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Steps towards mathematical modeling of microcasting process from mesoscopic point of view

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Abstract

Microcasting is one of the significant technologies for the production of metallic micro parts with high aspect ratio (ratio of flow length to diameter). The aim of this research is to investigate scaling effects on mathematical formulation of fluid flow in micro casting and present governing differential equations.

Keywords: microcasting,, microchannel, meso scele, fluid flow, mathematical modeling.

1. Introduction

Microcasting is one of the key technologies enable the manufacture of small structures in the micrometer range or of larger parts carrying microstructures by using a metal melt which is cast into a microstructured mold. This technology has been successfully applied for manufacturing of instruments for surgery and dental devices, instruments for biotechnology and miniaturized devices for mechanical engineering. Microcasting, is generally identified with the investment casting process, which is known as the lost-wax, lost-mold technique (Baltes *et al*, 2005;Mohammadi 2011, Baumeister et al. 2002, 2004),. Figure 1 shows the micro investment casting process steps. First the plastic or wax pattern is made and embedded in a ceramic slip. After drying the ceramic mold is heated and sintered and the pattern will be lost during this process due to melting and burning. Finally the preheated ceramic mold is filled with metal melt by vacuum-pressure or centrifugal casting. After solidification, the ceramic mold is mechanically removed without destroying or influencing the cast surface. Depending on the casting alloy and the ceramic mold material, additional chemical cleaning processes may be sometimes necessary. Finally, the single parts are separated from the runner system.

By decrease in the dimensions of casting part, some challenges like complete filling of the mold and determining suitable operational pressure and other parameters get more important in microcasting technique. Figure 2 shows a common failure in microcasting caused by incomplete filling of mold. Mathematical modeling and simulation techniques like FVM and multi scale modeling techniques can be used to overcome microcasting challenges. In this investigation a review on mathematical modeling of microcasting technique is done and the differential equations that can be used to model fluid flow in microcasting are introduced.

2. Structural dimensions in microcasting

Microcasting is the manufacturing process of small structures in sub millimeter or even micrometer range or of larger parts carrying microstructures by using a metal melt which is cast into a microstructured mold. For jewelry and dental casting, the sizes of the produced parts are in the millimeter up to the centimeter range with structural details in the millimeter and submillimeter ranges. Further development and improvement of these techniques allowed the casting of microparts with structural details even in the micrometer range, which was confirmed by the replication of small-scale LIGA structures with high accuracy.

Usually, the smallest achievable structure size depends on the aspect ratio, which is defined as the ratio of flow length to wall thickness. Wall structures down to 20 μm width were produced with an aspect ratio of 6. The flow length and aspect ratio achievable are mainly influenced by the preheating temperature of the ceramic mold and by the filling pressure.

The control of quality in microcasting products cannot be achieved without a knowledge base which incorporates fluid flow mechanics of microcasting. first step in flow modeling is to explore governing differential equations of the process.

3. Solidification system in casting

In order to model and simulate micro casting process and recognize its fluid mechanics it is necessary to review solidification phenomena in casting.

Consider casting alloy in the liquid state contained in a rectangular cavity insulated on three sides depicted in Figure 3. At time t = 0 the left face is lowered to a temperature T cold < TL (the liquidus temperature). At later times three regions will exist in the cavity (see Figure 3); a full solid region, a solid + liquid mushy region, and a full liquid region. In metals the mushy region usually has a dendritic crystalline structure. The mushy region is bounded by liquidus and solidus (or eutectic) isotherms. So the casting flow system is a solid-liquid two phase system and should be modeled for such a system (Stefanescu 2009). As self-reliant units, holons have a degree of independence and handle circumstances and problems on their particular levels of existence without reaching higher level holons for assistance. The self-reliant characteristic ensures that holons are stable, able to survive disturbances.

4. Point of view in casting mathematical modeling and simulation

In a casting process effective phenomena in depending its nature can be discussed at three different length scales, macro-, micro-, and nano-scale.

The macro-scale (macrostructure): this scale is of the order of 100 to 10^{-3}m. Elements of the macro-scale include shrinkage cavity, cold shuts, macrosegregation, cracks, surface roughness (finish), and casting dimensions. These macrostructure features may sometimes dramatically influence casting properties and consequently castings acceptance by the customer.

The meso-scale: this scale allows description of the microstructure features at grain level, without resolving the grain boundary. Generally, it can be considered that the mesoscale is of the order of 10^{-4}m. There is no clear demarcation between the liquid and the solid. In fact, three regions can be observed: liquid, mushy (containing both liquid and solid), and solid. The computational models that describe solidification at the mesoscale are typically based on the Cellular Automaton (CA) technique.

The micro-scale (microstructure): this scale is of the order 10^{-4}m to 10^{-6}m. The micro-scale describes the complex morphology of the solidification grain. In a sound casting, mechanical properties depend on the solidification structure at the micro-scale level. The CA technique or the phase field methods that are used for modeling microstructure evolution at this scale calculate all this information.

