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Three-dimensional cellular automaton-finite element modeling of solidification grain structures for arc-welding processes

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ABSTRACT

Solidification grain structure has significant impact on the final properties of welded parts using fusion welding processes. Direct simulation of grain structure at industrial scale is yet rarely reported in the literature and remains a challenge. A three-dimensional (3D) coupled Cellular Automaton (CA) – Finite Element (FE) model is presented that predicts the grain structure formation during multiple passes Gas Tungsten Arc Welding (GTAW) and Gas Metal Arc Welding (GMAW). The FE model is established in a level set (LS) approach that tracks the evolution of the metal-shielding gas interface due to the addition of metal. The FE method solves the mass, energy and momentum conservation equations for the metal plus shielding gas system based on an adaptive mesh (FE mesh). Fields are projected in a second FE mesh, named CA mesh. A CA grid made of a regular lattice of cubic cells is created to overlay the fixed CA mesh. The CA model based on the CA grid simulates the melting and growth of the grain boundaries in the liquid pool. In order to handle large computational domains while keeping reasonable computational costs, parallel computations and dynamic strategies for the allocation/deallocation of the CA grid are introduced. These strategies correspond to significant optimizations of the computer memories that are demonstrated. The 3D CAFE model is first applied to the simple configuration of single linear passes by GTAW of a duplex stainless steel URANUS 2202. It is then applied to a more persuasive example considering GMAW in spray transfer mode during multiple passes to fill a V-groove chamfer. Simulations reveal the possibility to handle domains with millions of grains in representative domain sizes while following the formation of textures that result from the growth competition among columnar grains.

1. Introduction

The Gas Metal Arc Welding (GMAW) process was introduced to industry in the late 1940s. It was originally developed with the use of a continuous fed aluminum wire electrode. At present, GMAW is the main welding process used to join metallic parts at industrial scale. This process can be applied to assemble a wide range of metallic materials such as aluminum or magnesium alloys, carbon steels or stainless steels. It is also well adapted to weld large thickness workpieces with high velocity and high added metal rate [1]. However the development of defects such as hot cracking can also be observed during cooling. These welding defects are mainly linked to the grain structure and the solidification path in the weld bead. Control is generally achieved by adjustment of the wire composition and tentative to form an equiaxed zone. Studies have been reported to model the grain structure developed in welding processing together with prediction of the internal pressure [2] or the liquid feeding ability at intergranular liquid channels [3]. The mechanical properties of the joints are also linked to the anisotropy of the grain structure developed in the weld bead, especially in case of multiples passes processes when large grains develop [4]. This demonstrates the need to reach better prediction of the solidification grain structure to master welding processing. It should also be outlined that the GMAW process can easily be automated in order to obtain a precise control of welding parameters and stable and repeatable final properties of the parts. Consequently, the prediction of welding microstructures is also of particular interest in the context of robotics welding applications that will replace in the future traditional manual welding. In this context, a multiscale approach is proposed in order to predict grain structure development in the weld beads.

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Metallographic inspections after welding generally reveals the presence of large grains in weld bead. Their orientation is linked to the local temperature gradient which is essentially perpendicular to the pool boundary [1]. Heat extraction toward the base metal leads to the growth of a columnar and textured structure, eventually later blocked by the development of equiaxed grains in the weld pool. The Cellular Automaton (CA) − Finite Element (FE) model for solidification grain structures, abbreviated as CAFE model, was initially introduced by Rappaz and Gandin [5,6] to simulate the nucleation and growth of a dendritic grain structures in the context of casting processes. Very rapidly, the technique was foreseen for application to welding and continuous casting [7,8]. However, limitations linked to computer resources prevented to deal with realistic three-dimensional (3D) predictions. Recent progresses of the CAFE model were in the coupling with macro-segregation caused by thermosolutal convection [9–12], and optimization of computations by parallel algorithms [12–14]. Chen et al. [15] then extended the 3D CAFE model to simulate the grain structure evolution during melting and solidification in Gas Tungsten Arc Welding (GTAW) processes. Recent progresses have also been reported in the literature for the grain structure prediction in laser welding [16]. The possibility to deal with large domains and several successive simulations for multiple passes were thus demonstrated, together with the propagation of the texture between passes due to epitaxial growth of the columnar grain structure from partially remelted previous passes. However, the development of the grain structure with the addition of the filler metal during welding processes, typically found in GMAW, was not yet possible.

The purpose of this paper is to present a model that permits simulation of multiple passes in GMAW for large computational domains based on 3D CAFE simulations. We first present the FE model that solve the volume average macroscopic conservation equations for the weld bead development based on the level set (LS) formulation to track the metal/shielding gas interface. We then introduce the grain structure model using the mesoscopic scale CA approach. The dynamic allocation strategies implemented to manage allocation/deallocation of cell information and data storage, as well as an illustration of the parallelization methodology are also given. The model is finally applied to GTAW single linear passes to reveal texture formation as a function of the process parameters as well as to GMAW multiple passes to fill a V-groove weld preparation. The alloy considered in this study is the URANUS 2202 steel grade.

