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# Simulation of convective flow and thermal conditions during ultrasonic treatment of an Al-2Cu alloy

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ABSTRACT

Grain refinement of an Al-2Cu alloy using ultrasonic treatment was investigated numerically. A finite element model coupling fluid flow and heat transfer was developed and validated by comparing the results of both numerical simulations and physical experiments. The model successfully describes hydrodynamic fields generated by ultrasonic treatment and its influence on heat transfer. The simulations were used to study the influence of the duration of ultrasonic treatment and the associated acoustic streaming on convection and the resulting temperature distribution. It was revealed that a relatively cold sonotrode applied during ultrasonic treatment for up to 4 min created a casting environment that promoted crystal nucleation and enabled their growth and survival during transport of these grains into the bulk of the melt by strong convection. The enhanced convection established a low temperature gradient throughout the melt which favours the formation of an equiaxed grain structure. Therefore, the convection induced by acoustic streaming plays a critical role in facilitating nucleation, growth, and transport of grains.

## 1. Introduction

The formation of the as-cast structure of metallic alloys is controlled by the nucleation, growth and transport of grains within the melt, which in turn is affected by heat and solute diffusion and convection which also control the morphology of crystals [1]. By controlling the nucleation and the growth processes, the as-cast grain structure of alloys can be modified to promote nucleation and restrict grain growth producing a refined structure.

It is well known that vibration induced ultrasonically, mechanically or electromagnetically, can cause grain refinement that is similar to or better than chemical nucleation [1–4]. Ultrasonic vibration characterised by high-intensity and low-amplitude is one of the physical/mechanical means that have been demonstrated to refine the as-cast grain structure without using inoculant particles [5–8]. Decades of research have revealed that UltraSonic Treatment (UST) is a potentially efficient, clean and versatile technology. However, UST is still mostly confined to the laboratory. There has been limited industrial application due to a lack of understanding of the interactions between the ultrasonic field, the subsequently generated flow in the molten metal, and solidification [9]. Hence, the development of computational models that quantitatively describe hydrodynamic fields induced by ultrasonics are needed in order to understand and optimise UST processes.

The basis of ultrasonic processing is the formation of cavitation bubbles, their pulsation and collapse in melts subjected to high-frequency, high-power vibrations, and the resulting acoustic streaming that extends the influence of ultrasound to a larger melt volume [10]. It has been proposed that nucleation due to cavitation is caused by some mix of (1) an increase in the melting point and thus undercooling of the surrounding liquid [11] and (2) an improved wetting of the insoluble inclusions by the melt [12]. The undercooling of the first mechanism occurs because of the increased pressure when bubbles collapse and, therefore, enhanced nucleation can be expected [11]. The increased wetting of the second mechanism combines with substrate activation, in which an inert particle (like an oxide, carbide or boride) floating in the melt becomes an active substrate through the physical action of cavitation. The expansion and collapse of cavitation bubbles produce melt jets and surges of high pressure and temperature that strip the particles of absorbed gas and facilitate filling of the surface defects with liquid aluminium – the so called sono-capillary effect [5,6,9].

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Another mechanism that may occur is the detachment of crystals that nucleate directly on the sonotrode surface [12,13]. When a cold sonotrode is immersed into the melt, there is a significant temperature drop that initiates solidification on the sonotrode surface. Depending on the condition of the surrounding melt and the sonotrode surface, the solidified grains will either remelt, continue to grow, or be detached and swept into the bulk of the melt. The grains formed on the radiating face of the sonotrode will be subjected to alternating tensile and compressive loads due to vibration at the rate of the ultrasonic frequency possibly facilitating detachment. Further, instantaneous fluctuations of pressure and temperature due to cavitation may affect grain stability on the sonotrode surface. These fluctuations may cause a repeating cycle of nucleation, growth and detachment of crystals from the radiating surface of the sonotrode. The released grains or fragments would then be transported by acoustic streaming into the rest of the melt. The mechanism of detachment may be similar to that of the fragmentation of dendritic grains which has been proposed as an important contributor to grain refinement by UST [5].

