Research Progress on Numerical Simulation of Welded Joints Microstructure

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Abstract. Since the integrity and mechanical properties of welded joints mainly depend on the solidification behavior of the weld pool and the microstructure characteristics of the welding heat affected zone, it is crucial for engineers and scientists to reveal the solidification behavior of the weld pool and the structural transformation of the welding heat-affected zone. With the dramatical improve of material calculation methods, the formation mechanism of the microstructure of some metal welded joints has been continuously revealed. In this article, the application of computer simulation in the study of welded joint microstructure is comprehensively analyzed. It focuses on the difficulties of simulating each area of welded joints, the advanced simulation methods applicable to each area and the current research status. Based on the characteristics of welded joint formation and simulation methods, some hot issues in research are proposed, aiming to provide effective help for researchers in related fields and open up new research ideas.

1. Introduction
The success of the welding process depends on the performance of the final welded joint, and the evolution of the microstructure determines the performance of the welded joint. Therefore, studying the microstructure of welded joints has significant scientific and practical engineering significance. Generally, welded joints are divided into weld zone, fusion zone and heat affected zone. In the molten pool area, the metal undergoes a metallurgical reaction process from melting to solidification and crystallization. In the heat-affected zone, phase transformation, recrystallization and grain growth are occurred. These two processes are both affected by the transient and high temperature characteristics of the welding process, resulting in the limitation of test methods to study the transient structure of the joint and its formation mechanism. With the evolvement of computational mathematics, numerical simulation methods have become indispensable research methods. Currently, the more commonly applied microstructure simulation methods include deterministic method, Monte Carlo method (MC), cellular automata method (CA), phase field method (PF) and particle method (or called discrete matrix method), finite element method combined with numerical model (phenomenological method).

2. The current situation of the research on the structure simulation of the weld zone

2.1. Nodus in numerical simulation of weld microstructure
First of all, the crystallization process of the weld belongs to the combined crystallization, which
increases the difficulty of simulation compared with the solidification process of casting\[1\]. Secondly, the welding seam solidification is an unbalanced dynamic continuous rapid cooling process, which has the characteristics of high temperature, transient, and local flow. Therefore, it is necessary to accurately establish the kinetic and thermodynamic data of dendrite growth in the molten pool during the simulation process. The determination of the boundary conditions is also very significant, which is able to ensure sufficient thermal diffusion of the solute at the front of the interface by maintaining the original temperature and composition of the solution away from the growth interface. Many uncertain factors in the welding process will increase the difficulty of simulation, which makes the simulation result and the test data quite different. The improvement of computer technology and the mathematical model of the welding process has accelerated the research of the weld solidification mechanism. At present, tremendous progress has been obtained in this field.

2.2. Current Status of Research on Numerical Simulation of Weld Structure Solidification

In the numerical simulation of weld solidification microstructure, three methods, Monte Carlo method, Cellular Automata method and Phase Field method are commonly adopted. However, the Monte Carlo method lacks a physical basis and cannot quantitatively analyze the effects of various physical phenomena, so it is rarely employed in weld solidification. Zacharia. T and Simunovic. S\[2\], Koseki. T\[3\] and Wei and Deb Roy\[4\] utilized respectively the MC method to conduct preliminary transient analysis on the solidification of the weld structure. The evolution of the grain structure and topology of the aluminum alloy GTAW weld was predicted in three-dimensional space.

In the CA method, local rules and spatial and time discrete are adopted to describe continuous physical phenomena. Multi-field coupling, including the coupling of the macro temperature field and the micro simulation, is employed by the CA method for microstructure simulation. Cellular automata has achieved remarkable results in the simulation of metal solidification microstructure, and it has also been praised by scholars and introduced it into the field of weld solidification structure simulation. Based on CA model, CA-PF model and CA-FE model, Pavlyk\[5\], Tan\[6\], Bordreuil\[7\], Chen\[8\], Rappaz\[9\], Jingwei Zhang and Frank Liou\[10\] etc. simulated the microstructure of welds respectively. Due to the CA model can not only introduce the temperature field and solute field, but also calculate the flow field and stress field, the dendrite growth morphology and grain size of various materials under different welding process conditions have been successfully reproduced by researchers. Shi Yaowu \[11\], Huang Anguo \[12\], Zhan Xiaohong\[13\], and Zhang Min \[14\] have carried out a lot of research work in the field of weld pool structure and morphology. For instance, in 2015, Zhang et al. \[14\] utilized the CA-FE method to couple the macro temperature field to discuss the transformation of the microstructure of the Fe-C alloy TIG weld. In 2016, Gu Chenguang and Wei Yanhong et al.\[15\] established a 3D-CA model, which was applied to study the growth process of dendrites during the solidification of Al-Cu binary alloy welds, and obtained 3D dendritic morphology and the distribution of the solute field, as shown in Figure 1.