2. Macroscopic FE modeling

In GMAW, a filler metal is added into the fusion zone due to melting of a consumable electrode. This creates a weld bead by addition of liquid droplets as schematically shown in Fig. 1, thus continuously changing the interface between the metal and its environment. A welding arc and plasma are developed during the process leading to the formation of melted droplets [17]. These droplets fall vertically and feed the weld pool leading to the continuous development of the weld bead. The process is considered to be in the spray transfer mode in the present approach due to the choice of process parameters for both power and electrode velocity. A continuous detachment from the vertical electrode of small droplets with a high frequency is assumed in the next GMAW simulations. Thus the liquid pool is fed with a stable rate in the axial direction of the electrode. An efficient approach to model the time evolution of this interface was developed by Desmaison et al. [18]. It is based on the LS method [19,20]. The model presented hereafter takes advantage of the LS interface to write a set of average conservation equations valid in a domain that encompasses the *metal* subdomain, $\mathbb{M}$, plus the *shielding gas* subdomain, $\mathbb{G}$ hereafter referred to as *gas*. A FE method is then used to solve the equations on a FE mesh as shown in Fig. 2 (b). This model, largely inspired from Ref. [18], thus overcomes the numerical difficulty inherent to a sharp interface tracking procedure of the metal/gas interface after successive passes in GMAW.

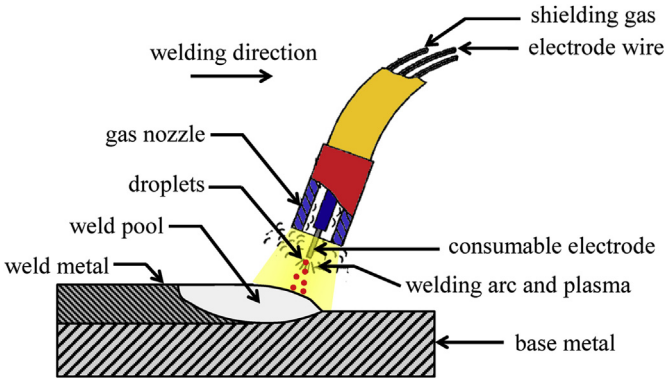

Fig. 1. Schematic of the Gas Metal Arc Welding (GMAW) process. The arc is developed between the consumable electrode and the metal. Droplets are formed at the base of the electrode and fall inside the weld pool. The development of the weld bead consecutive to the solidification of the liquid domain is shown on the left hand side part of the scheme [17].

2.1. LS modeling of the metal/gas interface

The LS function, ψ, is defined by the signed distance of any position M in the domain with respect to the metal/gas interface. Value $\psi = 0$ corresponds to the position of the interface. It is represented by the black curve in Fig. 2 (b). Negative values of ψ determine the points in the metal domain while positive values of ψ correspond to those in the gas domain. This corresponds to the mathematical definition:

$$\begin{cases} \psi < 0 \quad \text{, if } M \in \mathbb{M} & \text{: the position is in the metal domain.} \\ \psi = 0 \quad \text{, if } M \in \mathbb{M}/\mathbb{G} & \text{: the position is at the metal/gas interface.} \\ \psi > 0 \quad \text{, if } M \in \mathbb{G} & \text{: the position is in the gas domain.} \end{cases} \tag{1}$$

As a single FE mesh has been defined for both domains, material properties need to continuously evolve into this mesh from metal to gas. Thus, with the LS approach, any material property, χ, is averaged to $\langle\chi\rangle$ using the Heaviside function, $\mathscr{H}(\psi)$, defined on the basis of level set function:

$$\langle\chi\rangle = (1 - \mathscr{H}(\psi))\chi^{\mathbb{M}} + \mathscr{H}(\psi)\chi^{\mathbb{G}} \tag{2}$$

$$\begin{cases} \mathscr{H}(\psi) = 0 & \text{if } \psi < -\varepsilon (M \in \mathbb{M}) \\ \mathscr{H}(\psi) = \dfrac{1}{2}\left[1 + \dfrac{\psi}{\varepsilon} + \dfrac{1}{\pi} sin\left(\dfrac{\pi\psi}{\varepsilon}\right)\right] & \text{if } |\psi| \le \varepsilon \\ \mathscr{H}(\psi) = 1 & \text{if } \psi > \varepsilon (M \in \mathbb{G}) \end{cases} \tag{3}$$

$\langle\chi^{\mathbb{M}}\rangle$ and $\langle\chi^{\mathbb{G}}\rangle$ are the local intrinsic value of the property for metal and gas, respectively. The half-thickness of the transition zone between the metal sub-domain and the gas sub-domain is defined by ε, a length parameter of the LS approach taken as a small positive value. The boundaries of this transition zone are represented by the two red curves that surround the black curve in Fig. 2 (b). Analysis of Eq. (3) reveals that $\mathscr{H}(\psi)$ continuously evolves from 0 to 1 in the transition zone around the interface position delimited by ψ values in the interval $[-\varepsilon, \varepsilon]$. Also worth noticing is that $\langle\chi^{\mathbb{M}}\rangle$ is

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