

# Understanding Hot Cracking of Steels during Rapid Solidification: an ICME Approach

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**Abstract:** Cracking is a major problem for several types of steels during additive manufacturing. Non-equilibrium kinetics of rapid solidification and solid-solid phase transformations are critical in determining cracking susceptibility. Previous studies correlate hot cracking susceptibility to solidification sequence, and therefore composition, empirically. In this study, an Integrated Computational Materials Engineering (ICME) approach is used to provide a more mechanistic and quantitative understanding of hot cracking susceptibility of a number of steels in relation to the peritectic reaction and evolution of  $\delta$ -ferrite during solidification. The application of ICME and hot cracking susceptibility predictions to alloy design for additive manufacturing is discussed.

**Keywords:** rapid solidification; hot cracking resistance; ICME

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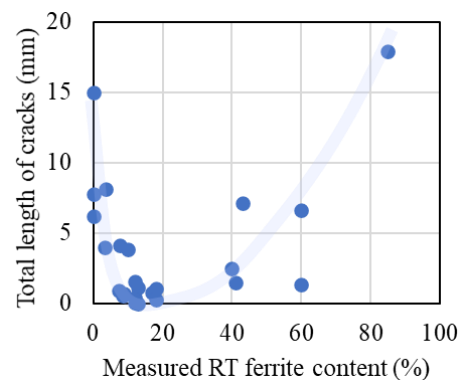
## 1. Introduction

Solidification cracking, also referred to as hot tearing, is one of the major problems for some types of steels during solidification in processes such as casting, welding, and additive manufacturing. It occurs when dendrites inhibit the flow of the remaining liquid in the interdendritic region to compensate for shrinkage and strain. Initial theories regarding hot cracking hypothesized that as the freezing range of an alloy, defined by the difference of liquidus and solidus temperature, is increased, the more susceptible it is to cracking, as large freezing ranges can lead to more interlocked dendrites that form in the later stages of solidification [1]. A more quantitative measure of solidification cracking, known as cracking susceptibility coefficient (CSC), proposed by Clyne and Davies [2], has been widely used to describe solidification cracking tendency. It is defined by Equation 1,

$$\text{CSC} = \frac{t_v}{t_R} \quad (1)$$

where  $t_v$  is the time period during solidification when the system is vulnerable to cracking which is taken as the liquid fraction between 0.1 and 0.01, and  $t_R$  is the time period during solidification when liquid feeding can readily occur, which corresponds to the liquid fraction between 0.6 and 0.1. Thus, if the window for stress relief is relatively large compared to the time period during which the alloy can readily crack, the probability for cracking during solidification is decreased, represented by the reduction of CSC. Three types of correlations were proposed to estimate cooling conditions: mode 1 with a constant cooling rate; mode 2 with a constant heat flow; mode 3 with a heat flow proportional to the square root of time [3].

Extensive studies have also shown that solidification cracking is closely related to the course of solidification and ferrite fraction at solidification temperatures, which are essentially composition-dependent. Kujanpää *et al.* [4] measured and correlated room-temperature  $\delta$ -ferrite content to total crack length for 24 austenitic and austenitic-ferritic welds with  $Cr_{eq}/Ni_{eq}$  between 1.11 and 3.25. It was identified that the least hot cracking is correlated to 10%-20%  $\delta$ -ferrite at room temperature, as indicated by Figure 1. However, using room-temperature ferrite content to explain solidification cracking behavior is mechanically insufficient, as the full evolution of ferrite content during solidification and cooling is not taken into account. While experimentally available information is usually limited to room temperature measurements, state-of-the-art computational techniques enables analysis of the evolution of phase contents during solidification, which is essential to understanding solidification cracking.



**Figure 1.** Total length of cracks vs  $\delta$ -ferrite content measured at room temperature for 24 austenitic and austenitic-ferritic welds in [4].