It is well known that ultrasound propagating through a viscous fluid can induce a mass flow known as acoustic streaming. This phenomenon can in general be regarded as any flow generated by the force arising from the presence of a gradient in the time-averaged acoustic momentum flux in a fluid [14]. More strictly, it is described as the time averaged flow circulating near a vibrating surface which is attributed to the friction at a solid boundary that is vibrating and in contact with a fluid [15], or the steady flow in a fluid driven by the absorption of high amplitude acoustic oscillations during the passage of an acoustic wave. The latter is called “quartz wind” because it was observed when ultrasound piezoelectric quartz came into use [16–18]. Acoustic streaming is a steady flow of fluid formed by viscous attenuation of an acoustic wave. Using these concepts, Lighthill derived a Navier–Stokes based equation describing acoustic streaming as a non-oscillatory Reynolds stress, i.e. a time-averaged momentum flux in a fluid generated by the presence of a spatial gradient in the oscillatory Reynolds stress [14]. This approach provided a sound theoretical basic with which to model acoustic streaming under ultrasonic fields.

Computational modelling is a good way to explore the physics involved in UST [19–21], even if the widely separated time and length scales have made UST simulation impractical due to the significant computing resources and time required. In this paper, a computational model is presented that simulates acoustic streaming induced by a sonotrode by simplifying the interface between the sonotrode and the melt with the introduction of a momentum source over a volume which equals the cavitation zone. The model is based on Lighthill’s acoustic streaming theory [22], and assumes that all the acoustic energy absorbed by the liquid is converted into turbulent motion, forming a jet under the sonotrode tip. Using this assumption, the Navier-Stokes equations were solved using a ESI Group’s ProCAST virtual casting software [23], to determine the hydrodynamic field in the melt. The model was validated subsequently by comparing the results from computational simulations against obtained from experiments.

## 2. Experimental procedures

Four kilogram batches of Al–2 wt%Cu alloy (Al-2Cu) were melted in an electric furnace from commercially pure aluminium (99.7%) and pure copper (99.9%).

The ultrasonic device used in this work consisted of a 2 kW commercial ultrasound generator, an air cooled 20 kHz transducer, and a sonotrode made of molybdenum based alloy with a tip 18 mm in diameter. About 1 kg of the alloy was melted and preheated inside a graphite-clay crucible with dimensions 90 mm top diameter, 60 mm bottom diameter and 120 mm in height. When the melt temperature reached 720 ± 5 °C the crucible was transferred from the furnace to the experimental platform. When the melt temperature reached 694 °C which is 40 °C above the liquidus temperature of 654 °C, the powered sonotrode was immersed into the melt with the radiating surface 15 mm below the top surface of the melt and left there for the following three time ranges:

Range I - the UST was terminated at 660 °C
Range II – the UST was terminated at 654 °C, and
Range III – the UST was terminated after 4 min

These three ranges are shown in Fig. 1b. The procedure followed to terminate UST was to remove the sonotrode from the melt, turn off the ultrasonic power and then allow the melt to solidify.

Two K-type thermocouples were placed in the melt to one side of, and below, the sonotrode: one close to the wall of the crucible and the other a further 12.5 mm from the wall. Both thermocouples were placed 45 mm above the bottom of the crucible as indicated in Fig. 1a. A data-acquisition system collected temperature data by sampling 4 readings per second.

The cast samples were vertically sectioned along the centre symmetrical axis and prepared for microscopic observation using standard metallographic techniques.

## 3. Computational model and validation

### 3.1. Mathematical model

The model is focused on the development of convective melt flow and its impact on the temperature distribution in a crucible similar to that used in the experiments described above. Fig. 2 shows the geometric representation of the computational model and details the boundary conditions applied at the various heat exchange interfaces. The heat transfer coefficients (HTC) and the reference temperature ($T_{ref}$) applied at each boundary are shown in the inset table. A $T_{ref}$ of ‘Calc’ indicates that ProCAST calculates the appropriate temperature based on the material temperatures adjacent to the boundary.

The external surface of the crucible and exposed surfaces of the sonotrode and melt are air cooled, and the bottom surface of the crucible has been defined with forced cooling conditions to accommodate contact with the brick floor, as shown by section CD in Fig. 2.

#### 3.1.1. Acoustic streaming model

Acoustically induced ultrasound streaming has been modelled by assuming that the volume underneath the sonotrode tip, shown in red in Fig. 2, is a source of momentum that accelerates the surrounding fluid downwards forming a jet. It is further assumed that the acoustic energy $P$ attenuates at a constant rate per unit length $r_a$ along the distance $c$, and the rate of momentum of the jet $r_m$ equals the total acoustic momentum rate $r_a = P/c$ emitted from the acoustic power source.

Lighthill [22] calculated acoustic streaming from the Navier-stokes equation at higher Reynolds numbers by the following equation:

$$\rho(\vec{v}\cdot\nabla\vec{v}) = -\nabla p + \mu\nabla^2\vec{v} + \vec{F} \quad (1)$$

where the force $F$ causing streaming is the spatial variation of the Reynolds stress: