

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 the cracking susceptibility. Previous studies correlate the hot cracking susceptibility to the 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 the hot cracking susceptibility of a number of steels in relation to the peritectic reaction and evolution of δ -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 inter-dendritic 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 the cracking susceptibility coefficient (CSC), proposed by Clyne and Davies [2], has been widely used to describe the 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 a reduction of the 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 the ferrite fraction at solidification temperatures, which are

essentially composition-dependent. Kujanpää et al. [4] measured and correlated the room-temperature δ -ferrite content to the total crack length for 24 austenitic and austenitic-ferritic welds with C_{req}/Ni_{eq} between 1.11 and 3.25. It was identified that the least hot cracking is correlated to 10–20% δ -ferrite at room temperature, as indicated by Figure 1. However, using the room-temperature ferrite content to explain the solidification cracking behavior is mechanistically insufficient, as the full evolution of the 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 enable analyses of the evolution of phase contents during solidification, which are essential to understand solidification cracking.

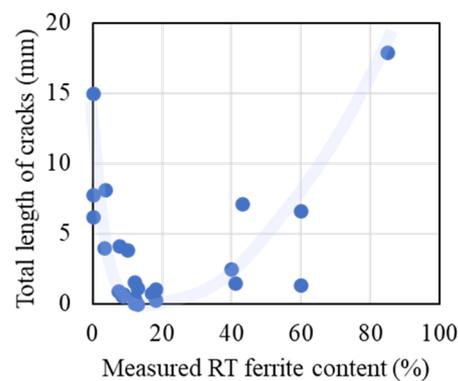


Figure 1. Total length of cracks vs. δ -ferrite content measured at room temperature for 24 austenitic and austenitic-ferritic welds in [4].

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

2. Methods

The solute redistribution with respect to the temperature during rapid solidification is simulated by the Scheil–Gulliver model using the Scheil Calculator within the Thermo-Calc software (version 2020b) [5]. It is a classical model for extreme non-equilibrium conditions which assumes that there is no diffusion in the solid phase and infinitely fast diffusion of all components in the liquid phase. Thermo-Calc Software TCFE10 Steels/Fe-alloys database is used for the calculations [6].

For diffusion-controlled phase transformations during solidification and continuous cooling, the Diffusion Module (DICTRA) [5] and Thermo-Calc Software MOBFE5 Steels/Fe-alloys mobility database [7] are used to predict cooling-rate-controlled kinetics. In this work, a cylindrical one-dimensional cell is used to represent the thickening of primary cell arms during solidification.

3. Results and Discussions

3.1. Hot Cracking Susceptibility (HCS)

CSC values for the 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, the CSC values under the mode 2 cooling condition are plotted against the carbon content in Figure 2 to manifest the carbon effect on the cracking susceptibility. Figure 2 suggests that for dilute solutions ($x < 0.2$ wt.%), the alloy system gets prone to cracking as the carbon content increases, whereas increasing carbon levels can reduce the CSC values when the carbon content is greater than 0.2 wt.%. However, this tendency in high carbon

regions is not well aligned with the experimental observation of the hot cracking sensitivity on the carbon content of the same alloy system carried out by Tamaki et al. [8]. Experimental evaluation of cracking percentage in steel welds suggests a dip in the cracking susceptibility at a medium carbon level, followed by an increased cracking susceptibility as the carbon content increases.

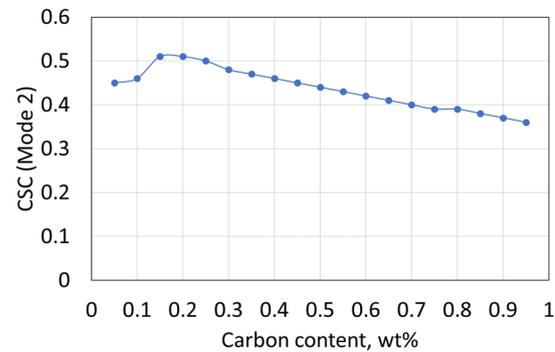


Figure 2. Cracking susceptibility coefficient (CSC, under mode 2 cooling condition) vs. carbon content for Fe-0.5Si- x C ($x = 0.05\text{--}0.95$, in wt.%) ternary system.

To address the disparity, a metric named HCS (hot cracking susceptibility) [9] is used to represent the cracking sensitivity. Figure 3 shows the plot of HCS values against varied carbon content in the Fe-0.5Si- x C ternary system in comparison with an isopleth of the equilibrium phase diagram. The tendency of the HCS curve matches well with the experimentally-determined cracking percentage curve in [8], with a dip at an intermediate carbon level indicating a less cracking-sensitive composition. Compared with the phase diagram in Figure 3b, the first bump of the curve corresponds to the alloy compositions with a peritectic reaction ($L + \delta \rightarrow \gamma$) occurring during solidification. This indicates that the hot cracking sensitivity is a combined effect of solidification temperature and solidification range. With peritectic reactions, the solidification range is expanded and therefore increases the susceptibility to hot cracking. Therefore, compared with the CSC curves, the HCS is a more comprehensive metric that can better represent the cracking sensitivity during solidification.

