Computers and Structures 186 (2017) 35–49

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

A numerical kinematic model of welding process for low carbon steels

Junyan Ni [a], Magd Abdel Wahab [b,c,d,*]

[a] Department of Electrical Energy, Systems and Automation, Faculty of Engineering and Architecture, Ghent University, Belgium
[b] Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
[c] Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
[d] Soete Laboratory, Faculty of Engineering and Architecture, Ghent University, Technologiepark Zwijnaarde 903, B-9052 Zwijnaarde, Belgium

ARTICLE INFO

Article history:
Received 10 January 2017
Accepted 13 March 2017

Keywords:
Phase transformation
Welding process
Finite element analysis
ABAQUS

ABSTRACT

A numerical metallurgical integrated model, based on Bhadeshia microstructure model, is developed to predict microstructure development of welding low carbon steels. The new model integrates the thermodynamic kinematics equations and provides the start and finish temperatures during continuous cooling, the transformation kinetics, as well as, the resultant volume fractions of each micro-constituents. Further, it is integrated into finite element (FE) commercial package ABAQUS and the laser welding process of DP600 blanks is numerically simulated. The temperature-dependent thermal properties are adopted to calculate the temperature field and history, which are used as input to describe the kinematics of phase transformation. Knowing the chemical composition in each node, the process of austenization and austenite-to-allotriomorphic ferrite/Widmannstätten ferrite/pealite/bainite/martensite are modelled, respectively. The results obtained using our proposed model are compared with those obtained using Kirkaldy model for S355 steel. Furthermore, the results predicted by both models are compared with experimental data. In addition, the predicted volume fractions are validated using experimental data at selected locations. The proposed thermo-metallurgical model serves as a useful tool to forecast the transformation products during and after welding.

1. Introduction

Several algorithms [1–7] have been proposed and adopted in finite element codes to predict the development of microstructure during welding process. Among those, Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation [6] is the most widely used. The derivation of JMAK equation assumes random nucleation and constant growth rate, and the application is limited to isothermal transition from one phase to another. This limitation is often overcome by the law of additivity so that the JMAK model can be extended to an isothermal condition [3,8,9]. Before implementation, the temperature-dependent growth parameters in JMAK equation need to be determined by several experiments [10], and the welding heat source and the cooling rate have to be carefully calibrated and predicted as well [11]. Comparably, Leblond et al. [2] developed an incremental function of temperature-dependent parameters, i.e., equilibrium volume fraction and characteristic time to describe the transformation kinetics, which is capable of predicting microstructure evolution in arbitrary thermal history. This model is relatively flexible and was applied to situation where the chemical compositions of base material and fusion zone are distinguished [11]. However, both models mentioned above need to be calibrated with time-temperature-transformation (TTT) and/or continuous cooling transformation (CCT) diagrams before implementation. As it is said, the coefficient and the exponent in the JMAK equation need to be determined with the knowledge of two points in TTT diagram at each temperature. Similarly, values of characteristic time in Leblond's model [2] need to be solved by comparing the austenite (γ)/austenite (γ) + ferrite (α) temperature boundaries at isothermal and anisothermal conditions. The JMAK model has already been integrated by several authors [9,12] in order to examine the effect of microstructure on the mechanical properties of welds. Similarly, the model proposed by Leblond et al. [2] has been also incorporated as the metallurgical algorithm in commercial software SYSWELD [13].

Independently from metallurgical diagrams, Kirkaldy et al. [1] expressed the increment of volume fraction in function of grain size, temperature and temperature histories. Their model was further extended by Watt et al. [4] to describe simultaneous decomposition and was implemented by Henwood et al. [14] in FE code to model microstructural development during welding process.

* Corresponding author at: Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam.
E-mail addresses: magd.abdelwahab@tdt.edu.vn, magd.abdelwahab@UGent.be (M. Abdel Wahab).

http://dx.doi.org/10.1016/j.compstruc.2017.03.009
0045-7949/

The start temperatures and parameters in growth functions were estimated simply based on empirical formulas of chemical composition. Börjesson et al. [15] adopted similar algorithm and included mechanical properties in finite element analysis.

Comparably, another self-dependent model was proposed by Bhadeshia et al. [16–19], in which the start and finish transformation temperatures are estimated based on thermodynamic theories rather than empirical functions. For transforming kinetics, the model, not only, assumes the reconstructive transformation to occur at grain boundaries, but also includes the possibility of inclusion nucleation. The nucleation rates were treated as temperature-dependent and the growth rates were determined by solving carbon diffusion equations [16]. The initiation of bainite growth was assumed to be displacive with a strain energy of 400 J/mol[20]. Besides, a new relationship was proposed for martensitic transformation [18]. The advantages of the serial work by Bhadeshia et al. [16–19] are:

(a) it omits the necessity of determining parameters with known results and
(b) it requires only the basic information i.e., the chemical composition, the temperature history and the austenite grain size at the beginning.

In the present work, the frameworks proposed by Kirkaldy and Bhadeshia are briefly described in Section 2. The corresponding predicted start and finish temperatures, and the volume fractions of various micro-constituents are presented and are compared to experimental data as well. In Section 3, the model by Bhadeshia et al. [16–18] is implemented in the commercial finite element package ABAQUS to predict the microstructure development over the welding area in case of two steels. The way to couple the metallurgical model with thermal analysis is summarized in a flow chart. The heat source model developed by Goldak [21] are presented. The corresponding temperature histories predicted through thermal analysis are compared with measured values at several selected sites. Finally, the plot contour of microstructure are analysed and compared to metallographic results. Although this research deals with the integration of the microstructure welding model in Finite Element Analysis, the authors believe that the future implementation of this model in a more advanced numerical technique, such as isogeometric analysis (IGA) [22–33], will be an interesting topic in predicting microstructure development of welding low carbon steels. Isogeometric analysis (IGA) was originally introduced by Hughes et al. [34,35] with the aim to integrate Finite Element Analysis with Computer Added Design (CAD) and showed some favourable features. In IGA, non-uniform rational B-spline (NURBS) basis functions are used to describe the exact geometry of a structure and approximate its field variables. For implementations and applications of IGA, the reader may refer to recent publications on this topic [36–41].

