



## Comparison of solidification behavior between in situ observation and simulation of Fe–C–Si system



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### ABSTRACT

Over the last few years, important advances have been made in the understanding and modelling of phase transformations of metallic alloys including (a) the coupling of phase equilibria and kinetics for computerised simulation of multicomponent alloys and (b) in situ time resolved X-ray imaging of phase transformations in real time. Both techniques can be complementary. However the quality of the simulation relies to a large extent on the accuracy of phase equilibria and diffusion data obtained from existing experimental studies. In situ X-ray techniques provide quantitative information on the evolution and proportion of phases, and can validate the thermodynamic/kinetic packages. This validation in-turn improves the computational models and databases. In the present work, the phase transformation in the Fe–C–Si system from liquid to  $\gamma$ -Fe and the reaction liquid  $\leftrightarrow$   $\gamma$ -Fe + Cementite was observed by using X-ray imaging at SPring-8 synchrotron. The relationship between fraction solid and temperature was obtained from the generated SPring-8 images. The results are compared with computer simulation using Thermo-Calc. and DICTRA. A critical analysis compares the results of the simulation with the real-time observations of the phase transformation.

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### 1. Introduction

Cast iron, represented by the Fe–C system, with Si as the main alloying element is one of the basic materials of the metallurgy industry. Its lower eutectic melting point of 1366 K [1], compared to that of stainless of 1600–1800 K [2], facilitates the casting processes and as a consequence the production of complex shaped objects. Although cast iron is sensitive to impact forces because of its brittleness and unsuitable for hot rolling or forging, low temperature casting has the potential to reduce the costs of production rendering the alloy useful for home appliances and frames of industrial machines [3].

In cast iron, the distributed proportions and shape of  $\gamma$ -Fe and graphite (cementite) define the mechanical properties. For instance, the formation of a large proportion of flake shape graphite (cementite) plays a major role in the brittleness of the material [4]. Thus, in order to improve their mechanical properties, the microstructure formed during cooling should be understood and controlled.

The conventional approach for studying and control of microstructure during casting solely relying on experimentation as a

pathway to alloy development is no longer the most efficient use of resources. The potential of alloy improvement through computer simulation has motivated the development of coupled thermodynamic and kinetic packages over the past twenty years. Examples of specific software are Thermo-Calc. and DICTRA [5]. These packages are based on the calculation of phase diagrams (CALPHAD), and on the finite difference simulation of diffusion controlled reactions in multicomponent alloys, respectively.

Alternatively, over the past decades, synchrotron based technology has been developed that enables direct observation of phase transformations in metals in real time [6–8]. Using those techniques, the phase evolution can be observed by using X-ray transmission imaging technology and simulated using commercial thermodynamic and kinetic packages.

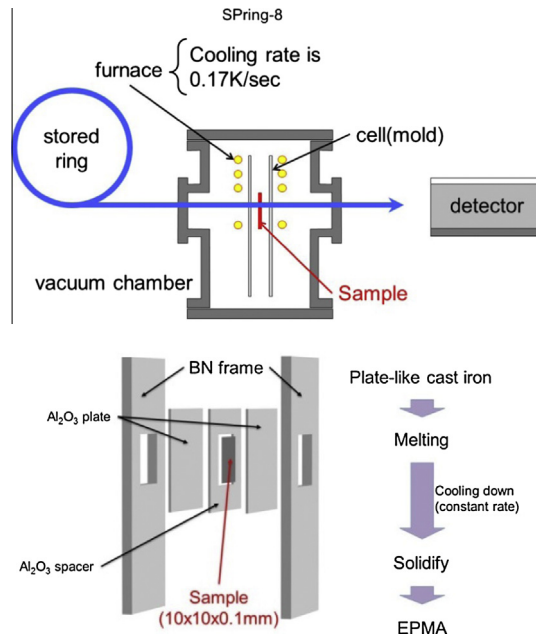
Among the phase transformation parameters able to be assessed during cooling of cast iron, the fraction of solids is one of paramount relevance. The following three statements illustrate the importance of it:

- Their relationships with mechanical properties are able to be estimated.
- It is an information easy to retrieve at condition of equilibria using appropriate phase diagrams.
- It is a parameter possible to control and evaluate during casting.

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**Table 1**  
Composition of samples.

Sample No.	ICP-MS compositional analysis of sample (wt%)			
	C	Si	P	S
Sample 1	3.17	<0.01	<0.001	0.003
Sample 2	4.50	<0.01	<0.001	<0.001
Sample 3	2.92	1.43	<0.001	<0.001
Sample 4	3.62	2.48	<0.001	<0.001



**Fig. 1.** Schematic experimental apparatus with details of the cell.

The equilibrium model represent one extreme where infinitely large diffusion is assumed in both solid and liquid phases. The Scheil approximation are the other extreme and assumes no diffusion in solids and infinitely large diffusion in the liquid [9]. In the Fe–C related systems, the carbon diffusion in solids is considerably fast, thus the Scheil model is not valid. A realistic description for the Fe–C associated systems are the simulations that include data

on diffusion coefficients and on the microstructure. Validity of the diffusion simulation models using the proportion of solids as a parameter of comparison has been tested for Stainless Steel under various conditions [10,11]. However, there is an absence of reported validations of the existing simulation packages for cast iron related alloy. Thus, it is the opinion of the authors that the in situ X-ray studies using X-ray imaging from SPring-8 provides a unique opportunity to compare in situ observations with results of computer simulation.

