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Origin of grain orientation during solidification of an aluminum alloy

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ABSTRACT

The evolution of grain morphology during solidification of a moving aluminum alloy pool is simulated by considering heat transfer, flow of liquid metal in the molten pool and solidification parameters. The computationally efficient model consists of a 3D coupled heat transfer and fluid flow simulation to predict the molten pool shape and temperature field, and a 2D model of grain formation in the molten pool. The results demonstrate that columnar grains grow in a curved pattern rather than along straight lines from the fusion boundary towards the center of the molten pool. The calculated results are validated with independent experimental data. The computed ratio of local temperature gradient to solidification rate, G/R, is used to model the columnar to equiaxed transition during solidification. The simulated results show that only curved columnar grains are formed when the scanning speed is low (2.0 mm/s). In contrast, a transition from curved columnar to equiaxed morphologies occurs at the higher scanning speeds of 8.0 mm/s and 11.5 mm/s, with higher equiaxed grain fraction at higher speed. The similarities between the physical processes governing fusion welding and additive manufacturing (AM) make the model capable of predicting grain orientation in both processes.

1. Introduction

In both additive manufacturing and fusion welding, a moving pool of molten metal leaves behind a unique solidification pattern depending on the temperature field near the solidifying interface and the grain orientation of the substrate [1–6]. Control of microstructure is critical to achieve the desired mechanical and chemical properties of the fabricated components. Moving heat sources such as a laser beam, an electron beam or an electric arc create a fusion zone (FZ), a heat affected zone (HAZ) and microstructural gradients that affect the properties and performances of the fabricated product. Understanding the thermal history that creates these gradients is important, and has been computed through 3D modeling of heat transfer and fluid flow during welding. HAZ and FZ models need to be developed to connect the temperature history and the microstructural changes that occur. HAZ models have been created through kinetic models of phase transformations and Monte Carlo modeling [7–9]. But comparatively little has been done to predict the FZ microstructure.

The grain structure of the weld metal in the FZ significantly affects its resistance to solidification cracking and mechanical properties [10,11]. Curved columnar grains have been observed in the FZ of aluminum, and other alloys [10,12–15]. Equiaxed grains also form and coexist with columnar grains under some welding conditions [10,16]. The columnar grains are generally coarse and are characterized by fibrous texture and anisotropic mechanical properties. In contrast, equiaxed grains are usually small, do not exhibit fibrous texture, and are isotropic, with more uniform mechanical properties [17–19]. Although a large volume of experimental data have been reported about the grain morphologies in the weld metal of aluminum alloys, very little work has been done to simulate the evolution of curved columnar and equiaxed grains in the FZ. Furthermore, the mechanism of formation of these grains has not been thoroughly examined based on solidification theory.

The grain structure in the weld metal is predominantly controlled by the base metal grain structure and the welding conditions [20]. Initial grain growth occurs epitaxially at the partially melted grains in the base metal. Grains then grow along a certain crystallographic direction during the solidification process [21]. The preferred crystallographic directions for solidification of face-centered cubic aluminum alloys are ⟨100⟩. Therefore, in polycrystalline specimens containing randomly oriented grains, preferred growth during solidification occurs when the grains oriented along ⟨100⟩ directions grow along the maximum heat flow

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direction. The heat flow direction at the solid/liquid (S/L) interface is dependent on the local curvature of the boundary of the molten pool which depends on various welding variables [22,23]. Columnar structures in the weld metal can be promoted from the competitive growth during the solidification process whereby dendrites that are more aligned with the temperature gradient outgrow slower growing misaligned dendrites [20]. Under certain solidification conditions the curved columnar grains may transit to equiaxed grains at the center region of the weld during their growth process in some aluminum alloys [10,13]. The local solidification conditions at the S/L interface of the molten pool must be known to predict this transition.

In this paper a model is developed to calculate the geometric aspects of the FZ grains. Elemental segregation and the finer scale of solidification that describes the formation of cells or dendrites within the grains are not included for simplicity, but can be added later if higher fidelity models are required. It is shown that a model with such simplification can give realistic simulation of the grain morphology and orientation evolution during the solidification process while being computationally tractable. The model is validated with independent experimental data [13–15] for grain growth at various scanning speeds.