Nano scale is of the order of 10^{-9}m (nanometers) and describes the atomic morphology of the solid-liquid interface. At this scale solidification is discussed in terms of nucleation and growth kinetics, which proceed by transfer of individual atoms from the liquid to the solid (Stefanescu 2009).

Microcasting encounters a reduction in length scale so elements like shrinkage cavity, filling of die, misruns, macrosegregation, cracks, surface roughness (finish), and casting dimensions which were of macroscale in macro casting, now should be treated as meso and microscale phenomena. This work presents basic differential equations to evaluate meso scale phenomena in microcasting.

5. Flow channel classification

As the flow channel size in processes such as casting becomes smaller, some of the conventional theories for (bulk) fluid, energy, and mass transport need to be revisited for validation. There are two fundamental elements responsible for departure from the "conventional" theories at microscale. For example, differences in modeling fluid flow in small diameter channels may arise as a result of:

(a) a change in the fundamental process, such as a deviation from the continuum assumption for fluid flow, or an increased influence of some additional forces, such as electrokinetic forces, etc.;

(b) uncertainty regarding the applicability of empirical factors derived from experiments conducted at larger scales, such as entrance and exit loss coefficients for fluid flow in channels, etc., or

(c) uncertainty in measurements at microscale, including geometrical dimensions and operating parameters.

Channel classification based on hydraulic diameter is intended to serve as a simple guide for conveying the dimensional range under consideration.

The classification proposed by Mehendale et al. (2006), divided the range from 1 to 100μmas microchannels, 100μm to 1mm as meso-channels,1 to 6 mm as compact passages, and greater than 6 mm as conventional passages.

The earlier channel classification scheme of Kandlikar and Grande (2003), is slightly modified, and a more general scheme based on the smallest channel dimension is presented in Table 1 (Kandlikar et al. 2006)

According to this classification, flow channels in micro casting usually are in the range of mesochannels and mathematical modeling should be done regarding to fluid flow in mesochannels.

Some researchers have found that, for fluid flow in cavities larger than 10 times of fluid molecular diameters, the continuum hypothesis will still be valid and navier-Stokes Equation can be used to analyze the flow (Xiangdong et al. 2011). The channels dimension in microcasting is in order of hundreds of micro meters that is sufficiently far from fluid molecular diameter thus continuum hypothesis and navier-stokes equations will still be valid with mesoscopic point of view.

6. Fluid flow equations of micro casting

The mathematical problem is to solve the mass, energy and momentum transport equations for the particular geometry and material of the casting.

If the fluid is incompressible and viscosity is constant across the fluid, the equation governing the shear stress, in its simplest form, states that a liquid, in parallel flow to a flat plate (boundary) will experience an x-directed tangential shearing stress, τ_{xy}. This shear stress is set up between two fluid layers (containing imaginary cuboids), in the presence of a shearing velocity gradient in the y-direction, according to:

$$\tau_{xy} = -\mu dU_x/dy \qquad (1)$$

In three dimensional flows, there can be a total of nine components of shear and normal stresses that need to be considered.

The combination of Newton's laws of viscosity and motion, plus continuity, leads to the famous Navier–Stokes (N-S) equation for flows within an incompressible, Newtonian fluid. In vectorial form, the N-S equation can be summarized as follows:

$$\frac{\partial}{\partial t}(\rho V) + [\nabla.\rho VV] = -\nabla P - [\nabla.\tau] + \rho g \qquad (2)$$

Where V is velocity vector, ρ is density and τ is shear stress and equals in fluid (Roderick & Guthrie 2009).

For a co-ordinate system, in which the "observer" to the flow, is stationary (Eulerian framework). This partial differential equation shows that the changes in values of the convective momentum terms (on the left hand side of the equation) as fluid passes through a fixed, infinitesimal volume element (e.g. an imaginary cuboid) within the flow field, is balanced by changes in pressure, together with shearing stresses at the surfaces of the micro-volume element, plus the forces of gravity.

There are two main difficulties in solving these equations for the problem of interest.Firstly, the application of these equations to a two-phase or multi-phase system, where all the quantities must describe not one but two phases; secondly, the formulation of the source terms for the various types of transport. Two main approaches, based on concepts from Continuum Mechanics, have been developed to solve the complicated problem of a two-phase system.

In the mixture-theory model each phase is regarded as a continuum that occupies the entire domain, and described by a set of variables that are continuous and differentiable functions of space and of time. Any location within the domain can be simultaneously occupied by all phases. The macroscopic transport equations are formulated using the classical mixture theory. Summation over the computational domain is used.

In the volume-averaged, all phases are considered separated. Phase quantities are continuous in one phase but discontinuous over the entire domain. Discontinuities are replaced by phase interaction relationships at interface boundary. Integration of microscopic equations over a finite volume is used (Stefanescu 2009).

