



# Modeling of morphological evolution of columnar dendritic grains in the molten pool of gas tungsten arc welding



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## ABSTRACT

A macro–micro coupled model for epitaxial nucleation and the subsequent competitive dendrite growth was developed to study the morphological evolution of both dendrite and grain structures in molten pool of the gas tungsten arc welding (GTAW) for Fe–C alloy. The simulation of heat and mass transfer in molten pool was conducted by the three-dimensional finite element (FE) model to obtain the transient solidification conditions. The process of epitaxial nucleation and the competitive dendrite growth was simulated by a two-dimensional cellular automata (CA) model. The size and random preferential orientations of substrate grains were considered in this model. The transient thermal conditions used in the CA model were obtained from the results of FE model through the interpolation method. In addition, the effects of the substrate grain size and the welding speed on the morphologies of both dendrite and grain structures were investigated. The simulated results indicate that dendrites with the preferential orientations parallel to the direction of the highest temperature gradient are more competitive during the competitive dendrite growth, and the morphology of resulting columnar grains is determined by the competition between different dendritic arrays. Under the same welding conditions, with the increase of substrate grain size, the average width of resulting columnar grains becomes larger, and the characteristics of dendrite structure within the columnar grains do not change obviously. Without considering the new nucleation in the melt, with the increase of welding speed, the dendrite structure in weld seam becomes much finer, and the average columnar grain width within the calculation domain of the CA model does not change obviously. The trend of the simulated results of dendrite arm spacing under various welding conditions are consistent with the analytical and experimental data.

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## 1. Introduction

Welding is one of the most important techniques for material processing and has a wide range of applications in many fields of manufacturing industry [1]. The solidification behavior of welding pool controls the size and shape of grains, the microstructure morphology, and the ultimate mechanical properties of the weld [2]. The solidification of welding pool begins from epitaxial nucleation on the partially melted substrate grains which located at the fusion boundary [1,3]. Then the competitive growth of dendrites with different preferential orientations occurs during the solidification process. The epitaxial nucleation and the subsequent competitive dendrite growth have significant impacts on the morphologies of both dendrite and grain structures which can exert influence directly on mechanical properties of the weld. Therefore, the investigation on the morphological evolution of both dendrite and grain

structures during the process of epitaxial nucleation and competitive dendrite growth is helpful to understand the solidification behavior in molten pool and can provide important information for the optimization of welding process. However, welding is a multi-field coupling, time dependent and highly non-linear process [4]. It is difficult to observe the highly dynamic solidification process and predict the morphology of solidification structures through the conventional experimental methods.

Fortunately, with recent advances in computational power and numerical models, the computer simulation has become an efficient method to predict the microstructure morphology. Phase field (PF) and CA methods are usually applied to simulate the morphology of solidification structures. The PF method [5–8] simulates the phase types by solving governing equations which describe the evolution of phase field variables for either pure metals or multi-component alloys. The CA technique [9–17] simulates the microstructure morphology by determining the solid/liquid interface based on temperature and solute fields. The CA method needs fewer computational resource and can be used for bigger

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calculation domain, although the CA mesh can introduce the artificial anisotropy [18].

Up to now, some investigations have been conducted to simulate the morphologies of solidification structures in molten pool. Pavlyk and Dilthey [3] calculated the temperature field and fluid flow in the welding pool, and simulated the dendrite arm spacing at different locations along the fusion boundary by using the CA model. Zhan and Wei [19–21] simulated the columnar dendrite growth during welding process and then proposed a limited angles method to improve their CA model. A two-dimensional model combining the FEM and the CA technique was developed to simulate dendrite growth in the molten pool during the laser-engineered net shaping process by Yin and Felicelli [18]. The empirical expressions were proposed to describe the relationship between cooling rate and dendrite arm spacing. Tan et al. [17] developed a combined CA–PF model to simulate the dendrite growth in the laser cladding process, which adopted PF method for calculation of growth kinetics and a basic CA technique to track the solid/liquid interface. Chen and Guillemot [22] proposed a coupled CA–FE model to predict the grain structure formation during GTAW process. The FE model was used to solve the heat flow problem based on an adaptive meshing, and the CA model was applied to simulate the development of the envelope of the grains in the liquid. Bordreuil and Niel [23] adopted a two-dimensional CA model to predict the grain structure in the weld. And based on this prediction, the hot cracking phenomenon during GTAW was studied. Farzadi et al. [24] simulated and compared the microstructure morphologies at two different locations along the fusion boundary during GTAW of Al–Cu alloy using the PF method. A PF model was coupled to a new heat transfer FE model to study the evolution of primary dendrite arm spacing under the directional solidification conditions in laser powder deposition of Ti–Nb alloys by Fallah et al. [25]. Considering the transient solidification conditions, Zheng and Dong et al. [4] developed a PF model to investigate the microstructure evolution near the fusion line during GTAW for aluminum alloy. From the above, the existing studies investigated the solidification structures in molten pool at two different scales. At the micro-scale, the existing studies mainly focused on the evolution of dendrite morphology during the solidification of molten pool, and the effects of solidification conditions on the dendritic characteristics, especially for the dendrite arm spacing [3,4,19,20,24,25]. Moreover, the competitive dendrite growth under different solidification conditions and the resulting dendrite structures were also investigated for the process of laser processing [17,18]. At the meso-scale, the grain structure in the weld after solidification was simulated directly by coupling the macro-scale heat transfer model for molten pool [22,23]. By the numerical models developed in these studies, many useful conclusions have been obtained.