This work is utilizing a CALPHAD-based ICME (Integrated Computational Materials Engineering) approach to quantify these metrics in order to evaluate solidification cracking tendency with respect to steel compositions in a more mechanistic manner.

## 2. Methods

Solute redistribution with respect to temperature during rapid solidification is simulated by the Scheil-Gulliver model using the Scheil Calculator within Thermo-Calc software. It is a classical model for extreme non-equilibrium conditions where there is assumed to be no diffusion in the solid phase and infinitely fast diffusion of all components in the liquid phase.

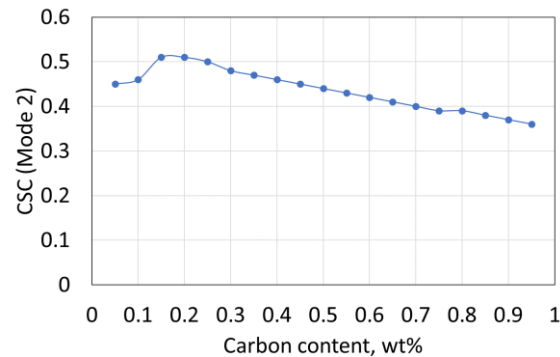
For diffusion-controlled phase transformations during solidification and continuous cooling, DICTRA is used to predict cooling-rate-controlled kinetics. In this work, a cylindrical 1-dimensional cell is used to represent thickening of primary cell arms during solidification.

## 3. Results and discussions

### Hot cracking susceptibility (HCS)

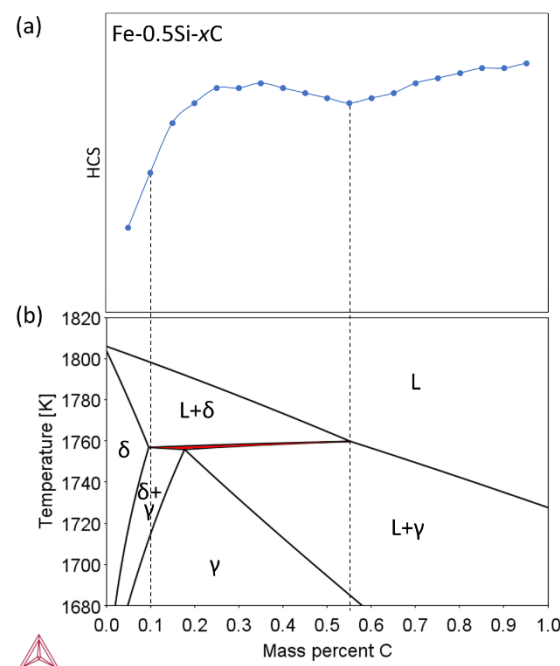
CSC values for Fe-0.5Si- $x$ C ( $x = 0.05$ - $0.95$ , in wt.%) ternary system are calculated from Scheil curves based on the model proposed by Clyne and Davies [2]. Since it is suggested that mode 2 and mode 3 give similar reasonable results on susceptibility prediction, CSC values under mode 2 cooling condition are plotted against carbon content in Figure 2 to manifest carbon effect on cracking susceptibility. Figure 2 suggests that for dilute solutions ( $x < 0.2$  wt.%), the alloy system gets prone to cracking as carbon content increases, whereas as carbon content is greater than 0.2 wt.%, increasing carbon level can reduce CSC values. However, this tendency at high carbon region is not well aligned with the experimental observation of hot cracking sensitivity on carbon content of the same alloy

system carried out by Tamaki *et al.* [6]. Experimental evaluation of cracking percentage in steel welds suggests a dip in cracking susceptibility at medium carbon level, followed by increased cracking susceptibility as carbon content increases.



**Figure 2.** CSC (under mode 2 cooling condition) vs carbon content for Fe-0.5Si-xC ( $x = 0.05\sim 0.95$ , in wt.%) ternary system.

