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Modelling the creation and destruction of columnar and equiaxed zones during solidification and melting in multi-pass welding of steel

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ABSTRACT

The authors present a novel meso-scale (mm–cm) numerical model of multi-pass welding of stainless steel based on the front tracking formulation. During a typical multi-pass notched butt weld, multiple cycles of melting and solidification occur throughout the weld pool, where previously solidified equiaxed zones are destroyed by melting and subsequently resolidify in columnar form. These thermal cycles result from the thermal effects of the current deposition of liquid filler metal being superimposed onto those of the previous pass. The advancement of the liquidus isotherm is employed to characterize melting, while both columnar and equiaxed dendritic growth in the undercooled melt are considered in the model of solidification. Columnar solidification is simulated using a front tracking method where computational markers are employed to explicitly define the advancing columnar front. Competing equiaxed solidification is modelled using a volume averaging approach. During the first and second welding passes of a case study, the weld pool solidifies as purely columnar. This is due to the high thermal gradient present in the weld pool, which results in a very small region of undercooled liquid ahead of the columnar front and subsequently low levels of equiaxed grain nucleation/growth. Towards the end of the third and final pass the equiaxed grains have sufficient dwell time in the undercooled liquid to form a coherent network and present a physical barrier to the advancing columnar front. A Columnar to Equiaxed Transition (CET) occurs and the remainder of the weld pool solidifies in a fully equiaxed microstructure. The results are compared with Hunt's analytical model of CET and the agreement is reasonably good. The occurrence of CET throughout the weld pool is directly predicted via this front tracking model without the need to rely on estimated thermal gradients and solidification rates. Further simulations indicate that CET can be promoted, even in early passes, by increasing the grain refiner level and/or by pre-heating the parent metal.

1. Introduction

Modelling of solidification structures has become a key component of research on industrial processes such as casting and welding where direct measurements of temperature and velocity fields are very difficult during experiments and the influence of operating parameters on the solidification structure is very complex. Solidification of alloys typically occurs via dendritic growth in an undercooled melt [1]. The very high thermal gradients and high temperatures reached within the weld pool make it impractical to capture real time temperature data. This makes modelling of the welding process essential to understanding the weld pool formation and subsequent solidification. The solidified microstructure has a strong influence on the mechanical properties of product, and thus it is highly desirable to exert as much control as possible on the final solidification structure by understanding and controlling the dendritic growth. The geometry and temperature field of the weld pool, upon the addition of molten filler material, have significant influence on the subsequent development of the solidification structure.

During welding, wetting of the solid parent metal by the liquid presents a favourable situation for initiation of columnar growth without having to overcome a significant nucleation energy barrier. Very low levels of undercooling will promptly result in columnar growth. However, a fully columnar grain structure weld is susceptible to centre line hot or cold cracking and exhibits weaker mechanical performance during plastic deformation. Thus it is desirable to promote a Columnar to Equiaxed Transition (CET) within the solidifying weld pool as central equiaxed grains show better resistance to crack formation and propagation [2]. The addition of TiN grain refiners have been shown to promote equiaxed nucleation and therefore growth ahead of the columnar

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front, leading to CET in steels [3–7], as will be discussed in Section 2.4.1. The new approach to modelling of welding, outlined herein, allows the position of the melting and/or solidifying front to be explicitly tracked as well as resolving the undercooled liquid ahead of the solidification front. This allows equiaxed nucleation and growth to be modelled ahead of the columnar front as well as the occurrence of CET as will be discussed in Section 2.

Hunt's analytical model [8] describes the selection of an equiaxed or columnar microstructure due to the competition between the advancing columnar interface and equiaxed grain nucleation and growth in a region of undercooled liquid ahead of an advancing solidification interface. Two criteria are determined relating the velocity of the advancing interface (v) and the thermal gradient (G). If the volume fraction of equiaxed grains reaches 0.49 then subsequent solidification is defined to be fully equiaxed; however if the equiaxed volume fraction is always less than 0.0066 the resulting microstructure is defined to be fully columnar. The model establishes upper and lower bounds for fully columnar or fully equiaxed microstructures on a log–log plot of the thermal gradient (G) *vs* the solidification interface velocity (v). Fig. 1 outlines a schematic of the transitional limits between the columnar structure (solid – blue) and equiaxed structure (dashed – red) as specified in G–v space by Hunt's analytical model. Between these limits CET is expected to occur. A example of a G–v trajectory for a given solidification system is shown in Fig. 1, in this case CET would be expected to occur as the trajectory enters the mixed columnar/equiaxed region. This approach to predicting CET is widely employed throughout the literature, however more accurate numerical models are available. A recently review by Mirihanage et al. [9] provides a comprehensive look at numerical models used to predict CET, from macro to micro length scales.