![Cellular automata three-dimensional simulation of columnar crystal growth in molten pool of aluminum-copper alloy \[15\]](image)

The phase field method is based on Ginzburg-Landau theory and adopts partial differential equations to solve the instantaneous physical state of the system in time/space under the action of diffusion, ordering potential and thermodynamics. It was introduced into the study of dendrite growth
in the 1970s. PF avoids tracking complex interfaces in the calculation process, greatly reducing the complexity of the PF model. By coupling with temperature field and solute field, it is easier to simulate the phenomenon of dendrite formation and solute segregation during solidification, and the specific morphology and fine substructure of dendrites can be supplied in detail. In 2008, Farzadi et al. [16] carried out a phase-field simulation of the solidification structure of Al-3%Cu alloy TIG welds. The influence of welding speed on the morphology of the solidification structure was discussed. V. Fallah et al.[17] established a coupling model of PF and temperature field, and revealed the solidification of the molten pool of Ti-Nb alloy powder laser cladding. In 2014, Wei Yanhong et al. [18] launched the exploration of the solidification process of the welding pool utilizing the phase field method, and established a temperature field equation with the characteristics of the welding pool cooling. In addition, Al-4%Cu alloy was employed to study the transformation behavior of weld structure, the growth rate of dendrites, and the preferential growth orientation of crystals of associated crystals.

3. Current status of research on welding heat affected zone organization simulation

3.1. Nodus in numerical simulation of welding heat-affected zone structure
Due to the different thermal cycles experienced by each point in the welding heat-affected zone, the grain size of each location in the heat-affected zone is not consistent. The process of grain growth involves grain merger and grain boundary migration. In this process, although the grain boundary energy is decreased by the driving force, the existence of the second phase particles will have a significant influence on the growth of the grains. Therefore, the deterministic method has become a common method for predicting the grain size in welded parts, such as Monte Carlo method and cellular automata method.

Besides, affected by the thermal cycle, the diffusion-type phase transformation, martensite transformation and recrystallization and other structural transformations were occured in the heat-affected zone. Therefore, in the simulation of the microstructure of the heat-affected zone, many difficulties are caused by solute diffusion, interfacial energy, subcooling and other factors during the solid phase transition.

3.2. Research status of grain growth simulation in heat affected zone
The Monte Carlo method (MC) is a type of deterministic method, which is a numerical method based on probability that adopts random sampling and statistical methods to explain physical processes. The MC method only involves the growth process of crystal grains and does not involve the theoretical system of initial nucleation of crystal grains. Based on this, the MC method is widely applied in the simulation of grain growth in the heat-affected zone of welded joints. In 2004, Debroy and Mishra[19] used the MC method to reproduce the grain topological morphology and grain distribution characteristics of the heat affected zone of Ti-6Al-4V alloy TIG welding. In 2008, Xu Yanli[20] simulated the grain growth behavior of SUS316 stainless steel and Nimonic263 nickel-based alloy welding heat-affected zone respectively, based on the modified EDB (Experimental Data Based) model. Wu Chuansong[21], Kim[22], Zhang[23] have successfully obtained the grain growth behavior of the heat-affected zone by using the MC model, including the heat-affected zone of ferritic stainless steel by laser-pulse MIG hybrid welding, and carbon steel welding Heat-affected zone, aluminum alloy friction stir welding joints.

