3-D multi-scale modelling of deformation within the weld mushy zone

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Abstract

The deformation of the fusion weld mushy zone, as a critical factor in solidification cracking, has been simulated by combining a 3D multi-scale model of solidification and microstructure with a deformation model that includes the effects of solidification shrinkage, thermo-mechanical forces and restraining forces. This new model is then used to investigate the role of welding parameters on the deformation rate of micro liquid channels during Gas Tungsten Arc welding of AA6061. It is shown that the internal normal deformation rate due to solidification shrinkage and also the external normal deformation rate caused by external forces are both highest for the micro liquid channels at the center of the mushy zone where solidification cracks usually occur. Furthermore, the model shows that welding travel speed and welding current strongly influence the deformation rate of the weld mushy zone and consequently the solidification cracking susceptibility of the weld. The model can be also used to link micro-scale phenomena with the macro-scale characteristics of solidification cracking during welding.

Keywords: Welding; Modeling; Micro liquid channel; Multi-scale; 3D.

1. Introduction

The semisolid region of a weld, called the mushy zone, consists of grains forming a solid body within a network of micro liquid channels covering each grain [1-3]. At high solid fraction, the

micro liquid channels may deform due to the solidification shrinkage, if a lack of feeding is present, and consequently induce local tensile deformation [3-6]. Note that the deformation of a micro liquid channel refers to enlargement of the space confined inside the channel due to separation of channel walls, and not deformation as generally applied within solid mechanics. The mushy zone can also deform because of external forces acting on the weld pool. Specifically, the thermo-mechanical force field evolving during solidification [7, 8], along with the restraining forces explicitly applied to the base metal [3, 9-10], externally distort the mushy zone.

Fusion welding is made difficult due to the propensity for defect formation in the semisolid state, especially solidification cracks [11]. Several studies have been carried out to investigate the mechanism behind solidification cracking [12-14]. These studies link the formation of solidification cracks to two key factors: 1) the metallurgical characteristics of the weld, and 2) the deformation of the weld mushy zone. As shown in reviews by Eskin et al. [11] and Cross et al. [15], deformation of the semisolid structure is a key factor in the formation of this defect. In general, models of solidification cracking were developed for casting processes and then adapted to welding as required. The majority of these models are applicable at the macro-scale, involving only the average deformation characteristics of the semisolid [16]. For instance, according to the strain theory [17], a solidification crack forms if the average strain within the semisolid exceeds a critical strain value. Other macro-scale examples include strain rate-based models [18, 19], in which the semisolid cracks once the average strain rate rises beyond a critical value. At the micro-scale, Rappaz et al. [20] developed the so-called RDG solidification cracking criterion based on a mass balance performed over the entire mushy zone that links the pressure drop within a micro liquid channel and consequently the formation of solidification cracks to both the

local flow rate of the channel and the normal separation rate of the channel walls. Recently, Kou applied a similar mass-balance technique but focused on the grain boundary instead of the mushy zone as a whole to develop a differential equation that provides a cracking criterion inside a micro liquid channel [4]. Unlike the RDG model in which the differential control volume consists of both the liquid films and the solid grains, the Kou model focuses on only the micro liquid channels.

Multi-scale modelling of solidification, including the well-known cellular automaton approach for microstructure development (e.g. [3, 21-22]) and more recently the granular modelling approach (e.g. [23-25]), is useful for understanding the relationships between phenomena occurring at different length-scales. Micro-scale models of solidification cracking, like Rappaz's and Kou's criteria, appear to suite multi-scale modelling of solidification since they can be applied to each micro liquid channel within a representative network of channels to examine local solidification cracking susceptibility. However, in order to implement micro-scale solidification cracking models within a multi-scale context, the local characteristics of a single micro liquid channel, i.e. the deformation and flow rate, have to be determined. Vernède et al. [24] and Sistaninia et al. [6, 23, 25] have developed a sophisticated numerical method for multi-scale modelling of solidification cracking during casting. Following reconstruction of the network of micro liquid channels using a granular model of solidification, they simulated the local flow rate [23] and the separation of the walls of every single channel [25]. Similar studies in welding are less advanced. Cross et al. [26] modeled the separation of grains during welding using a simplified 2D structure with horizontal and vertical micro liquid channels. Bordreuil et al. [3] predicted the local characteristics of the micro liquid channels during welding using a 2D replica of the mushy zone developed by cellular automata. However, the results were limited by

the use of 2D geometry, which both induces discontinuity in the liquid network [1], and poorly represents the morphology of the solidifying weld microstructure. Also, these models did not consider the effects of external thermo-mechanical forces on the deformation of the micro liquid channels, and therefore cannot yield the deformation characteristics of the channels in a self-restrained welding condition.

As the first step towards multi-scale modelling of solidification cracking in welding, this study presents a method to estimate the deformation characteristics of micro liquid channels. Both the internal deformation rate of the micro liquid channels due to solidification shrinkage, and the external deformation rate of the mushy zone considering the thermo-mechanical and restraining forces are included. The external deformation rate is distributed to each micro liquid channel by means of a modified partitioning method. Finally, the role of various parameters including solid fraction and welding parameters on the deformation rate of micro liquid channels is investigated. Although this model is specifically developed for Gas Tungsten Arc (GTA) welding of aluminum 6061 alloys, the methodology is applicable to a wide range of welding processes and alloys.