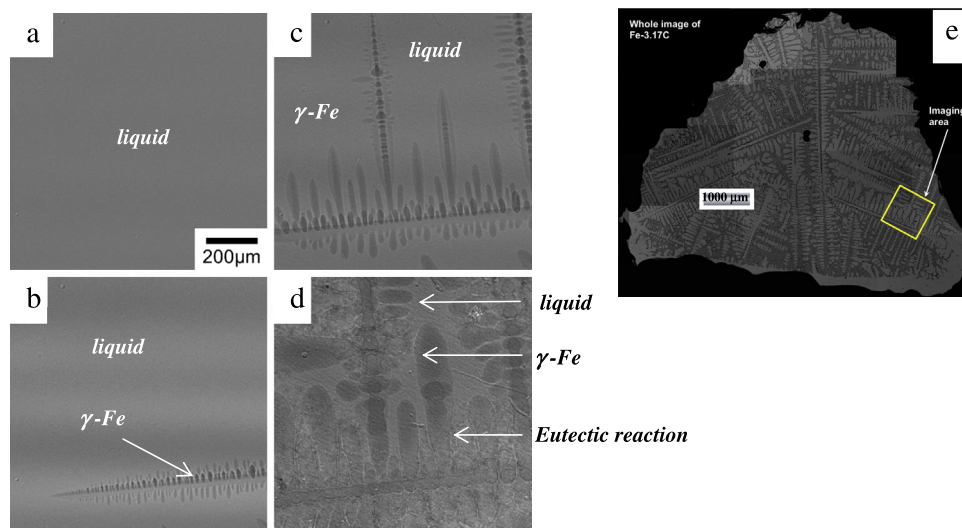
The present work undertakes an analysis of the proportion of solid phases during cooling for the Fe–C and Fe–C–Si systems at selected compositions to compare the results obtained using simulation with that of real-time observation of phase transformation. We expect to generate information to optimize the kinetic parameters and subsequently, obtain more reliable databases and simulation results.

## 2. Experimental procedure

The samples at the target composition were pre-melted using an Arc-melting method and high purity materials, such as 99.99 wt%Fe, 99.99999 wt%C and 99.99999 wt%Si. The selected composition of the samples as analysed using ICP-MS can be seen in Table 1. The four compositions correspond to two hypoeutectic and two hyper-eutectic for each of the Fe–C and Fe–C–Si systems.

The direct observation was carried out using a BL20XU in SPring-8. The schematic experimental apparatus shows in Fig. 1. The sample with dimensions 10 mm × 10 mm × 0.1 mm was set in the centre of the cell, which was located between heaters. The cell consisted of the BN frame, Al<sub>2</sub>O<sub>3</sub> window, and Al<sub>2</sub>O<sub>3</sub> spacer. The furnace, including the cell, was placed in the vacuum chamber. The pressure in the chamber was adjusted to about 1 Pa. In order to control the temperature of the furnace, the thermocouple was set close to the sample. The cooling rate of the sample was fixed at 0.17 K/s. The X-ray beam from the stored ring passed through the chamber and the sample before reaching the detector where a series of sequential transmission images were obtained. Further detailed experimental conditions can be found elsewhere [8].

As an example, Fig. 2 shows the sequential direct observation image of Fe–3.17 wt%C (sample 1). During the experiments, the sample was completely melted as is shown in Fig. 2(a), prior to cooling down at a constant rate of 0.17 K/s. As indicated in Fig. 2(b), a dendrite of  $\gamma$ -Fe appeared from the left side. The density of the solid phases  $\gamma$ -Fe are higher than that of liquid phase, thus, the dendrites of  $\gamma$ -Fe became the darkest region. The primary  $\gamma$ -Fe grew as indicated in sequential image Fig. 2(c) until the sample reached the eutectic reaction as can be seen in Fig. 2(d). The experiment continued until the end of the eutectic reaction when the sample was let cool down to room temperature. A typical sample at the end of the experiment is shown in Fig. 2(e), the sample indicates the approximate section of the direct observation which corresponds to a rectangular area of approx. 1 mm × 1 mm.



**Fig. 2.** Sequential direct observation image of Fe–3.17mass%C. (a) liquid sample; (b) precipitation of dendrite of  $\gamma$ -Fe; (c) starting of the eutectic reaction; (d) end of the eutectic reaction; (e) SEM image of the whole sample at the end of the experiment.

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