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Three-dimensional modeling of grain structure evolution during welding of an aluminum alloy

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ABSTRACT

The structure and properties of welded and additively manufactured alloys are affected by the microstructural evolution in the fusion zone (FZ) and heat affected zone (HAZ). The motion of the liquid pool and the interdependence of grain growth in both the solid and liquid regions are important in the evolution of the final grain structure. Previous investigations of microstructure evolution have been limited to either the HAZ or the FZ and in many cases in idealized isothermal systems. Here we report the evolution of grain structure and topology in three dimensions in both the FZ and the HAZ considering the motion of the liquid pool. Temporal and spatial distributions of temperature obtained from a well-tested heat transfer and liquid metal flow calculation are combined with Monte Carlo and topology calculations in a computationally efficient manner. The computed results are tested against independent experimental data for arc welding of an aluminum alloy. The average size of the columnar grains in the FZ and the equiaxed grains in the HAZ are shown to decrease with increasing scanning speed. For a given weld, the size and aspect ratio of the columnar grains in the longitudinal and horizontal planes are shown to decrease with distance from the weld interface. It is further shown that the grain size distributions and topological class distributions in the HAZ are largely unaffected by the temporal and spatial variations of the temperature created by different welding parameters.

1. Introduction

The mechanical properties of additively manufactured and fusion welded components depend critically on the evolution of microstructure during solidification of a molten pool of liquid metal [1–3]. The unique solidification pattern originates from a combination of the motion of the liquid pool, the temperature field near the solidification front and the grain structure of the adjacent solid [4–6]. Understanding the thermal history and the evolution of grain structure and topology is important because they affect the microstructure, properties and performance of fabricated components. Well tested computationally efficient models for the calculation of three dimensional (3D) temperature fields are now available [7,8]. However, very little work has been done to connect the transient 3D temperature field with grain growth in the fusion zone (FZ) and the adjacent heat affected zone (HAZ).

Both additive manufacturing (AM) and welding involve spatially and temporally variable heating and cooling conditions [9–12]. The evolution of microstructure in these systems can only be revealed by considering the movement of the liquid pool and the interdependence of grain growth in both the solid and liquid regions. This is because the FZ microstructure is influenced by the evolution of HAZ microstructure and both are affected by the transient three dimensional temperature field which depend on process variables [13,14]. At the solidification front, grains start growing epitaxially with the partially melted grains in the solid region. The subsequent growth is influenced by both the preferred crystallographic direction and the dominant local heat flow direction at the growth interface [13,14]. For face-centered cubic aluminum alloys, the preferred crystallographic directions for solidification are <100>. Therefore, the most rapid growth of partially melted, randomly oriented, poly-crystalline grains occurs when the maximum heat flow direction aligns with the <100> directions. Other, misoriented, grains progress more slowly and are overtaken by faster moving grains.

Grain growth models for the HAZ have been proposed based on Monte Carlo (MC) technique using kinetic models of phase

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transformations [15–18]. Additionally, grain structure evolution in the FZ has been simulated by combining a two dimensional (2D) grain growth model with a 3D heat transfer and fluid flow model [5]. However, the 2D FZ model cannot take account of the impingement effects of columnar grains with various orientations in 3D space and the results are most useful in certain symmetry planes and not in the entire 3D component. Many of the applications of cellular automata and phase field models have considered either 2D calculations or 3D calculations in isothermal idealized systems to make the computationally intensive calculations tractable [19–21]. However, these simulations do not represent realistic welding or additive manufacturing conditions. In some other efforts, 3D grain growth utilized a computationally intensive cellular automaton model in the FZ, while ignoring grain growth in the HAZ which is known to affect the evolution of grain structure in the FZ [22–24]. Recent progress has also been reported for the grain structure prediction in the FZ and the HAZ during electron beam welding using a MC approach [25]. However, the temperature field and solidification parameters were obtained from a simplified model, which did not incorporate a detailed fluid-thermal consideration in the results.