5. Summery

Mathematical modeling of microcasting fluid flow can be done in three dimensional scale which are mesoscale include filling of cavity, crack formation, time of solidification, measure of suitable machine pressure and mold temperature, microscale dimension including morphology of the solidification grain and microsegregation, and nonoscale point of view which include the atomic morphology of the solid-liquid interface and nucleation and growth kinetics of grains. As the flow channel size becomes smaller, some of the conventional theories for (bulk) fluid, energy, and mass transport may need to be revisited for validation. The channels dimension in microcasting is in order of hundreds of micro meters that is sufficiently far from fluid molecular diameter thus continuum hypothesis and navier-stokes equations will still be valid with mesoscopic point of view.

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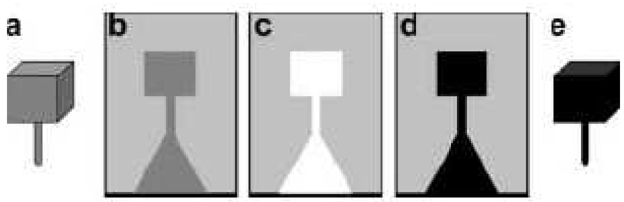

Figure 1: Micro investment casting process, **a** plastic pattern, **b** embedded in ceramic slip, **c** hollow form, **d** gold filled mold, **e** cast part

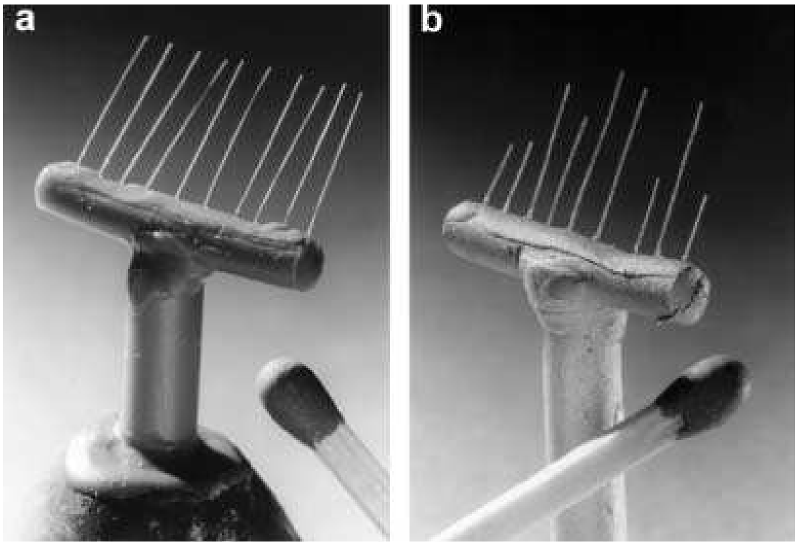

Figure 2: a casting pattern of micro wires, b incomplete filling of micro wires [4].

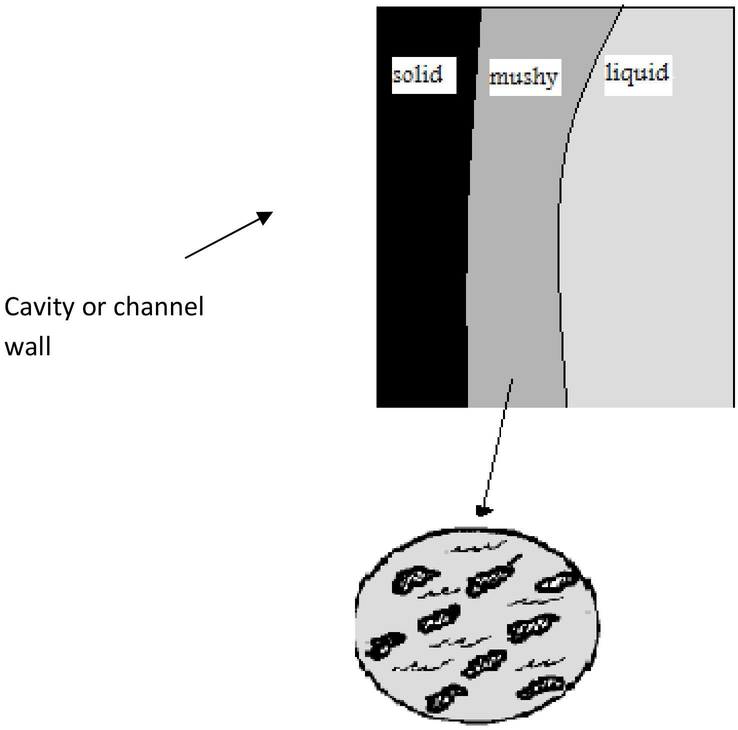

Figure 3: three regions in casting fluid in cavity

Table 1: flow channel classification

TYPE OF CHANNELS	DIMENSIONAL RANGE
Conventional channels	> 3 mm
mesochannels	3 mm > D > 200 μm
microchannels	200 μm > D > 10 μm
Transition microchannels	10 μm > D > 1 μm
Transition nanochannels	1 μm > D > 0.1 μm
Nanochannels	0.1 μm > D