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Acta Materialia 60 (2012) 6793–6803

Acta MATERIALIA

www.elsevier.com/locate/actamat

A 3-D coupled hydromechanical granular model for simulating the constitutive behavior of metallic alloys during solidification

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Received 16 May 2012; received in revised form 22 August 2012; accepted 30 August 2012
Available online 23 September 2012

Abstract

A three-dimensional (3-D) coupled hydromechanical granular model has been developed and validated to directly predict, for the first time, hot tear formation and stress–strain behavior in metallic alloys during solidification. This granular model consists of four separate 3-D modules: (i) the solidification module is used to generate the solid–liquid geometry at a given solid fraction; (ii) the fluid flow module (FFM) is used to calculate the solidification shrinkage and deformation-induced pressure drop within the intergranular liquid; (iii) the semi-solid deformation module (SDM) simulates the rheological behavior of the granular structure; and (iv) the failure module (FM) simulates crack initiation and propagation. Since solid deformation, intergranular flow and crack initiation are deeply linked together, the FFM, SDM and FM are coupled processes. This has been achieved through the development of a new three-phase interactive technique that couples the interaction between intergranular liquid, solid grains and growing voids. The results show that the pressure drop, and consequently hot tear formation, depends also on the compressibility of the mushy zone skeleton, in addition to the well-known contributors (lack of liquid feeding and semi-solid deformation).

Keywords: Microstructure; FE modeling; Semi-solid; Discrete element method; Hot tearing

1. Introduction

Hot tearing is one of the major casting defects that occurs during the solidification of metallic alloys. Previous studies have revealed that two phenomena lead to the formation of this defect: (i) a lack of intergranular melt flow to feed solidification shrinkage and (ii) thermally induced deformations caused by the combination of solid contraction and mechanical constraints. In order for simulations to successfully predict the formation of hot tearing, both the interaction between the solid and liquid phases and the evolution in microstructure that occurs during solidification must be included. It has recently been demonstrated that partially solidified alloys can exhibit the characteristics of a cohesionless granular material, including Reynolds's dilatancy, jamming, arching and stick–slip flow [1–3]. In this regard, semi-solid behavior is quite complex in comparison with the constitutive response of solids (small strains and high stresses) and liquids (low stresses and large strains). This difference is due to the very large change in viscosity that occurs concurrently with solidification [4]. Not surprisingly, modeling hot tear formation remains a challenging task.

The standard method for investigating semi-solid mechanical behavior, and by extension hot tearing, has been to treat the semi-solid as a continuum with mechanical properties represented by averaging methods (e.g. [5–8]). The main weakness of such approaches is that they cannot account for the localization of straining and feeding at grain boundaries, a feature that has been recently clearly demonstrated by in situ X-ray tomography tensile testing experiments [3].

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http://dx.doi.org/10.1016/j.actamat.2012.08.057

In the past few years, there has been interest in using granular methods in order to capture both stochastic effects and the solid–liquid interaction when simulating equiaxed globular solidification [9–11], semi-solid mechanical behavior [12–15] and liquid feeding [16–20]. In this method, the microstructure is usually approximated by polyhedral shapes based on the Voronoi diagram of a random set of nuclei, resulting in irregular grain arrangements. This approach has been used by Vernède et al. [13] to simulate the fluid flow in two dimensions caused by solidification shrinkage and grain movement, as well as by Phillion et al. [12] to investigate two-dimensional (2-D) semi-solid deformation at relatively small strains. In the latter work, the fluid was modeled as a solid material with a low elastic modulus and a small flow stress. Most recently, Sistaninia et al. have developed a series of 3-D models based on a combined finite element/discrete element method in order to investigate both the mechanical behavior of semi-solids under rather large deformations [15] and the corresponding fluid flow in a two-phase granular structure [19]. In the simulation of semi-solid deformation, the solid grains have been modeled using an elasto-viscoplastic constitutive law, while the remaining liquid films at the grain boundaries were approximated by flexible connectors. This allowed for relatively large deformations (up to $\epsilon \simeq 0.02$) to be achieved, while reducing the number of elements in the domain significantly, and avoided the issue of excessive deformation in the liquid elements seen in Ref. [12].