2. Model description

2.1. 3-D granular solidification model for welding

The microstructure of the weld mushy zone can be reconstructed using a solidification model simulating the evolution of the solid skeleton and the network of micro liquid channels. The majority of solidification models in welding are based on either phase field [27-30] or cellular automaton [3, 21-22]. Due to computational costs, phase field is restricted to only few grains and is thus not suitable for multi-scale modelling. Although cellular automaton can model the

microstructure of the entire weld pool, the liquid network suffers from a discontinuity problem [3]. Recently, Zareie Rajani and Phillion [1] developed a transient mesoscale model to reproduce the mushy zone during GTA welding of aluminum AA 6061 that is based on a granular method for modelling solidification [24]. The model is sensitive to welding conditions, creating different microstructures based on the choice of welding parameters. The base idea behind the granular solidification model for welding (further details given in [1]) is that the weld microstructure can be approximated using a sequence of Voronoi tessellations or nearest neighbor diagrams. Solidification within each grain is then simulated assuming that each polyhedron within the Voronoi diagram represents one grain. The present study utilizes this solidification model to create a continuous 3D network of micro liquid channels for further study of the deformation characteristics of a semisolid weld. For a given set of welding parameters, a representative volume element (RVE), i.e. a section of the weld pool is first generated by the model. Only one side of the weld is modeled due to symmetry. A schematic showing the placement of the RVE within the entire weld pool, along with the global X-Y-Z coordinate system corresponding to the penetration direction, lateral direction, and weld line, respectively, is provided in Fig. 1. The size of the RVE is given by welding experimental data (depth of penetration and half-width). Specifically, the dimension along the X direction is given by “depth of penetration” +200 μm , and along the Y dimension is given by “half-width of the weld” +200 μm . The extra 200 μm in X and Y were added to include a small amount of the base metal within the RVE. The Z dimension, along the weld line, is set to 1000 μm . This value was chosen as a compromise between capturing the entire mushy zone and computational cost. Within the RVE, an unstructured grid is then generated to represent the structure of the weld at the macro-scale (size and shape) and micro-scale (size of equiaxed and columnar grains) based on the input welding

parameters. Specifically, a Voronoi tessellation is applied to nuclei placed pseudo-randomly throughout the weld to create columnar and equiaxed grains. As Fig. 1 shows, the columnar grains extend from the fusion boundary towards the center of the weld, while the equiaxed grains are located at the center of the weld. Due to the use of experimental input data, different microstructures are created for different welding conditions. For instance, for high welding travel speeds and lower welding currents, the reconstructed microstructure consists of a small weld with a mainly columnar structure, while for lower welding travel speeds and high welding currents, the overall reconstructed RVE is larger, with also a larger equiaxed region. Due to the use of experimental data for the dimensions of the weld, this model indirectly accounts for the effects of thermal phenomena and fluid flow on the shape and size of the weld. However, this model cannot reconstruct the dendritic feature of the grains, nor can the columnar grains be curved because of the intrinsic characteristic of a Voronoi tessellation.

Since this granular solidification model for welding [1] is sensitive to welding conditions and requires experimental input data, a series of welding experiments were first carried out to acquire macro-scale (size and shape) and micro-scale (size of equiaxed and columnar grains) features of the weld over a large set of welding parameters. The details regarding the welding experiments and the methodology for their link to the RVE were presented in Ref. [1]. In brief, a series of 28 bead-on-plate weld experiments were performed on aluminum AA6061 plates, 200 mm long, 100 mm wide, and 3 mm thick, at various travel speeds and welding currents using an automatic GTA welding machine as shown in Fig. 2a. At the completion of the experiments, each welded specimen was analyzed via optical microscopy in order to quantify the weld microstructure. The relevant process-microstructure maps are given in Figure 3 of reference [1].

After generating the weld microstructure, each grain is split into smaller tetrahedral elements. Solidification is then simulated through tracking of the solidification fronts that split each element into separate solid and liquid regions. As presented in [1], tracking the motion of each solidification front within the weld pool occurs by combining an evolving temperature field generated by the 3D Rosenthal equation [31] with a solid fraction curve for AA 6061 generated by Thermocalc under Scheil solidification conditions. The Rosenthal equation predicts the thermal field, T , during welding as a function of spatial coordinates R_c (radial distance from the center of the weld) and D_c (distance from the center of the weld along the weld line),

$$\frac{2\pi(T - T_o)KR_c}{Q} = \exp\left[\frac{-V(R_c - D_c)}{2\alpha}\right] \quad (1)$$

where T_o is the initial temperature of the workpiece, V is the travel speed of the torch, Q is the heat transferred from the torch to the metal, K and α are the thermal conductivity and diffusivity of the base metal. The main unknown in Eq. (1) is Q , since the actual heat transferred from the torch to the metal will depend on the welding conditions. This heat transfer coefficient was used as a fitting parameter to match the predictions made by the Rosenthal equation to thermocouple data from each of the 28 welding experiments with each experiments having a different Q value. Since the Rosenthal equation does not account for time, but instead outputs the thermal field around the weld pool at steady-state, the quasi-static approximation was applied. Specifically, as the welding torch travels, the quasi-static isothermal surfaces attached to the weld pool also travel. Thus, a given point on the workpiece experiences variations in temperature during welding. In this model, the isothermal surfaces given by the Rosenthal equation were moved with the same traveling speed as of the welding torch to plot the thermal histories of the desired points. The results from one example fitting exercise are given in Fig. 2, for a weld fabricated at welding speed of 5 mm/s and welding current of 140 A. Fig. 2a and b show the location of these

points in relation to the weld line. The obtained thermal histories corresponding to three thermocouples are shown in Fig. 2c. As can be seen, an excellent fit is found between the experiments and the predictions from the fitted Rosenthal equations.

