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Modeling of microstructural evolution during divorced eutectic solidification of spheroidal graphite irons

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Abstract—A two-dimensional multiphase cellular automaton model is proposed for the simulation of microstructural evolution during divorced eutectic solidification of spheroidal graphite (SG) irons. The model adopts a previously proposed local solutal equilibrium approach to calculate the driving force for the growth of both graphite and austenite phases. The growth kinetics of graphite also includes the effect of the density difference between iron and graphite. The model is applied to simulate the microstructural evolution of both hypoeutectic and hypereutectic SG irons. The simulated microstructures, cooling curve and graphite nodule sizes at various cooling rates compare reasonably well with the experimental data, demonstrating the quantitative capabilities of the proposed model. The simulation results reveal some dynamic features of the divorced eutectic solidification, such as the interactive and competitive growth between austenite dendrites and graphite nodules, and the graphite growth controlled by carbon diffusion through the solid austenite shell.

Keywords: Microstructural modeling; Solidification; Divorced eutectic; Spheroidal graphite; Ductile iron

1. Introduction

Spheroidal graphite (SG) cast iron is characterized by the presence of quasi-spherical graphite nodules distributed in the metallic matrix. The spheroidal shape of the graphite reduces the stress concentration and provides higher strength and toughness than that of gray (lamellar graphite) iron. Since the discovery of SG cast iron (1938–1948 independently by Adey, Millis and Morrogh), it has been used extensively in industry because of its good mechanical properties, castability, machinability and competitive price compared with many other materials [1].

The mechanical properties of SG iron depend mainly on the shape, size and distribution of graphite nodules, and on the microstructure of the iron matrix. While the matrix can be modified/improved through subsequent heat treatment, the graphite shape and distribution are mostly the results of solidification, and can be only slightly affected by heat treatment.

Computer modeling has now become an effective tool for understanding and describing the mechanisms of microstructural evolution during solidification. However, the complex solidification of SG iron is one of the most difficult liquid-to-solid transformations to describe through computational modeling, as the eutectic is a divorced eutectic where the graphite (Gr) growth is mostly through solid diffusion through an austenite (γ) shell, as demonstrated experimentally by Patterson and Scheil [2] as early as 1953. Scanning electron microscopy (SEM) images of microshrinkage in SG iron (Fig. 1) [3] suggest that, while the austenite grows anisotropically into the liquid along its preferred crystallographic orientation, restrictions imposed by isotropic diffusion growth will force an increased isotropy on the system. The dendritic shape of the austenite will be altered and the γ/liquid interface will exhibit only small protuberances instead of clear secondary arms. A further complication is that the eutectic grain of SG iron consists of SG surrounded by eutectic austenite deposited on primary austenite dendrites. Such a grain is difficult to outline through classical metallographic procedures. Color etching metallography [4], special etching techniques (direct austempering after solidification) [5] and microshrinkage SEM pictures (Fig. 1) demonstrate that the SG iron eutectic grain is made of several graphite nodules surrounded by quasi-spherical austenite envelopes. For a more in-depth description of the solidification of SG iron, the reader is referred to Ref. [6].

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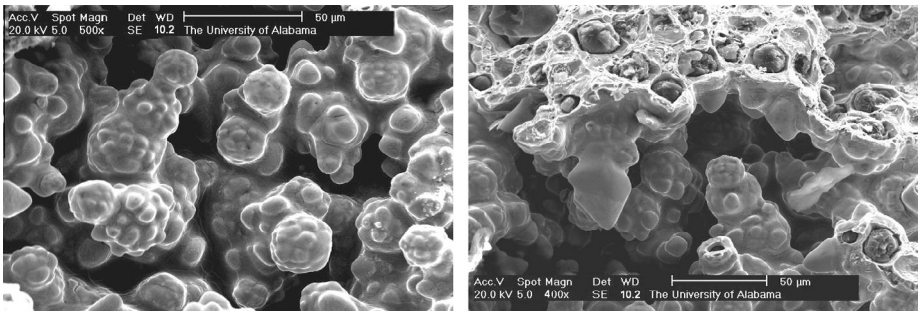

Fig. 1. SEM images of the divorced graphite–austenite eutectic in SG iron. The images are from a shrinkage cavity and can be considered as resulting from interrupted solidification [3].