2. Models and methodology

The modeling of grain morphology and orientation evolution of aluminum alloys is implemented by incorporating a 3D heat transfer and fluid flow model [24,25] and a 2D grain growth model. The temperature and velocity fields, solidification parameters and the molten pool geometries are calculated using the well-tested, three dimensional, transient, heat transfer and fluid flow model. The computed results of temperature fields and solidification parameters are then used as input for the grain growth model, which simulates the evolution of grain structures. This grain growth model is newly developed to study the grain morphology and orientation evolution process in the FZ. The salient features of the models and the computational scheme for the grain growth process are presented below. Gas Tungsten Arc (GTA) welding of aluminum-magnesium-silicon alloy 6082 is considered as an example to illustrate the evolution of grain morphology and orientation.

2.1. Heat transfer and fluid flow model

3D heat transfer and fluid model has been used to simulate the temperature and velocity fields by solving the equations of conservation of mass, momentum and energy. The details of the governing equations, boundary conditions and the algorithm are available in our previous papers [24,26–28] and are not repeated here. The composition of the aluminum alloy is presented in Table 1. The data used for the numerical calculation are included in Table 2 and the welding parameters are listed in Table 3.

2.2. Grain growth model

2.2.1. Assumptions

The grain growth model focuses on the geometric aspects of grains and macrostructure in the FZ. The following simplifying assumptions are made to achieve computational efficiency: (1) The formation of planar, cellular or dendritic structures inside the grains is not considered. (2) Solute redistribution and local heat transfer in micro scale during the grain growth process are not considered. (3) The segregation of solutes is disregarded. (4) The competitive growth among grains with different crystallographic orientations is not considered for simplicity.

Table 2
Data used for numerical calculations.

Variables	Value
Arc radius (mm)	1.8
Arc energy efficiency	0.80
Solidus temperature (K)	855
Liquidus temperature (K)	925
Density of metal (kg m^{-3})	2700
Thermal conductivity of solid (W m^{-1} K^{-1})	180
Effective thermal conductivity of liquid (W m^{-1} K^{-1})	376
Effective viscosity of liquid (kg m^{-1} s^{-1})	0.009
Temperature coefficient of surface tension (N m^{-1} K^{-1})	−0.35
Specific heat of solid (J kg^{-1} K^{-1})	0.90
Specific heat of liquid (J kg^{-1} K^{-1})	1.18
Coefficient of thermal expansion (K^{-1})	2.30×10^{-5}

It is assumed that the columnar grains grow along location dependent directions and speeds as the molten pool moves along, and that the shape and size of the pool does not change with time when steady state is attained. However, more grains grow as the pool moves along at a constant speed. Geometrically, it appears that the grains are “pulled” by the curvature of the trailing edge of the molten pool which has a major influence on their shapes. The incremental growth of grains for each time step modifies the local directions and velocities, which change for all the grains as they tend to align parallel to the scanning direction toward the center of the molten pool.

The model does not predict the critical G/R value for transition from columnar to equiaxed grains. The existing theories for such transitions were developed for castings considering one dimensional heat conduction without any rigorous fluid flow considerations. These difficulties are apparent from the previous research [14], [29]. Here the formation of equiaxed grains in the FZ are determined from the critical G/R values obtained from independent previous research [14].

2.2.2. Grids and time steps

Grids are spaced uniformly 10 μm apart in both x- and y-directions for the grain growth calculations. The grids used in the heat transfer and fluid flow calculations are non-uniform and 5 to10 times larger in size. The temperature field obtained from the heat transfer and fluid flow model is interpolated to obtain local temperatures at each grid node of the finer grids used in the grain growth model. The time step Δt used in the calculation of grain growth is obtained by:

$$\Delta t = C\frac{a}{R_{\max}} \tag{1}$$

where C is a constant greater than 1, a is the mesh size, and $R_{\max}$ is the maximum solidification rate or the scanning speed. The molten pool moves a distance of $C{\cdot}a$ in every time step.

Table 1
Chemical compositions of aluminum alloy 6082 (wt%) [13].

Mg	Si	Fe	Mn	Cr	Ti	Ni	Cu	Zn	B	V	Zr	Al
0.75	0.86	0.42	0.43	0.06	0.032	0.01	0.09	0.07	0.0001	0.01	0.003	Bal.