Although the previous granular models of solidification and semi-solid deformation have provided insight into hot tear formation, they were not successful in modelling hot tearing failure per se, i.e. the initiation and growth of a hot tear. In order to reach such a goal, the formation and percolation of voids within the intergranular liquid channels need to be considered. Furthermore, the inherent assumption of previous fluid flow models [16–20], i.e. that the grains remained fixed during solidification, needs to be addressed. In the present study, a 3-D coupled hydromechanical granular model of semi-solid deformation is developed to overcome the limitations and for the first time directly predict the formation of a hot tear in a two-phase medium. This has been achieved through development of a new three-phase interactive technique that couples the interaction between intergranular liquid, solid grains and growing voids.

2. Model development

The coupled hydromechanical granular model of semi-solid deformation is described below. It consists of four separate 3-D modules: (I) a solidification module (SM), for generating the initial solid–liquid geometry; (II) a fluid flow module (FFM), for the pressure drop calculation and localization of feeding; (III) a semi-solid deformation module (SDM), for the localization of deformation; and (IV) a failure module (FM), for modeling crack initiation and propagation. Modules II–IV are coupled together through the pressure in the liquid and the deformation of the solid in order to predict hot tear formation.

2.1. The solidification module

The solid–liquid geometry is generated using a 3-D granular solidification model known as GMS-3D [10,15]. The model is appropriate for grain-refined alloys with an equiaxed globular microstructure and assumes that the final grain structure is close to the Voronoi tessellation of random nucleation centers, as shown in Fig. 1a. To simplify the solidification calculation, the Voronoi regions are subdivided into small pyramids (see Fig. 1c), which are further divided into tetrahedral elements Fig. 1d. Because of their regular shape, solidification within a tetrahedron is reduced to a 1-D microsegregation problem, with infinite mixing in the liquid and back-diffusion in the solid. The master diffusion equation controlling the evolution of the solid–liquid interface in a tetrahedron is then given by [10]

$$v^* x^{*^2}(k_o - 1)C_\ell + \frac{1}{3}\left(L^3 - x^{*^3}\right)\frac{\dot{T}}{m_\ell} + x^{*^2} D_s \frac{\partial C_s}{\partial x}|_{x^*} = 0 \qquad (1)$$

where C_s and C_ℓ are the solid and liquid composition, v^* is the solidifying velocity of the interface, x^* is its actual position, k_o is the partition coefficient, D_s is the diffusion coefficient in the solid, $\dot{T}$ is the cooling rate and m_ℓ is the slope of the liquidus line. At the end of the solidification sequence, tetrahedrons from opposing grains come into contact with each other, and coalesce.

The solidification module used in the present work contains two major modifications compared to Refs. [10,15]: coalescence and undercooling, and rounded corners.

2.1.1. Coalescence and undercooling

Coalescence during solidification corresponds to the point at which two neighboring solid grains come into contact with each other and coalesce or bridge [21]. This occurs near the end of solidification, when the width, $2h$, of the liquid layer remaining between two grains becomes on the order of the diffuse solid–liquid interfacial thickness, δ. In this granular model, the liquid channel widths diminish to a small value only by the process of solidification. However, in reality the forces applied to the grains due to hydrostatic liquid pressure and gravity can accelerate this process and cause the grains to come into contact at lower g_s. Solidification of this last liquid film depends on the interfacial energies of the (dry) grain boundary, γ_{gb}, and of the solid–liquid interface, $\gamma_{s\ell}$. As shown by Rappaz et al. [21], the coalescence undercooling ΔT_b in a pure material required to have a dry boundary is given by

$$\Delta T_b = \frac{\gamma_{gb} - 2\gamma_{s\ell}}{\Delta s_f}\frac{1}{\delta} \qquad (2)$$

where Δs_f is the entropy of fusion per unit volume. γ_{gb} varies between 0 and $\gamma_{gb,max}$ as a function of grain misorientation $\Delta\theta$, and is shown in Fig. 2a for a [1 0 0] symmetric tilt