However, the morphologies of both dendrite and grain structures which are determined by the epitaxial nucleation and the subsequent competitive dendrite growth have significant effects on the mechanical properties of the weld. The welding parameters can affect the competitive dendrite growth by controlling the solidification conditions in molten pool, and then determine the morphologies of both dendrite and grain structures in the weld. Therefore, it is important to investigate the formation process of both dendrite and grain structures during the epitaxial nucleation and competitive dendrite growth. To date, the study on the morphological evolution of both dendrite and grain structures with various welding conditions by simulating the epitaxial nucleation and subsequent competitive dendrite growth in molten pool has not been presented.

In present paper, a macro-micro coupled model is developed to simulate the epitaxial nucleation and the subsequent competitive growth of dendrites with different growth directions in the molten

pool of GTAW. The simulation of heat and mass transfer during welding process is performed by a three-dimensional FE model to obtain the transient solidification conditions. The process of epitaxial nucleation and the competitive dendrite growth is simulated by a two-dimensional CA model. The size and random preferential orientations of the substrate grains are considered in present model. The transient thermal conditions used in the CA model are obtained from the results of FE model through the interpolation method. Based on the simulated results, the formation process of both dendrite and grain structures in molten pool are analyzed, and the effects of substrate grain size and the welding speed on the morphologies of dendrite and grain structures are investigated. In addition, the simulated dendrite arm spacing of the solidification structures are compared with the analytical and experimental data.

## 2. Model description

### 2.1. FE model for GTAW

The transient thermal conditions in welding pool can strongly affect the solidification behavior and the resulting solidification structures. To obtain the accurate solidification conditions during welding process, a three-dimensional FE model of GTAW process is developed in this section. In this model, the complicated fluid flow in welding pool which caused by buoyancy, electromagnetic force, arc plasma and Marangoni force is considered. To simplify the numerical model, some basic assumptions have been made as follows: (1) this problem is symmetric in the longitude plane along the welding direction, (2) the fluid flow in the welding pool is laminar, incompressible and Newtonian, and (3) the deformation of the free surface during welding process is ignored. To obtain the simulated results of velocity field in welding pool and the temperature field of entire workpiece, it is necessary to solve the equations of energy, mass and momentum conservation. These conservation equations in three-dimensional Cartesian coordinate system are detailed described in our formerly published work [26].

In general, the heat transfer and the competitive dendrite growth in welding pool occur in the three-dimensional space. In this situation, the thermal conditions and the formation process of solidification structures are complicated. In order to obtain the simpler solidification conditions and study the formation process of solidification structures easily, a thin plate-shaped workpiece and the full penetration process are applied in present work. This simplified method for the investigation of solidification structures in welding pool is also applied in many previously reported experimental works [27–30]. Under such conditions, the temperature field and the resulting solidification structures in welding pool do not change obviously along the workpiece thickness direction, and can be approximately considered as two-dimensional problems on the upper surface of the workpiece. Therefore, the workpiece used in the FE model is a carbon steel plate with the length of 70 mm, width of 40 mm, and thickness of 2 mm. In addition, the thermal properties of the carbon steel used in present simulation are obtained from Ref. [31]. It should be noted that, even under such simplified conditions, the limitation also exists in its present stage. The simulated result of the competitive dendrite growth on the upper surface of the workpiece which obtained by a two-dimensional microstructure model can only approximately represent the formation process of the solidification structures in actual welding pool. To completely eliminate this limitation, a three-dimensional microstructure model should be developed to study the competitive dendrite growth in actual welding pool. However, it is difficult to develop the three-dimensional dendrite growth model for the entire welding pool within the near future owing to the huge requirement of computational resource.

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