. In order to overcome the deleterious effect of coarse grains, the computer modelling of alloy continuous casting process by appropriate technique is a necessity. Here we demonstrate, by numerical calculations that the complex thermal and mass transport phenomena are within the reach of the present computational framework. We have developed realistic model that simulates full continuous casting process of Cu-based SMAs using ProCAST software package. Our casting system is depicted schematically on Fig (1b) and is realized with ceramic vessel, graphite crystallizer and water cooling system made from copper. Despite apparent production simplicity, when it comes to physically model, such a casting process we face several theoretical challenges. This paper is organized as follows: in the second section, we explain main physical features of the simulation, in the third we present some numerical results and in the fourth we provide conclusion remarks as well as some future research directions.

Physical modeling

Purpose of a physical model is to get a better understanding of the different physical phenomena, their interaction and the impact on continuous casting process. Here we use commercial software package ProCAST[1] that is specifically designed for casting process simulation. Within the software we have designed continuous casting process simulation that resembles system in the LAB as shown in Fig. (1a and b). As is well known it is rather complicated to device appropriate physical model that captures all necessary features during nonequilibrium time evolution. Some important characteristics are:

1. enlarging of the space domain filled with alloy (here we use Mixed Lagrangian-Eulerian (MiLE) algorithm [12] for non-steady modelling of continuous casting) is accomplished by "accordion" technique which start with two regions filled with alloy, one is stationary (1) and one is moving (2). As the moving domain go away new layers are introduced filling the gap between and they form third domain (3). New layers are introduced on the interface between region 1 and 3.
2. time dependent boundary conditions between alloy and crystallizer where we have to take care that we have noncoincident mesh contact that is caused by relative motion of the casting and crystallizer
3. highly demanding numerical tools within the finite elements (FE) approach are necessary to take into account intricacies of the boundary and various surface effects (as can be seen on Fig 1b there is plenty of sharp angles in the geometry of the system)
4. we have also utilize mirror symmetry through yx plane so that computation time is highly reduced

Here we model system by taking into account chemical, thermal and mechanical properties of the Cu based alloy.

[1] ProCAST is trademark of ESI Group

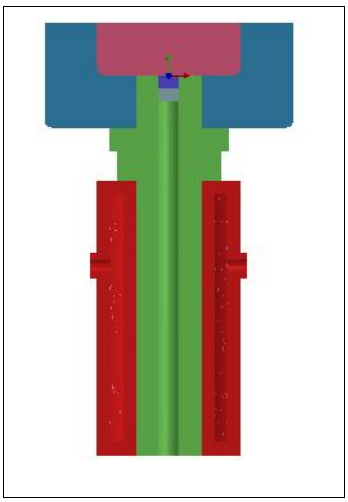

Figure 2. Continuous casting systemmodel system parts (green: graphite crystallizer 145 mm height; blue: ladle; violet/rose: alloy; red: copper water cooler)

One of the major difficulties in performing realistic thermomechanical simulation is connected to correctly take into account various contact thermal resistance characteristics because as is well known they depend in complicated way on the phase of the alloy (increase when solid phase is formed due to reduced contact surfaces). Since we do not have precise experimental values from the experiment, we use typical literature values with the hope that we catch right physics on the average. It is tedious and intractable at the moment tot take into account myriad nonequilibrium effects. We have to consider space and time resolution that is calculated in finite amount of time. Here we set smallest FE element to 0.5 mm and time is adaptive (readjust with every evolution step but around 0.01 s).

Results

In our LAB setting casting speed profile is essentially regular sequence of 5 mm pulls and 0.5 – 0.7 s waiting intervals. Water cooling system was set at 6 l/min. We started at 1250ºC, which is well above liquidus temperature. In the experiment and in the simulation we let system redistribute temperature field in order to minimise transient starting effects which are of no practical use (in simulation we let system thermalize for 30 s without mass transport).

Material thermal properties: liquidus is estimated (equilibrium thermodynamic phenomenological value) at T_l=1058ºC and solidus T_s=1020ºC, latent heat 233 kJ/kg and thermal conductivity, density, specific heat, solid fraction are all given as functions of temperature with typical forms for aluminum bronzes.

Fig 3 shows typical simulation result and specifically on (a) we present temperature field after it became almost stationary (75 s form simulation start) and (b) solid fraction at the same time that gives typical form of the solid liquid interface in continuous casting. From the simulation results we conclude that during casting the main thermal transport route is through the rod itself which is easy to understand since the thermal conductivity is highest along this direction. The main control parameter at hand to process adjustment is the casting speed (here speed profile is given in Fig.3). For the best results the best practice turn out to be shift sequencing so that rolls pull alloy rod following appropriate waiting intervals that enable local thermal equilibration. Waiting time increase is consequence of the graphite crystallizer heating up during the process since in continuous casting process heat and material constantly enter the system from the ladle.

