Computational Materials Science 131 (2017) 35–43

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Identification of key liquid metal flow features in the physical conditioning of molten aluminium alloy with high shear processing

Mingming Tong [a,1], Jayesh B. Patel [b], Ian Stone [b], Zhongyun Fan [b], David J. Browne [a,*]

[a] School of Mechanical and Materials Engineering, University College Dublin, Ireland
[b] BCAST, Brunel University, UK

ARTICLE INFO

Article history:
Received 15 September 2016
Received in revised form 27 January 2017
Accepted 29 January 2017
Available online 9 February 2017

Keywords:
Rotor-stator mixer
High shear processing
Computer simulation
Shear rate
Flow rate
Aluminium alloy

ABSTRACT

Although treating molten alloy with high shear processing (HSP) can dramatically refine the microstructure of solidified aluminium alloys, it was also recently employed as part of an effective route to purification of contaminated aluminium alloy scrap. The key mechanisms of HSP include the dispersion of large aluminium oxide films and clusters into very fine oxide particles by the high shear rate, and the redistribution of bulk melt by the agitation. These fine oxides act as nucleation sites for iron-based intermetallic phases, the formation of which is a pre-cursor to purification of the alloy. Macroscopic flow features of HSP, such as flow rate and shear rate, influence its performance significantly. Simulation based on Computational Fluid Dynamics was used to predict key features of fluid flow during HSP in a static direct chill (DC) caster. It was found that the distribution of shear rate and mass flow rate is highly nonuniform in the caster, and only in the close vicinity of the mixing head is there a relatively high level of shear rate and effective melt agitation. Therefore, effective dispersion of oxide films and clusters, and resulting significant nucleation of the intermetallics and/or primary aluminium phase, can only occur near the mixing head, and not throughout the whole crucible. Confidence in the model validity was built, by comparison with post-solidification microstructures in a previous experiment with similar process parameters and geometry.

1. Introduction

Treating liquid metal with high shear processing (HSP) has been found to have significant influence on the properties of solidified aluminium alloys and magnesium alloys. As reviewed by Fan and co-workers [1,2], shearing the molten alloy in the liquid state using a rotor-stator mixer can dramatically refine the microstructure of direct chill (DC) cast aluminium alloys. Specifically, the HSP process can produce very fine equiaxed dendrites in the cast alloy [3] without using grain refiners. The high shear rate generated by the closed coupled rotor-stator mixer effectively fragments large aluminium oxide films and clusters into fine individual particles [4]. In high grade aluminium alloys, in which the content of iron and manganese is relatively low, the oxide particles were found to have very low lattice misfit with the α-Al phase on close packed crystallographic planes [5]. On cooling liquid aluminium alloys that have a relatively high level of iron (e.g. 1 wt% or higher), the iron-bearing intermetallics normally precipitate before the appearance of α-Al phase [6]. The lattice misfit between the aluminium oxide and iron bearing intermetallics was also found to be very low [7]. Therefore, the fine oxide particles act as potent nucleation sites for both the intermetallic and α-Al phases [8,9], during the solidification of aluminium alloys, and hence refine the microstructure of corresponding cast samples. Haghayeghi and Nastac have also reported [10] that shearing of a molten aluminium alloy prior to solidification resulted in a finer equiaxed grain size.

Besides the influence on microstructure refinement, it has recently been realized that HSP has great potential in purifying contaminated aluminium alloys. Iron is a very common and usually detrimental impurity in recycled aluminium alloys. An excessive level of iron can dramatically reduce the mechanical properties of the cast products. Due to the related thermodynamic features of such alloys [6,8], iron-bearing intermetallics (e.g. α AlFeMnSi) can effectively collect the iron component from molten scrap alloy while the primary α-Al solid solution phase is not yet formed [11]. Because the solid intermetallics are denser than the rest of the molten alloy, they can be separated from the bulk material by using a sedimentation technique, and hence the level of iron in the treated material is decreased. Such physical conditioning of the molten alloy using HSP is being used as the major technique in research on alloy purification, whereby the authors are trying to manufacture high performance aluminium alloys by processing contaminated recycled aluminium scrap.

---

[*] Corresponding author.
E-mail address: david.browne@ucd.ie (D.J. Browne).
[1] Present address: Mechanical Engineering, NUI Galway, Ireland.

http://dx.doi.org/10.1016/j.commatsci.2017.01.050
0927-0256/© 2017 Elsevier B.V. All rights reserved.

With the purpose of purifying the contaminated material, the key factor of HSP is the shear of molten metal by the rotor-stator mixer. The nucleation of iron-bearing intermetallics or primary α-Al phase is only effective when there is large number of available potent nucleation sites present. As presented in previous work [12], the shear rate was found to have a dominant influence on the breakage of oxide clusters during HSP. In order to systematically understand the influence of HSP process parameters on the resultant size of oxides, the flow features of the liquid metal (including particularly the shear rate and flow rate of melt) during the HSP with rotor-stator mixer have to be characterised.

Although there are a variety of experimental methods that are capable of measuring the features of fluid flow, such as Laser Doppler Anemometry and Particle Image Velocimetry, they are very difficult to apply in the measurement of flow features inside an opaque liquid metal. Because the molten metal is non-transparent, at high temperature and maybe flammable (e.g. magnesium alloys), it is infeasible or dangerous to place such experimental measurement equipment very close to the liquid that is being treated by HSP when operating the mixer. Therefore, computer modelling and simulation provide a very good alternative to calculate the related key features of melt flow during HSP.