Fig. 3 shows the semisolid structure at two different average solid fractions (0.55 and 0.8) that were welded using a welding travel speed of 2 mm/s and a welding current of 120 A; the empty space represents the liquid phase. This particular simulation consisted of 582 columnar grains each 200 μm in length, 1674 equiaxed grains each 60 μm in diameter, and $\sim 10,000$ total elements. As can be seen in the figure, the evolving semi-solid results in the formation of micro liquid channels at the grain boundaries. The main output of the model is the channel width and velocity of the channel walls as a function of time during welding. The geometry of a single micro liquid channel is shown in Fig. 4a, along with the applied local coordinate system. The origin is fixed on one of the channel walls and the local z axis is orthogonal. The corresponding network of micro liquid channels, obtained by assembling the individual channels, is shown in Fig. 4b. As solidification evolves, the channel widths decrease until the grains coalesce.

2.2. Modelling the deformation rate of the micro liquid channels

At any given time, a network of micro liquid channels within the weld mushy zone can be assembled using the granular solidification model for welding. This RVE is then used to investigate semi-solid deformation. Although the RVE can be characterized using an average fraction solid, the actual fraction solid will vary with position since a weld contains strong temperature gradients.

Assuming that the walls of the micro liquid channels within the RVE remain parallel during welding [4], the deformation rate vector $\overrightarrow{\delta^i}$, where i is a counter representing the channel

number, can be decomposed into two components. The first is the normal deformation rate along the local z direction ($\vec{\delta}_z^i$), representing the separation rate of the channel walls. The second is the shear deformation rate ($\vec{\delta}_{xy}^i$), characterizing the relative displacement of the walls parallel to the local xy surface. According to the micro-scale models [4, 20], it is only the separation rate of the channel walls that affects the formation of solidification cracks within the micro liquid channel. Thus, the shear component of the deformation rate vector can be ignored. Note that the term “normal” refers to the direction perpendicular to the orientation of the micro liquid channel.

The normal deformation rate ($\dot{\delta}_z^i$) can be further divided into internal and external components based on the source of deformation,

$$\dot{\delta}_z^i = \dot{\delta}_{z,int}^i + \dot{\delta}_{z,ext}^i \quad (2)$$

where $\dot{\delta}_{z,int}^i$ corresponds to the internal normal deformation rate caused by solidification shrinkage, and $\dot{\delta}_{z,ext}^i$ is the external normal deformation rate induced by the external sources that act on the mushy zone and distort the entire network of micro liquid channels.

2.2.1 Internal normal deformation rate

It has been already shown that the recession rate of a solidification front due to solidification shrinkage is given by βv^* [23], where v^* is the velocity of the solidification front, $\beta = (\rho_s/\rho_l - 1)$ is the shrinkage factor, and ρ_l and ρ_s are the densities of the liquid and solid. As a result, the separation rate of the walls of any individual channel along the local z direction and consequently the internal normal deformation rate can be obtained by:

$$\dot{\delta}_{z,int}^i = \beta(v_1^* + v_2^*) \quad (3)$$

where v_1^* and v_2^* are the velocities of the two channel walls, given by the solidification model, that make up an individual micro liquid channel. The velocity of a channel wall is directly proportional to $\frac{dT}{dt} \frac{\partial f_s}{\partial T}$, i.e. the product of the cooling rate and the solidification rate. The solidification rate for AA 6061 and consequently the velocity of the channel walls becomes significantly reduced as the temperature decreases and the solid fraction increases [1, 4]. The present model utilizes Eq. (3) and the output of the solidification model to determine the evolution of the internal normal deformation rate of every single micro liquid channel within the weld pool at a given time.

2.2.2. External normal deformation rate

Unlike the internal normal deformation rate, the external normal deformation rate applied to individual micro liquid channels cannot be directly determined through solidification models. Instead, it is quantified using a two-stage process. First, the average strain rate of the entire weld mushy zone, denoted global strain rate, $\dot{\epsilon}$, is determined and then translated to a global deformation rate, $\dot{\delta}$. Second, the global deformation rate is partitioned amongst each micro liquid channel to yield $\dot{\delta}_{z,ext}^i$. Note that the global deformation/strain rate refers to only the lateral tensile component (Y-dir in Fig. 1), i.e. the component perpendicular to the weld line since it is tensile deformation in this direction that governs solidification cracking in welding [7, 26, 32].