The heat transfer to the crystallizer is critical to model correctly since the heat transfer from the shell is severely affected by shrinkage of the alloy with crystallization. The meniscus shape (see Fig 3b) is outcome of the heat transfer topology and we make no further assumptions. Present geometry prevents significant impact of the complex flow patterns like vortices or turbulences. It is essentially really surprising that foundries are very successful in adjusting optimal set of process conditions without complex physical models like this one (especially steelmakers have been very smart in twiddling parameters in very complex physical set ups [13]). It is fair to say that in this systems everything

counts and physical modeling is just a right way to take complex mutual interactions into account properly.

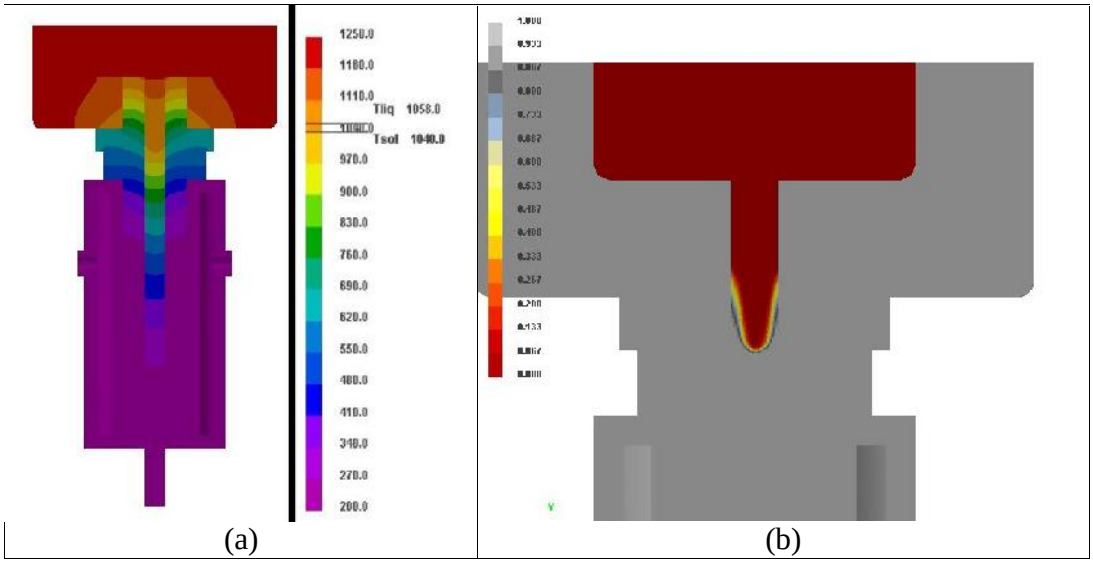

Figure 3. Simulation results at 75 s on mirror symmetry plane: (a) thermal field (b) solid fraction field depicting meniscus representing solid liquid interface.

Conclusion and outlook

- A FE thermo-mechanical model was developed in ProCAST software suite and applied to investigate casting speed for continuous casting of Cu based SMA alloys, assuming nonsteady conditions and average values of the transport properties. An accurate thermal and stress model, temperature dependent material properties, and non-equilibrium phase transformation temperatures.
- High casting speed leads to hotter material at the mold exit and may easily contain substantial amount of mushy content
- Efficient water cooling of the graphite crystallizer is essential since elevated temperatures cause severe drop in thermal conductivity and therefore increase percentage of the mushy phase
- Demanding noncoincident thermal contact of the alloy and the crystallizer make very difficult to generate satisfactory FE volume mesh
- In order to increase casting speed the best practice is to enlarge crystallizer length
- In thermal-stress calculation it is verified that stresses develop within the alloy and mould which can deform geometry leading to gap creation at the contact resulting in substantial increase in contact thermal resistance
- Several improvements can be made to present model to improve correspondence to real casting experiment that has been performed in the LAB
    - programmatically calculate contact thermal resistance to properly take into account various environments of the alloy during transport and solidification

- Perform microstructural simulations using Cellular Automata and Finite Element (CAFE) [14] calculation that effectively works on two scales (FE and cellular automata grid) in order to model microstructure development nucleation and growth of the grains.

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