To address to the disparity, a metric named HCS (hot cracking susceptibility) [5] is used to represent cracking sensitivity. Figure 3 shows the plot of HCS values against varied carbon content in the Fe-0.5Si-xC ternary system, in comparison with an isopleth of the equilibrium phase diagram. The tendency of HCS curve matches well with experimentally-determined cracking percentage curve in [6], with a dip at intermediate carbon level indicating a less cracking-sensitive composition. Compared with the phase diagram in Figure 3(b), the first bump of the curve corresponds to the alloy compositions with peritectic reaction ( $L + \delta \rightarrow \gamma$ ) occurring during solidification. This indicates that hot cracking sensitivity is a combined effect of solidification temperature and solidification range. With peritectic reactions, solidification range is expanded and therefore increases susceptibility to hot cracking. Therefore, compared with CSC curves, HCS is a more comprehensive metric that can better represent the cracking sensitivity during solidification.

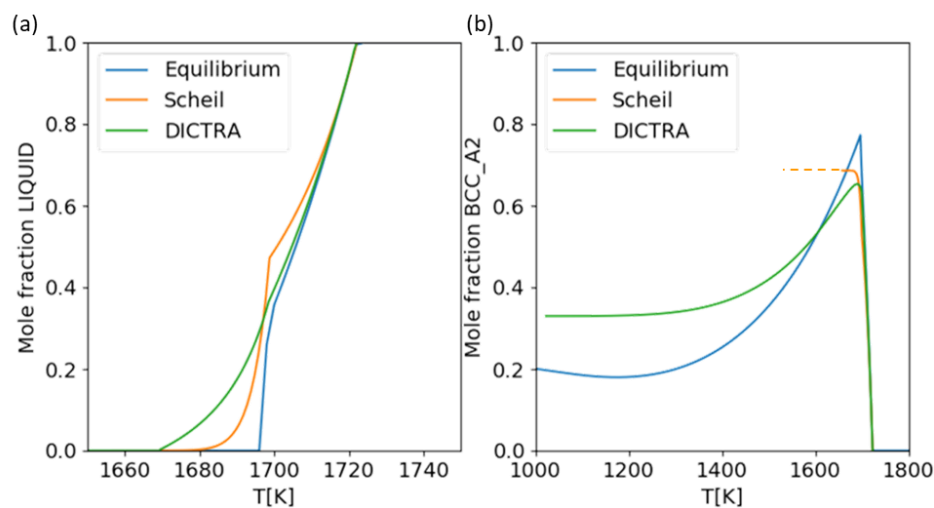


**Figure 3.** Relation between HCS and equilibrium phase diagram of the Fe-0.5Si-xC ( $x = 0.05\sim 0.95$ , in wt.%) ternary system.

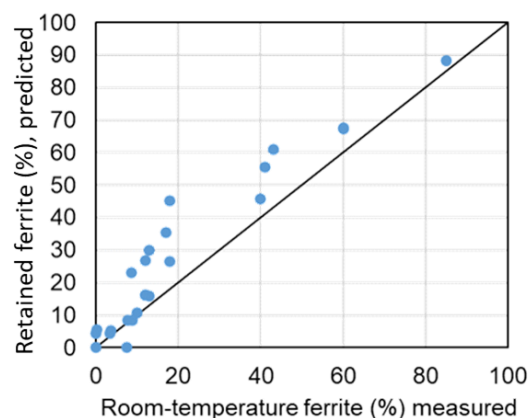
### $\delta$ -solidification

$\delta$ -ferrite fraction is another effective metric that needs to be well-controlled to ensure low solidification cracking susceptibility. Empirically, Schaeffler diagrams are used to dictate  $\delta$ -ferrite fraction and therefore cracking sensitivity with respect to  $Cr_{eq}$  and  $Ni_{eq}$  values, especially for austenitic stainless steels. Using the ICME approach, it is feasible to predict  $\delta$ -ferrite fraction for multicomponent systems with greater reliability, without needs to estimate  $Cr_{eq}$  and  $Ni_{eq}$  values.