2.2.2.1. Calculation of the Global strain rate

As the mushy zone solidifies, the base metal thermo-mechanically reacts to the thermal shrinkage and solidification shrinkage of the weld, and also temperature variations in the heat affected zone, evolving a transient thermo-mechanical force field that distorts the mushy zone [7,

33-35]. Concurrently, the mushy zone can deform as a result of the restraining forces applied to the base metal [36]. Hence, the global strain rate consists of:

$$\dot{\epsilon} = \dot{\epsilon}_{th} + \dot{\epsilon}_{re} \quad (4)$$

where $\dot{\epsilon}_{th}$ and $\dot{\epsilon}_{re}$ are the strain rates induced by the thermo-mechanical forces and the restraining forces. While the restraining strain can be directly controlled and measured based on the restraining forces explicitly applied to the base metal [36], the thermo-mechanical component of the global strain rate has a complex nature and cannot be simply controlled and measured.

There are two common approaches for treating the thermo-mechanical component of the global strain rate. First, $\dot{\epsilon}_{th}$ can be neglected assuming that $\dot{\epsilon}_{re}$ is significantly large and therefore dominates the deformation of the mushy zone. This assumption suits solidification crack sensitivity tests such as Varestraint in which high external strain rates are applied to the base metal. However, this approach cannot be applied to self-restrained welding conditions where $\dot{\epsilon}_{re} = 0$. The self-restrained welding condition is defined as a welding condition in which every point on the edges of the workpiece is tightly clamped, and therefore the edges of the workpiece are fixed in all directions. Alternatively $\dot{\epsilon}_{th}$ can be experimentally measured [9, 26]. However, the extensometer is usually located across the weld root in order to avoid a collision with the welding torch, which can cause significant measuring errors. Recently, Zareie Rajani and Phillion [7] have modeled the evolution of thermo-mechanical stresses that act laterally on the fusion surface to deform the mushy zone during GTA welding of AA 6061 alloys. The restraining strains are modelled in one of two ways. In the case where self-restraint is imposed, a Dirichlet boundary condition is applied to the edge of the workpiece, restricting the displacement of this surface. This condition mimics the effect of clamping on the thermo-mechanical stresses.

In the case when a restraining force is imposed, a known displacement rate is applied to the edge of the workpiece, in a direction perpendicular to the weld line. This previous study showed that the thermo-mechanical stress begins to evolve at high solid fractions once the mushy zone is percolated, i.e. once a continuous solid bridge forms across the mushy zone. Welding current and welding travel speed were also shown to strongly affect this thermo-mechanical tensile stress. In the present study, this lateral stress acting on the fusion surface is coupled with a visco-plastic constitutive equation for semisolid AA 6061 [37] to calculate $\dot{\epsilon}_{th}$.

The constitutive equation for semisolid AA 6061 is of the form:

$$\sigma = e^{(a-bT)}(\epsilon + \epsilon_o)^n(\dot{\epsilon} + \dot{\epsilon}_o)^m(1 - \alpha f_l) \quad (5)$$

where a , b , n , m , $\dot{\epsilon}_o$, ϵ_o , and α are empirical constants [37], T represents the average temperature of the mushy zone in Kelvin and f_l is the average liquid fraction of the mushy zone. By rearranging Eq. (5), one can express the thermo-mechanical strains at t_2 and t_1 , i.e. ϵ_2 and ϵ_1 , as a function of their corresponding thermo-mechanical stress values, i.e. σ_2 and σ_1 :

$$\epsilon_2 = \left[\frac{\sigma_2}{e^{(a-bT)}(\dot{\epsilon}_2 + \dot{\epsilon}_o)^m(1 - \alpha f_l)} \right]^{1/n} - \epsilon_o \quad (6)$$

$$\epsilon_1 = \left[\frac{\sigma_1}{e^{(a-bT)}(\dot{\epsilon}_1 + \dot{\epsilon}_o)^m(1 - \alpha f_l)} \right]^{1/n} - \epsilon_o \quad (7)$$

Further, $\dot{\epsilon}_{th}$ can be given by the difference in strain between one time increment and the next,

$$\dot{\epsilon}_{th} = \frac{\epsilon_2 - \epsilon_1}{t_2 - t_1} \quad (8)$$

Assuming a small time interval, $\Delta t = t_2 - t_1$, such that $\frac{\partial \dot{\epsilon}_{th}}{\partial t} \big|_{t \in \Delta t} \approx 0$ and that liquid fraction remains unchanged, $\dot{\epsilon}_2 = \dot{\epsilon}_1 = \dot{\epsilon}_{th}$. Substituting Eqs. (6) and (7) into Eq. (8) leads to:

$$\dot{\epsilon}_{th} = A(\dot{\epsilon}_{th} + \dot{\epsilon}_o)^{-m/n}, \quad A = (1/\Delta t) \left[\frac{1}{e^{(a-bT)(1-\alpha f_l)}} \right]^{1/n} (\sigma_2^{1/n} - \sigma_1^{1/n}) \quad (9)$$

Eq. (9) being implicit, is solved at different time values using the Newton-Raphson method. The $\dot{\epsilon}_{th}$ value calculated above is then added to restraining strains $\dot{\epsilon}_{re}$ to yield the variation in the global strain rate $\dot{\epsilon}$ with time. Finally, $\dot{\epsilon}$ is translated into the global deformation rate as:

$$\dot{\delta} = l\dot{\epsilon} \quad (10)$$

where l is the initial lateral length of the mushy zone. Note that the weld mushy zone has a variable lateral length along the global X direction due to the shape of the weld pool and therefore Eq. (10) cannot be applied directly to the mushy zone as a single body. Instead, the weld mushy zone is discretized into lateral bar elements as shown in Fig. 5 that lie along the global Y direction. Each bar element has a unique length and cross section area given by the grain size.