2. Framework of two metallurgical models

Austenite (γ) decomposes into several products, i.e. allotriomorphic ferrite (α), Widmannstätten ferrite (α_w), pearlite (α_p), bainite (α_b) and martensite (α') during welding process. According to classical transformation theories, two typical transition types i.e., reconstructive and displacive transformations, occur during continuous cooling.

2.1. Transformation model proposed by Bhadeshia

Reconstructive phase transformation includes transition from γ to α and α_p. Below the A_{e3} boundary, the transformation to α becomes possible. In the framework of Bhadeshia's model, the theoretical calculation for A_{e3} was proposed by Shiflet et al. [42] as:

$$\Delta\mu_{Fe}^{\gamma\to\alpha} = RT\ln a_{Fe}^{\gamma} - RT\ln a_{Fe}^{\alpha} \tag{1}$$

where $a_{Fe}^{\alpha}=1$. $\Delta\mu_{Fe}^{\gamma\to\alpha}$ is the molar Gibbs free energy difference of iron between α and γ, and a_{Fe}^{γ} and a_{Fe}^{α} are the activities of iron in α and γ respectively. The parameter a_{Fe}^{γ} is further expressed as [42]:

$$\ln a_{Fe}^{\gamma} = 5\ln\left(\frac{1-x_\gamma}{1-2x_\gamma}\right)+6 \times \ln\left(\frac{1-2J_\gamma+(4J_\gamma-1)x_\gamma-[1-2(1+2J_\gamma)x_\gamma+(1+8J_\gamma)x_\gamma^2]^{1/2}}{2J_\gamma(2x_\gamma-1)}\right) \tag{2}$$

where x_γ is the carbon concentration in γ and $J_\gamma = 1-e^{-\omega_\gamma/RT}$. ω_γ is the pairwise interaction energy between adjacent carbon atoms in γ, which is calculated as a function of chemical compositions [43]. By solving the above equations, the A_{e3} boundary can be obtained.

The eutectoid temperature A_{e1} is estimated based on thermodynamic equilibrium as A_{e3} but calculated by assuming carbon concentration equilibrium in both γ and cementite θ (Fe_3C, M_3C). The equilibrium condition is expressed as [44,45]:

$$\frac{1}{3}x_{Fe}^{\gamma}\left(4\mu_{Fe_3C}-3\mu_{Fe}^{\gamma}-\mu_C^{\gamma}\right)+\frac{1}{3}x_M^{\gamma}\left(4\mu_{M_3C}-3\mu_M^{\gamma}-\mu_C^{\gamma}\right)=0 \tag{3}$$

where M is the alloying element. x_{Fe}^{γ} and x_M^{γ} are mole fractions of iron and substitional element in γ, respectively. μ_{Fe}^{γ}, μ_C^{γ} and μ_M^{γ} are molar Gibbs free energies of iron, carbon and alloying element in γ respectively. μ_{Fe_3C} and μ_{M_3C} are the molar Gibbs free energies of cementite. As long as the temperature falls below A_{e3} and the above equilibrium condition is satisfied, transition to α_p becomes possible. The thermodynamic equilibrium based algorithm is implemented in model of Bhadeshia [16].

As the temperature drops drastically, the transformation procedure becomes displacive. In the framework of Bhadeshia, the start temperature and growth mechanism of Widmannstätten ferrite (α_w) are considered different from allotriomorphic ferrite (α). The start temperature of α_w is denoted as W_s, which is determined by [20]:

$$|\Delta F^{\gamma\to\gamma+\alpha}| \geqslant F_{\alpha_w} \tag{4}$$

and

$$|\Delta F^{\gamma\to\gamma+\alpha}| \geqslant \Delta F_N \tag{5}$$

where $\Delta F^{\gamma\to\gamma+\alpha}$ is the change of partial Gibbs free energy when γ transforms to α in an equilibrium carbon concentration. ΔF_N is the energy difference needed to obtain a detectable nucleation [46]. The stored strain energy in Widmannstätten ferrite F_{α_w} is supposed to be about 50 J/mol [16]. $\Delta F^{\gamma\to\gamma+\alpha}$ can be further expressed as:

$$\Delta F^{\gamma\to\gamma+\alpha} = RT\left[(1-x_\gamma)\ln\frac{a_{Fe}^{\gamma}}{a_{Fe}^{\alpha}}+x_\gamma\ln\frac{a_C^{\gamma}}{a_C^{\alpha}}\right] \tag{6}$$

where a_C^{γ} and a_C^{α} are the activities of carbon in α and γ respectively and the rest are defined the same as in Eq. (1). The start temperature of bainite B_s is determined similarly as α_w, but with different energy gap $\Delta F^{\gamma\to\alpha'}$. Bainitic ferrite forms when the following conditions are satisfied [20]:

$$|\Delta F^{\gamma\to\alpha'}| \geqslant F_{\alpha_b} \tag{7}$$

and

$$|\Delta F^{\gamma\to\gamma+\alpha}| \geqslant \Delta F_N \tag{8}$$