Using computational fluid dynamics (CFD), computer simulation has been extensively employed in the prediction of flow features of metal processing, including such as casting [13] and welding [14,15]. In comparison, CFD modelling of melt conditioning is relatively rare. The majority of this has been dedicated to the degassing processes taking place in the gas stirred ladle of liquid metals [16–18]. CFD modelling has been applied to precipitation processes occurring in a mechanically agitated tank [19], in which a standard combination of baffle and impeller is used to agitate the fluid. However, the rotor-stator mixer that is used in HSP is such a closely coupled device [1,20] that it is inherently different from such a baffle-impeller combination. The published CFD modelling that is most relevant to the HSP process of our interest is the work by Utomoa et al. [21,22], in which a variety of flow features were analysed in the 3D CFD modelling of treating water with a rotor-stator mixer [21,22]. However, respective results were only analysed along the radius of the mixer and there were no analyses of flow features through the depth of the tank. Moreover, the rotor-stator mixer that was employed in the research of [21,22] is a type of commercially available mixer with major applications in food, cosmetics, chemical and pharmaceutical industries. The novel rotor-stator mixer that is employed in the HSP of liquid metal [1,20] is a recently invented device. Its design is very different from that of the conventional mixer (e.g. those used in [21,22]). Taking the dramatic differences between the properties of liquid metal (e.g. liquid aluminium alloy) and those of water into account (e.g. in terms Weber number and Prandtl number), we have had to develop a new CFD model in order to understand and predict the flow features of interest in the case of treating liquid metal with HSP.

In this paper, we firstly specify the configuration of the experimental device and computational case study. Then we present the details of our computational model and computer software. The key features of fluid flow simulations are analysed. Key computational predictions are compared with available experimental results from an HSP-treated solidified ingot, in order to provide confidence in the model.

2. Configuration of the case study and CFD model

The detailed configuration of treating liquid metal with HSP by using rotor-stator mixer can be found in Fig. 1 of [23]. Fig. 1a of the current paper schematically illustrates the overall setup of HSP of liquid metal, and Fig. 1b specifies some key dimensions of the mixing head, the 3D shape of which can be seen in Fig. 2. In the crucible (or mould), the impeller operates at relatively high speed. At the side of the stator near the mixing head, there are rows of small holes, numbered as shown in Fig. 1b. At the bottom of the mixing head, there is a relatively large opening. The liquid metal can flow in and out of the mixing head through these holes and opening.

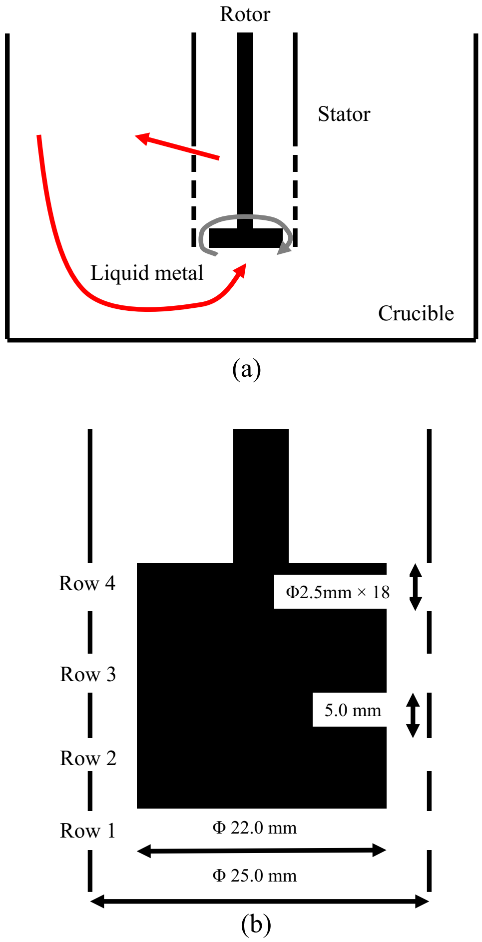

Fig. 1. Configuration of HSP process including the (a) overall setup, and (b) key dimensions of the mixing head.

The static DC caster is a cylindrical container of 60 mm in diameter. It is filled with liquid AA6060 aluminium alloy, to a depth of 120 mm. The rest of the caster contains air, above the liquid metal. The intent is to model the experiment carried out by Jones et al. [23], in which the mixer was removed from the superheated melt prior to alloy solidification. The mixer consists of a high speed spinning rotor and a stationary stator, which are coaxial and separated by a very small gap. The rotor consists of a long shaft with an impeller at its end, having four flat blades. The stator is a hollow tube, near the end of which is a series of circular holes in the wall. The geometry of the head of the mixer (i.e. the mixing head) can be seen in Fig. 1. As stated, the specific 3D geometrical features of the mixing head are illustrated in Fig. 2. The outer and inner diameters of the stator are 25 mm and 22 mm, respectively, and the diameter of the impeller is 21.5 mm. The rotor-stator annular gap is therefore 0.25 mm. There are 72 radial holes of 2.5 mm diameter in the stator, which are aligned along four rows or rings (of 18 equally spaced holes each). The impeller blades are 19 mm long. The mixer is placed inside the static DC caster at a depth of 70 mm relative to the bottom of the mixing head. The impeller speed is 4000 rpm.