2.2.2.2. Partitioning to individual micro liquid channels

A partitioning technique proposed by Coniglio and Cross [9, 26] is utilized to distribute the global deformation rate of a bar element among the micro liquid channels within it. This method treats the mushy zone as a composite material composed of solid and liquid phases and decomposes the global deformation rate vector into a series of local deformation rate vectors. The local vectors have the same direction as the global vector and are applied to every fully solid grain and every micro liquid channel between partially solidified grains. Therefore:

$$\dot{\delta} = \sum_{j=1}^{j=\dot{N}} \vec{\delta}_{Grain}^j + \sum_{i=1}^{i=N} \vec{\delta}_{ext}^i \quad (11)$$

where $\vec{\delta}_{Grain}^j$ are the local deformation rate vectors of the solid grains, $\vec{\delta}_{ext}^i$ are the local deformation rate vectors of the micro liquid channels induced by the external sources, and $\dot{N}$ and N are the number of solid grains and micro liquid channels. Since the liquid phase is significantly weaker than the solid phase, the role of the solid grains in partitioning the global deformation rate can be neglected. Therefore, Eq. (11) can be reduced to:

$$\vec{\delta}_{ext}^i = \frac{\dot{\delta}}{N} \quad (12)$$

assuming that the micro liquid channels equally contribute to the global deformation rate. Fig. 5 depicts the visual interpretation of Eq. (12) for a bar element in a 2-D view.

This method does not yet consider the dendrite coherency phenomenon at high solid fractions [9, 26]. Dendrite coherency corresponds to the moment when the secondary dendrite arms on the walls adjoining grains merge and form a solid bridge across the micro liquid channel [38]. From a mechanical point of view, the walls of a bridged channel are interlocked and cannot separate unless the bridging dendrite arms break apart. Therefore, the bridged channels behave similar to solid grains [3, 4] and their contribution to the deformation of the mushy zone is negligible. With the same reasoning, an isolated cluster of micro liquid channels that is fully surrounded by the bridged channels and not connected to the base metal or the surface of the weld do not contribute to the distribution of the global deformation rate either. In order for this partitioning technique to reflect the effect of the dendrite coherency, Eq. (12) is modified as follows:

$$\vec{\delta}_{ext}^i = \eta \frac{\dot{\delta}}{N_u}, \quad \begin{cases} \eta = 0 & \text{if } f_s \geq f_s^{coh} \\ \eta = 1 & \text{if } f_s < f_s^{coh} \end{cases} \quad (13)$$

where N_u is the number of the unbridged channels of a bar element that do not belong to an isolated cluster, f_s represents the solid fraction in the vicinity of the micro liquid channel i , and f_s^{coh} represents the solid fraction at which the dendrite coherency occurs, assumed to be 0.95.

As Fig. 5 shows, the micro liquid channels have random orientations within the mushy zone and they are not necessarily perpendicular to their local deformation rate vectors, *i.e.* $\vec{\delta}_{ext}^i$ is not parallel to the local z direction of channel i . Hence, Eq. (13) is further modified to yield the component of $\vec{\delta}_{ext}^i$ along the local z direction of the channel i as,

$$\dot{\delta}_{z,ext}^i = \eta \frac{\dot{\delta}(\vec{e}_Y \cdot \vec{e}_z^i)}{N_u} = \eta \frac{l(\dot{\epsilon}_{th} + \dot{\epsilon}_{re})(\vec{e}_Y \cdot \vec{e}_z^i)}{N_u}, \quad \begin{cases} \eta = 0 & \text{if } f_s \geq f_s^{coh} \\ \eta = 1 & \text{if } f_s < f_s^{coh} \end{cases} \quad (14)$$

where $\vec{e}_Y$ and $\vec{e}_z^i$ represent unit vectors in the global Y direction, and the z direction for channel i .

3. Results and discussion

The deformation characteristics of the mushy zone of a fusion weld are determined as follows. First, the solidification model is applied for a given set of welding parameters, and the network of the micro liquid channels within the weld mushy zone is assembled for a given average fraction solid. Second, the internal normal deformation rate for each micro liquid channel is calculated using Eq. (3). Third, a mechanical simulation is performed on the base metal [7] using the Abaqus commercial finite element software to determine the lateral stress acting on the fusion surface. Fourth, the global deformation rate across the mushy zone is calculated following the method explained in section 2.2.2.1. Finally, the global deformation rate is partitioned using Eq. (14) to determine the external normal deformation rate for each channel. Note that the analysis of deformation within micro liquid channels is focused on only RVEs with high average

solid fractions, i.e. when the RVE is not close to the weld pool. The end goal of this model is the multi-scale modeling of solidification cracking in welding, and it has already been shown [6] that solidification cracks do not survive in low solid fraction semi-solid since sufficient liquid is present to refill the cracks. In any case, the model is not applicable to low-fraction-solid regimes where the idea of deformation of micro liquid channels has no meaning.

3.1. Internal deformation rate

The variation in the internal normal deformation rate within the reconstructed mushy zone of a weld is depicted in Fig. 6 for two different average solid fractions, 0.66 and 0.92. The numerically reconstructed mushy zone corresponds to a welding velocity of 4 mm/s and a welding current of 120 A. For a constant average solid fraction during welding, the results show that the internal normal deformation rates are highest when the channels are closer to the symmetry surface, *i.e.* closer to the center of the mushy zone. This result indicates, through Eq. (3), that the micro liquid channels at the center of the weld have higher solidification velocities and consequently experience larger solidification shrinkage. As discussed in Section 2.2.1, higher temperatures and higher cooling rates increase the solidification velocity and lead to faster separation of the walls of the micro liquid channels. Therefore, this variation in the internal normal deformation rate can be associated with a nonuniform thermal field within the mushy zone. Fig. 7 shows the distribution of the cooling rate over a reconstructed mushy zone corresponding to a welding travel speed of 4 mm/s and a welding current of 120 A. As can be seen, the cooling rate is highest at the center of the mushy zone. Also, the micro liquid channels at the center of the weld have the highest temperatures since they are closer to the heat source [31].

Comparison of Figs. 6a and b reveals that the variation in the internal normal deformation rate is strongly dependent on the average solid fraction of the domain. In order to analyze this relationship, the average internal normal deformation rate, $\bar{\delta}_{z,int}$, has been calculated at various average solid fractions as:

$$\bar{\delta}_{z,int} = \frac{\sum_{i=1}^{i=N} \delta_{z,int}^i}{N} \quad (15)$$

Here N represents the total number of micro liquid channels within the mushy zone at a specific average solid fraction.

Fig. 8 shows the variation in $\bar{\delta}_{z,int}$ as a function of average solid fraction for various welding conditions. In this figure, and also Fig. 12, each welding condition is labeled by a format of VXIXXX where the single digit after V shows the simulated welding travel speed in mm/s and the digits following I indicate the simulated welding current in Amperage. Examining any one curve, *e.g.* V2I95, it can be seen that increasing the average solid fraction of the mushy zone significantly reduces $\bar{\delta}_{z,int}$. This effect can be linked to the fact that at higher average solid fractions the mushy zone becomes colder and the cooling rate also drops, see Fig. 7, leading to a reduction in the solidification velocity. By comparing different curves, it can be seen that (1) increasing the welding travel speed increases $\bar{\delta}_{z,int}$ for a given average solid fraction and (2) lower welding currents at a constant welding travel speed slightly increase the average internal normal deformation rate. These observations can be associated with the role of welding parameters on the thermal field of the mushy zone; lower welding currents at a constant welding travel speed lead to higher maximum cooling rates within the mushy zone and consequently

higher $\bar{\delta}_{z,int}$. The maximum cooling rate inside the mushy zone as a function of average solid fraction for the various welding conditions is shown in Fig. 9.

Additional simulations, not shown, indicate that the effect of the weld microstructure on the internal normal deformation rate is negligible. Specifically, applying the same thermal field to various weld microstructures shows little variation in the average internal normal deformation rate. This demonstrates that welding parameters modify the internal normal deformation rate mainly because of their ability to change the thermal field, and not the corresponding change in weld microstructure.

3.2. External deformation rate

In addition to the internal normal deformation rate of the micro liquid channels caused by solidification shrinkage, the model also provides the normal deformation rate induced by external forces, *i.e.* the external normal deformation rate comprised of a thermo-mechanical component based on $\dot{\epsilon}_{th}$, and a restraining component, $\dot{\epsilon}_{re}$. The variation in $\dot{\epsilon}_{th}$ with time is shown in Fig. 10 for three different welding procedures. Note that the welding current was varied between 110 and 130 A, while the welding speed remained constant (4 mm/s). The effect of this change in welding parameters on the microstructure is to expand the equiaxed region and make the weld larger. Note also that the welding time of zero corresponds to the time at which the weld pool begins to solidify. As can be seen in the figure, the lateral deformation of the mushy zone induced by thermo-mechanical forces occurs primarily at later times, corresponding to the last stages of solidification [7]. The rapid rise in $\dot{\epsilon}_{th}$ at later times is due to the coalescence effect. However, near the end of welding, the rigidity of the semisolid weld increases since coalescence has largely occurred and thus the growth rate of $\dot{\epsilon}_{th}$ decreases. If the thermo-

mechanical stress field is not strong enough, as seen in the case with a welding current of 110 A, $\dot{\epsilon}_{th}$ will drop at the very end of the solidification. Comparing the different curves of Fig. 10, it can be seen that an increase in the welding current leads to an increase in $\dot{\epsilon}_{th}$. This observation can be linked to the fact that higher welding currents amplify the lateral component of the thermo-mechanical tensile stress acting on the mushy zone [7]. These model estimates of external deformations can also be compared against experimental data, at least to a qualitative level. In a prior set of studies, Coniglio and Cross [39] used an extensometer located across the weld root to measure the evolving thermomechanical strain rate across the weld mushy zone during welding. For welding speed of 4 mm/s and welding current of 130A, this measured thermomechanical strain rate for AA6061 was reported to rise from 0 to 0.01 s^{-1} from the start to end of welding. The estimates made by the thermomechanical model for the same welding conditions show an increase from 0 to 0.0058 s^{-1} over the same period. Considering all the assumptions made in the model, the similarity in the two values is exceptional.

Through Eq. (14), the model calculates the external normal deformation rate of each micro liquid channel based on the variation in the global strain rate with time. Fig. 11 shows the external normal deformation rate of the micro liquid channels within the reconstructed mushy zone of a weld for two different average solid fractions, 0.66 and 0.92. The weld corresponds to a welding velocity of 4 mm/s and a welding current of 120 A under a restraining strain rate of 0.1 s^{-1} . As can be seen in the figure, the external normal deformation rate is very low near the fusion boundary, indicating that the channel walls in this region do not separate too much due to the external forces. This observation can be linked to dendrite coherency since the micro liquid channels near the fusion boundary have higher solid fractions as compared to the center of the weld [1] and therefore experience coherency earlier in the welding process. Thus, the walls of

these bridged channels become interlocked and therefore cannot accommodate any external deformation, forming an unaffected region in the vicinity of the fusion boundary. A comparison of Figs. 11a and b reveals that this unaffected region grows towards the center of the mushy zone, as expected, since an increase in the average solid fraction must also lead to an increase in the number of bridged channels.

As is well known, the choice of welding parameters affects the quality of a weld, inducing porosity, solidification cracking, etc., depending on the choice of variables. Figs. 12a, b, and c illustrate the effect of welding parameters on the average external normal deformation rate of the mushy zone, $\bar{\delta}_{z,ext}$, for three different values of $\dot{\epsilon}_{re}$. Arithmetic averaging similar to Eq. (15) is used to calculate $\bar{\delta}_{z,ext}$. Note that the bridged channels are not considered in averaging the external normal deformation rate of the micro liquid channels since they do not participate in deformation. A comparison of Figs. 12a, b, and c indicates that welding parameters do not affect the $\bar{\delta}_{z,ext}$ of a self-restrained mushy zone ($\dot{\epsilon}_{re} = 0$) and an externally-restrained mushy zone ($\dot{\epsilon}_{re} \neq 0$) in the same way. This difference in behaviour can be understood by examining the mechanisms by which welding parameters affect the external normal deformation rate of the channels. For the self-restrained mushy zone shown in Fig. 12a, welding parameters strongly affect both $\dot{\epsilon}_{th}$, and also the mushy zone morphology since different welding parameters generate different microstructures [1, 4]. As can be seen in Figure 12a, a welding travel speed of 4 mm/s accompanied by a welding current of 130 A yields the maximum $\bar{\delta}_{z,ext}$. However, for the externally-restrained mushy zones shown in Figs. 12b and c, $\dot{\epsilon}_{re}$ becomes the dominant source of deformation as compared to $\dot{\epsilon}_{th}$ and therefore the change in the mushy zone morphology is the

only mechanism by which welding parameters noticeably affect the average external normal deformation rate.

In terms of the weld microstructure and the mushy zone morphology, welding conditions that lead to finer grains reduce the external normal deformation rate. This is because weld microstructures with smaller grains have more micro liquid channels. Based on Eq. (14), the global deformation rate is then partitioned amongst more micro liquid channels, resulting in a decrease in the external normal deformation rate in any individual channel. As can be seen in Fig. 12, the largest $\bar{\delta}_{z,ext}$ for externally-restrained mushy zones occurs for a welding travel speed of 2 mm/s and a welding current of 95 A. The weld microstructure contained a low number of micro liquid channels as compared to all other simulations.

As Figs. 11 and 12 show, the external normal deformation rate of the micro liquid channels increases significantly with an increase in the average solid fraction. In other word, the micro liquid channels near the solidus surface have higher external normal deformation rates. As the average solid fraction rises, more liquid channels meet the dendrite coherency criterion and consequently the number of unbridged channels decreases. This is because, through Eq. (14), the transformation of unbridged micro liquid channels into the bridged ones as fraction solid increases lowers N_u . Consequently, the deformation of the mushy zone localizes over a few micro liquid channels, increasing the susceptibility of those channels to formation of solidification cracks.

Although this model is not intended to predict the formation of solidification cracks, it can however explain the formation of centerline cracks [32] that very commonly occur as part of solidification cracking. As shown above, the micro liquid channels at the center of the weld have

the greatest internal and external normal deformation rates. Therefore, based on the micro-scale models of solidification cracking [4, 20, 23], the centerline of the weld will be highly susceptible to the formation of solidification cracks. The model also shows that welding parameters can affect the deformation rate of the channels and consequently impact the degree of the solidification crack susceptibility of welds.

3.3. Model limitations

Although the presented model successfully calculated the deformation of micro liquid channels during welding, several limitations must be mentioned. First, the dendritic feature of welding microstructure is overlooked as it is assumed that the liquid flow is confined between two parallel facets of the grains. Although this is a strong assumption, it matches the geometrical features of the micro liquid channels defined by the micro-scale models of solidification cracking [4, 20, 23], and therefore will benefit the future studies on developing the multi-scale models of solidification cracking based on the existing micro-scale models. Second, although the modified partitioning technique used to distribute the global external deformation rate among the micro liquid channels has improved the existing partitioning methods, it does not yet include the role of the solid grains. In addition, this model assumes that each micro liquid channels equally contribute to the global deformation rate. Although it has been shown [23, 24] that the ability of the micro liquid channels to accommodate strain correlates with the width of the channels, where the channel walls can separate more easily in wider channels, this effect is only significant at lower average solid fractions where the semisolid weld contains a wide range of channels with different widths and therefore different capabilities to contribute to semisolid deformation. As this model focuses on solidification cracks, which occur at high average solid fraction, the application of this partitioning technique is appropriate. Third, only the lateral component of the