The CA method is based on the physical mechanism of grain nucleation and the kinetic theory of grain growth and the actual grain nucleation and growth process is basically consistent. Therefore, the CA method has been favored by many scholars in the study of mesoscale microstructure simulation[24]. In 2007, Raghavan[25] simulated the grain growth and dynamic recrystallization process with the aid of the CA method, and proposed a new method to calculate the local curvature of the grain boundary. In 2009, Li Yubin et al.[26] explored the correspondence between the heat-affected zone grain distribution and the welding temperature field distribution based on the CA
method. In 2009, Ma Rui, Dong Zhibo, et al.[27] further revised the above model, combined the flow field and CA model for coupling calculation, and successfully analyzed the influence of the flow field on the growth process of columnar and equiaxed crystals in the molten pool. In 2014, Song Kuijing[28] carried out CA simulations on the grain growth process of the heat-affected zone during TA15TIG welding.

3.3. Research status of solid-state phase transition in heat-affected zone

The final structure and phase composition of welded joints are mainly determined by the solid-state phase transformation process. Currently, there are three main methods for the evolution of solid phase change structure. The first method, analytical model based on phase change thermodynamics and phase change kinetics, including the JMA equation. The second method, based on isothermal transition TTT diagram, continuous cooling transition CCT diagram and continuous cooling transition SHCCT diagram of simulated welding heat affected zone. The third method is the particle model method used to simulate the transformation of the mushy zone and the microstructure phenomenological model suitable for solid-state welded joints.

The first two methods are feasible for predicting the dynamic behavior of phase change and the phase change fraction of each stage under different conditions, but it is impossible to predict the morphology of the tissue dynamically and in real time. In order to obtain the phase morphology, Benoit Appolaire [29] assumed that the morphology of the precipitated phase was parabolic, and then applied the Ivantsov analytical model to calculate the growth of grain boundary α phase, widmanstatten α phase, and intracrystalline acicular α phase. However, due to the prominent widmanstatten anisotropy, the parabolic hypothesis is far from its actual geometric shape.

The particle model is a new technology that was originally employed to simulate the solidification of spherical particles of equal size[30]. One advantage belongs to this method, that is, by using discrete elements to simulate a larger non-isothermal mushy zone. Zareie Rajani et al.[31] realized the mesoscale simulation of Al-Mg-Si alloy welding process through the coupled temperature field.

The model successfully reproduced the evolution process of the continuous liquid film and solidifying grains in the mushy zone of the weld.

The phenomenological model of microstructure refers to a model that establishes a quantitative relationship between the parameters describing the evolution of the structure and the deformation parameters (deformation temperature, strain rate, strain) through experimental methods. It is perfect to simulate the microstructure of friction welding joint with this model. It has been applied in the field of material recrystallization structure simulation in the 1970s. In 2013, Bennett et al. [32] introduced the phenomenological model to the microstructure simulation of welded joints, and finally obtained the distribution and volume fraction of austenite grains in Aermet 100 and SCMV inertial friction welded joints. Xu Wei et al.[33] established a two-dimensional axisymmetric thermal-mechanical coupled finite element model of the FGH96 alloy inertial friction welding process based on the finite element calculation software MSC.Marc. Through secondary development, the microstructure evolution process was simulated, and the distribution of dynamic recrystallization fraction and average grain size was verified, as shown in figure 2.

![Average grain size distribution in the process of IFW](image_url)
4. Conclusion and Outlook
In order to explore the complex evolution process and physicochemical mechanism of the microstructure of welded joints, the numerical simulation method of multi-field and multi-scale coupling is adopted. Moreover, quantitative, qualitative, and visual dynamic research has been obtained, which shows that computer simulation has broad prospects in the field of numerical simulation of welded joint microstructure. However, for the current numerical simulation model of microstructure, it is necessary for the following four points: (1) Supplement the coupling relationship between the numerical model and the relevant physical parameters of the actual process, such as time, temperature, solute, flow field. (2) Optimizing the structure of the current microstructure numerical model and exploiting universally applicable microstructure simulation software. (3) Improving the calculation efficiency of the model and enlarging the simulation area to reproduce the structural transformation of the entire welded joint. (4) A three-dimensional model should be used for calculations to obtain dynamic solidification and transformation behaviors closer to actual welded joints.

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