Koseki et al. [10] modelled equiaxed nucleation and growth during welding via a Monte Carlo (MC) method. This work simplified the weld to a 1D problem (although the simulation domain is 2D) similar to a case of full penetration welding. While the MC method was used to model nucleation and growth of solid, nucleation was simply assumed to occur instantaneously on TiN particles that become undercooled. The model does not take account of a size distribution of inoculant particles or a size *vs* undercooling relationship. While this model performed well in terms of agreement with experiments (e.g. prediction of CET), it is reliant on key inputs taken from these same experiments to which the model is compared.

Montiel et al. [11] modelled CET in resistance spot welding via a Phase Field (PF) method. The PF model was coupled to a simple heat conduction model to provide the time-dependent temperature profile in the weld pool, while a probabilistic nucleation model was employed to model heterogeneous nucleation. As regards predicting solidification structure, this model is only able to specify the positions of the solidus and liquidus isotherms, and does not explicitly track the position of the undercooled solidifying front This results in having to roughly estimate where the intersection of the G–v trajectory and the CET curves should occur as per the Hunt CET map illustrated in Fig. 1. Direct comparison to the experimental results is not possible as the phase field simulation does not account for the evolution of latent heat. Also the very small domain size (0.1×0.1 mm) precludes predicting whether CET occurs near the centre of a weld pool which is significantly larger.

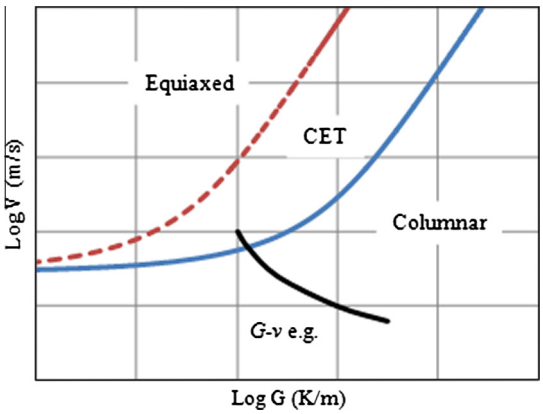

Fig. 1. Schematic of Hunt's CET map of solidification velocity (V) versus thermal gradient (G) in the liquid, showing fully columnar, fully equiaxed, and CET regions, and an example of a G–v trajectory entering the CET region.

Bailey and Shin [12] modelled laser spot conduction welding of 304 stainless steel, by employing a multiscale approach whereby a macroscale model is linked to a microscale Cellular Automata (CA) model which is combined with a PF model i.e. the CAPF model [13] (essentially linking 3 models). The implicit finite volume macroscale model considers the conservation of mass, momentum and energy in 3D and a simple linear relationship was used to model the evolution of solid fraction within the mushy zone (temperature range between solidus and liquidus temperatures, where the alloy is a mixture of solid and liquid). This model provides the weld pool geometry and the thermal history as direct inputs for the 2D microscale CAPF model. In the CAPF model the CA model tracks the dendritic morphology as well as the solute redistribution. In order to track the dendritic growth the PF model supplies the CA model with the local solidification kinetics for each cell. In turn, in order to calculate the solidification kinetics, the PF model requires key inputs from the CA model. This CAPF model is thus fully coupled with information flowing back and forth between models. In order to increase the computational efficiency of the model a database of growth kinetics is employed. The macro model compared well with experiments in relation to the predicted geometry of the weld pool and thermal history. The micro model replicates competitive grain selection and accurately predicts finer dendrite arm spacing at different locations throughout the weld pool due to the different local cooling rates. Equiaxed nucleation/growth is not addressed in the models. The domain size at the micro scale is ~0.25 mm $\times$ 0.18 mm, which is too small to account for solidification phenomena across the whole weld pool. Similar to the previous models, in this case the micro–macro linking is only one way i.e. the CAPF model does not pass information back to the macroscale model as regards the solid fraction evolution in the columnar mushy zone, which could be used to provide a more accurate update of the Darcy source term, as solidification proceeds.

While predicting the fine details of microstructure, these microscale models are typically only capable of working on very small simulation domains due to their inherently high computational costs. Modelling welding at the scale of a component with these microscopic models is normally very difficult or even unfeasible. The current meso-scale front tracking model addresses this deficiency and is capable of simulating the weld at the mm–cm length scale, while incorporating the direct prediction of CET in particular. As per the prediction of CET, most of the models that are applicable to the full scale of welding rely solely on the inputs of G and v [7,11,14–18] to be used in conjunction with the Hunt diagram [8] or the numerical solution posed by Gäumann et al. [19]. These G and v rates are difficult to measure experimentally and these models rely on simple heat transfer models to supply these inputs.

Some preliminary results of this front tracking model of multi-pass welding were presented in [20]. In this earlier implementation CET was not predicted. This was due to a number of assumptions which have been changed in the current version of the model. Previously the addition of welding passes was carried out at set time intervals which did not allow for complete