global external deformation rate is considered, *i.e.* the effects of the other components are ignored. Four, the model geometry, specifically, the parallel micro liquid channel walls, does not exactly match welding microstructure since in reality the grain boundaries are not parallel to each other during solidification. This is a strong assumption, however, it has been successfully used in previous applications of granular models of solidification to investigate new phenomena related to solidification cracking during casting processes [5, 6, 23-25]. If the channels walls are not assumed to be parallel, then it is not possible to determine the external deformation rate vector. Further, the solidification velocity vector $(\vec{v}_1^*, \vec{v}_2^*)$, resulting in the internal deformation rate vector, would have to be defined through two separate terms, *i.e.* βv_1^* and βv_2^* , rather than a single parameter ($\delta_{z,int}^i = \beta(v_1^* + v_2^*)$). Finally, unlike real semisolids in which solid grains have smooth surfaces with rounded corners, the grain edges within the reconstructed mushy zone are sharp due to using the Voronoi tessellation algorithm. These sharp edges do not allow the model to form large liquid pockets at grain triple joints and therefore for a given micro channel width, the model overestimates the solid fraction. The overestimation of the solid fraction will induce a premature drop in the number of micro liquid channels, potentially leading to an artificial rise in the external deformation rate (Eq. (12)).

4. Conclusions

A 3D multi-scale model has been developed to characterize the deformation rate of the weld mushy zone. Specifically, the normal separation rate of the walls of the micro liquid channels induced by both solidification shrinkage and external forces can be predicted as a function of welding conditions. Since the formation of solidification cracks within semisolids is strongly linked to the deformation rate of micro liquid channels, the results of this model can be used to

study the effects of GTA welding process parameters on the solidification cracking susceptibility of AA 6061 welds. Also, this model is able to simulate the variation of the deformation rate through the weld mushy zone. This can be used to locate the areas inside the weld that are more prone to solidification cracking. From the simulations, four main conclusions can be made:

- (1) Welding parameters (travel speed and current) strongly influence the internal deformation rates of the micro liquid channels induced by solidification shrinkage. The model suggests that increasing the welding travel speed increases the internal deformation rate of the weld mushy zone. Also, it is shown that lower welding currents at a constant welding travel speed increase the internal deformation rate of the mushy zone and therefore can induce solidification cracking.
- (2) Welding conditions also impact the external deformation rate of the weld mushy zone induced by external forces and thermo-mechanical stresses. The model shows that in an externally restrained welding condition, the external force is the dominant factor where larger forces cause higher external deformation rates. For self-restrained welding conditions in which the external force is eliminated, the model suggests that higher welding speeds increase the external deformation rate and can cause solidification cracking.
- (3) The internal normal deformation rate due to solidification shrinkage and also the external normal deformation rate caused by external forces are both highest for the micro liquid channels at the center of the mushy zone. This phenomenon explains the common occurrence of solidification cracks at the center of the weld.
- (4) The internal normal deformation rate of the micro liquid channels induced by solidification shrinkage increases near the weld pool where the solid fraction is low, whereas the external normal deformation rate caused by external forces is the lowest in this area.

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Figure captions

Fig. 1 Schematic of the base welding geometry: the model domain and the resulting unstructured grid.

Fig. 2 a) Experimental setup before welding; b) Schematic of the location of the thermocouples, and c) the numerical and experimental thermal histories of the three points shown in part b).

Fig. 3 Evolving semi-solid weld microstructure fabricated using a welding travel speed of 4 mm/s and a welding current of 120 A. The average fraction solid in (a) and (b) are 0.55 and 0.8.

Fig. 4 a) The geometry of a single micro liquid channel sandwiched between two parallel solidification fronts; b) the reconstructed network of micro liquid channels for the mushy zone shown in Fig. 2.

Fig. 5 The decomposition of the global deformation rate vector into external normal deformation rate vectors.

Fig. 6 The internal normal deformation rate of the micro liquid channels within the reconstructed mushy zone of a weld for a) an average solid fraction of 0.66 and b) an average solid fraction of 0.92. The weld is fabricated by a welding velocity of 4 mm/s and a welding current of 120 A.

Fig. 7 The cooling rate over the mushy zone of a weld fabricated by a welding travel speed of 4 mm/s and a welding current of 120 A.

Fig. 8 The variation of the average internal normal deformation rate as a function of average solid fraction for various welding parameters.

Fig. 9 The variation of the maximum cooling rate along the mushy zone of six welds fabricated by different welding parameters.

Fig. 10 The calculated transient thermo-mechanical component of the global strain rate for a weld fabricated by a welding speed of 4 mm/s and three different welding currents.

Fig. 11 The external normal deformation rate of the micro liquid channels within the reconstructed mushy zone of a weld for a) an average solid fraction of 0.66 and b) an average solid fraction of 0.92. The weld is fabricated by a welding velocity of 4 mm/s and a welding current of 120 A and under a restraining strain rate of 0.1 (1/s).

Fig. 12 The effect of various welding parameters on the average external normal deformation rate of the mushy zone for three different restraining strain rates: a) 0 (1/s), b) 0.005 (1/s), and c) 0.1 (1/s).

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