In this work, DICTRA simulations are performed to simulate phase transformation during solidification and continuous cooling. Although Scheil simulation can also give a reasonable solidification curve (see Figure 4), it overpredicts room-temperature  $\delta$ -ferrite content in the microstructure, as it does not consider  $\delta$ - $\gamma$  transformation. In contrast, DICTRA can describe both the formation and back-transformation of  $\delta$ -ferrite as a function of cooling rate and cell size during the continuous cooling process. As compared to the experimental results, DICTRA gives better prediction of room-temperature  $\delta$ -ferrite amount (see Figure 5).



**Figure 4.** Comparison of cooling simulations under equilibrium condition, and under non-equilibrium conditions performed by Scheil and DICTRA. (a) Comparison of fraction of liquid during solidification; (b) Comparison of  $\delta$ -ferrite fraction during continuous cooling.

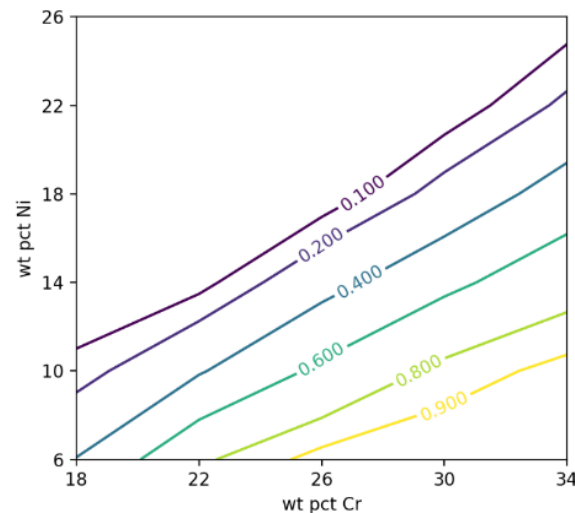


**Figure 5.** Comparison of predicted ferrite fraction by DICTRA simulations and measured values in [4].

### ICME-guided materials design

As described in previous sections, HCS and fraction of  $\delta$ -ferrite are composition-dependent metrics to evaluate solidification cracking susceptibility of alloys. They therefore

can be adopted in compositional designs for improved cracking resistance based on selected benchmark materials. Figure 6 exemplifies a simple ICME-predicted “Schaeffler diagram” generated with  $\delta$ -ferrite fraction data points obtained from DICTRA simulations. For identified  $\delta$ -ferrite fraction, the composition can be adjusted based on sensitivity, with constraints from HCS values.



**Figure 6.** ICME-predicted “Schaeffler diagram”.

#### 4. Conclusions

In this study, the ICME approach to provide a more mechanistic and quantitative understanding of solidification cracking susceptibility of steels during solidification has been demonstrated. Representative metrics, including CSC, HCS and  $\delta$ -ferrite fraction, are discussed quantitatively with CALPHAD-based simulations. Compared with experimental data, it is found that HCS is a more effective and reliable metric to describe hot cracking sensitivity than CSC which is generally used. In addition, DICTRA simulation can successfully be used to predict the evolution of  $\delta$ -ferrite fraction during solidification and continuous cooling. With reliable predictions from ICME tools, compositional design for improved solidification cracking resistance can be achieved.

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## Appendix A

The appendix is an optional section that can contain details and data supplemental to the main text—for example, explanations of experimental details that would disrupt the flow of the main text but nonetheless remain crucial to understanding and reproducing the research shown; figures of replicates for experiments of which representative data is shown in the main text can be added here if brief, or as Supplementary data. Mathematical proofs of results not central to the paper can be added as an appendix.

## Appendix B

All appendix sections must be cited in the main text. In the appendices, Figures, Tables, etc. should be labeled starting with “A”—e.g., Figure A1, Figure A2, etc.

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