Detailed reviews of the analytical and computational models for the solidification of SG iron have been provided in a series of recent papers, including Ref. [7]. Only the references with direct relevance to this work will be further discussed. An analytical model that has survived the test of time is that proposed in 1972 by Wetterfall et al. [8] in which calculations of diffusion-controlled steady-state growth of graphite through the austenite shell were made based on Zener's growth equation for an isolated spherical particle in a matrix of low supersaturation. This model, or modifications of this model [9], is used in practically all the deterministic models attempting to describe the solidification of SG iron (e.g. Refs. [10–12]). All these models solve the transport equation for a volume element with uniform composition and temperature, and thus microstructure, and are unable to generate microstructural visualization. A number of cellular automaton (CA) models tackled the problem of microstructural visualization. An early CA model developed by Charbon and Rappaz [13] used the classic model for diffusion-controlled graphite growth through the austenite shell. The results revealed that each grain included only one graphite nodule, contrary to current understanding and experimental results. Using Object Oriented Programming in C++, Beltran-Sanchez and co-workers [3] included solidification of primary austenite grains, which allowed for a more realistic description of the divorced eutectic growth of SG iron. Graphite growth was initiated once the graphite nuclei came in contact with the austenite grains. Their model produced pictures of multi-nodule austenite grains.

Burbelko, Kapturkiewicz and co-workers [14–16] proposed CA models that take into account the continuous nucleation of austenite and graphite grains from liquid, and the subsequent growth of the graphite–austenite eutectic under non-steady-state temperature distribution. The interface migration rate was considered to be a linear function of the local kinetic undercooling. Thus, a kinetic growth coefficient must be properly determined if quantitative simulation is to be pursued. The model was adopted to investigate the effect of the growth of graphite spheroids on the inhomogeneity of the carbon concentration field and on the growth of the austenite dendrite. Nevertheless, the influence of process variables such as cooling rate on the microstructural features, including the size and density of graphite nodules, was not simulated. Moreover, the model does not include the effect of difference in density between graphite and iron, which should have an important impact on the solidified microstructures.

The present authors [17,18] proposed a multiphase CA model to simulate the solidification of the divorced eutectic microstructures of SG cast iron. In the model, the growth kinetics of both graphite nodules and austenite dendrites were determined using a local composition equilibrium approach previously proposed by Zhu and Stefanescu [19], which allows reasonable calculation of the growth velocities for both austenite and graphite phases without the need to introduce kinetic coefficients. However, in calculating the growth velocity of the graphite phase, an average concentration was used. In addition, the growth kinetics of graphite did not account for the effect of the difference in density between iron and graphite. Consequently, the simulated graphite fraction and average nodule size were lower than the experimental data.

The present paper presents an improved version of the multiphase CA model. It takes into account the effect of the difference in density between iron and graphite in calculating the increment of graphite fraction. Moreover, the actual local carbon concentration, rather than the average concentration, is used to determine the growth kinetics of graphite nodules. The model is adopted to simulate the microstructural evolution during solidification of both hypoeutectic and hypereutectic SG irons. The mechanisms of the interactive and competitive growth between austenite dendrites and graphite nodules are discussed. The effects of cooling rate on the size and density of graphite nodules are studied. The simulation results are compared with those obtained experimentally.

2. Governing equations and numerical algorithm

2.1. Description of model

The focus of the present work is to model the microstructural evolution during the solidification of both hypoeutectic and hypereutectic SG iron alloys, which involves divorced eutectic reactions. The computation domain is divided into uniform square cells (grids). Each cell is characterized by several variables, such as composition, temperature, phase fractions (liquid, austenite and graphite), crystallographic orientation (for austenite dendrite), index (for graphite nodule) and states, including liquid cell ($f_L = 1$), graphite cell ($f_{Gr} = 1$), austenite cell ($f_\gamma = 1$), the graphite/liquid (Gr/L) interface cell ($0 < f_{Gr} < 1$, and $f_\gamma = 0$), the austenite/liquid (γ/L) interface cell ($0 < f_\gamma < 1$, and $f_{Gr} = 0$), the graphite/austenite (Gr/γ) interface cell ($f_{Gr} > 0$, $f_\gamma > 0$, and $f_{Gr} + f_\gamma = 1$), and the graphite/austenite/liquid (Gr/γ/L) interface cell ($f_{Gr} > 0$, $f_\gamma > 0$, and $f_{Gr} + f_\gamma < 1$), where f_L, f_{Gr} and f_γ are the fractions of liquid, graphite and austenite, respectively. The cells that