The FZ grain structure affects mechanical properties and resistance to solidification cracking [13]. Both equiaxed and columnar grains form during welding and additive manufacturing and curved columnar grains have been observed in the FZ of aluminum alloys [13]. These grains are generally coarse and are characterized by anisotropic mechanical properties. In contrast, equiaxed grains that form in and around welds are usually small and are isotropic with uniform mechanical properties [26,27]. Although a large volume of experimental data have been reported about 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 examined during welding or additive manufacturing.

Here we examine the formation and growth of curved columnar grains in the FZ and the evolution of the equiaxed grains in the HAZ in three dimensions considering their interdependence. The effects of scanning speed on the orientation, size and aspect ratio of the columnar grains are also studied. Furthermore, the grain size distribution and topological class distribution of the equiaxed grains in the HAZ are investigated under various scanning speeds using MC simulations. The numerical model can reveal the temporal evolution as well as the spatial distribution of grain morphologies and orientations and provide valuable insights in understanding the grain structure and topology during the solidification process. GTA welding of 1050A aluminum (99.5% Al) is considered as an example to examine the grain growth process to validate the calculated results with independent experimental data.

2. Models and methodology

2.1. Heat transfer and fluid flow model

A 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 [7,8,28,29] and are not repeated here. The composition of the aluminum alloy, the data used for the numerical calculation, and the welding parameters are presented in Tables 1–3, respectively.

2.2. Grain growth model

2.2.1. Assumptions

The following assumptions are made in the model to achieve computational efficiency:

(1) The weld pool is at steady state, i.e. FZ and HAZ geometry does not change with time. For continuous linear welding, the validity of this assumption is well recognized. A major exception is spot welding and the analysis presented in this paper is not valid for spot welding. Another exception is for rapid welding using high power density when the instability of the keyhole precludes attainment of a steady state weld geometry.
(2) The grain growth direction is parallel to the maximum heat flow direction which is normal to the solidifying surface of the weld pool. Grains in the HAZ have random crystal orientations and during solidification grains in the FZ start to grow from these randomly oriented grains. Grains with crystallographic directions closest to the heat flow direction compete more favorably over other grains and dominate the grain structure very close to the weld pool boundary [13].
(3) The formations of planar, cellular or dendritic substructures inside the grains are not considered. The development of the subgrain structure does not have significant effect on the macroscopic grain structure for polycrystalline materials [13]. The propagating direction of a grain is determined by the local maximum heat flow direction [13].
(4) Solute redistribution and segregation during solidification are not considered because the material used was nearly pure aluminum (99.5% Al).
(5) Undercooling during solidification is not considered because it is small under the conditions examined in this paper. The kinetic undercooling due to high interface velocities are unimportant at welding speeds of ~10 mm/s, since the kinetic undercooling becomes important at 50 or 100 times these speeds [30,31]. Constitutional undercooling can also be neglected because the material used in this study was nearly pure aluminum. As a result, it is fair to assume that the solidification front is located on the solidus isotherm of the weld pool.

Table 2
Data used for the calculation and temperature and velocity fields.

Variables	Value
Arc radius (mm)	1.8
Arc energy efficiency	0.75
Solidus temperature (K)	917
Liquidus temperature (K)	930
Density of metal (kg m^{-3})	2700
Thermal conductivity of solid (W m^{-1} K^{-1})	211
Effective thermal conductivity of liquid (W m^{-1} K^{-1})	126
Effective viscosity of liquid (kg m^{-1} s^{-1})	0.01
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}

Table 1
Chemical compositions of 1050A aluminum (wt. %) [40].

Mg	Si	Fe	Mn	Cr	Ti	Ni	Cu	Zn	B	V	Zr	Al
0.001	0.09	0.24	0.004	0.001	0.008	0.004	0.01	0.01	0.0003	0.01	0.001	Bal.