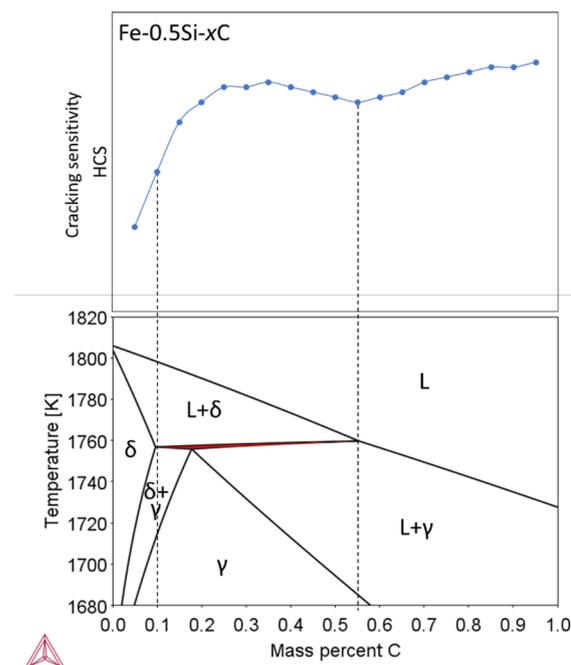


Figure 3. Relation between hot cracking susceptibility (HCS) and equilibrium phase diagram of the Fe-0.5Si- x C ($x = 0.05\text{--}0.95$, in wt.%) ternary system.

3.2. δ -Solidification

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

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

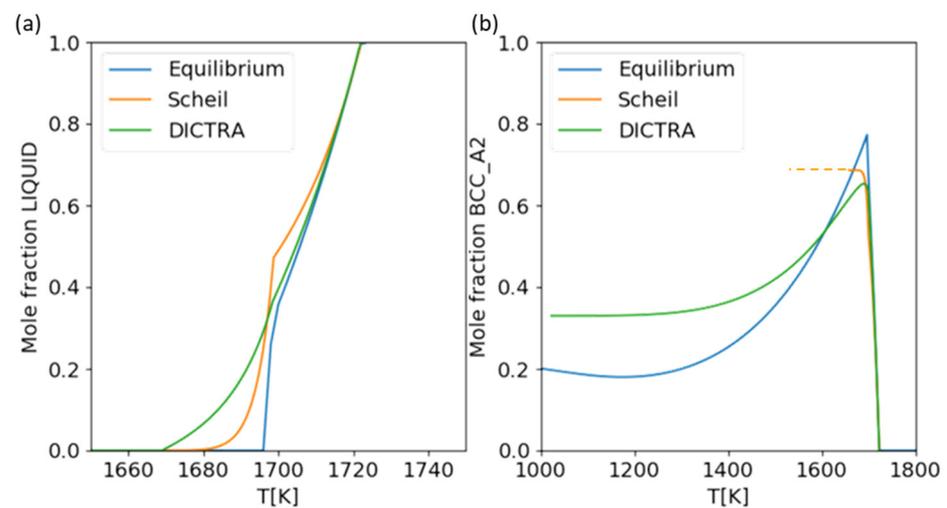


Figure 4. Comparison of cooling simulations under equilibrium condition, and under non-equilibrium conditions performed by Scheil and DICTRA. (a) Comparison of fraction of liquid during solidification; (b) comparison of δ -ferrite fraction during continuous cooling.

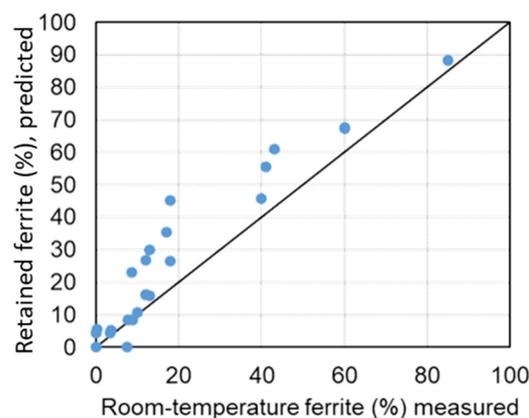


Figure 5. Comparison of predicted ferrite fraction by DICTRA simulations and measured values in [4].

3.3. ICME-Guided Materials Design

As described in previous sections, the HCS and the fraction of δ -ferrite are composition-dependent metrics to evaluate the solidification cracking susceptibility of alloys.

Therefore, they 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 δ -ferrite fraction data points obtained from DICTRA simulations. For an identified δ -ferrite fraction, the composition can be adjusted based on sensitivity, with constraints from the HCS values.

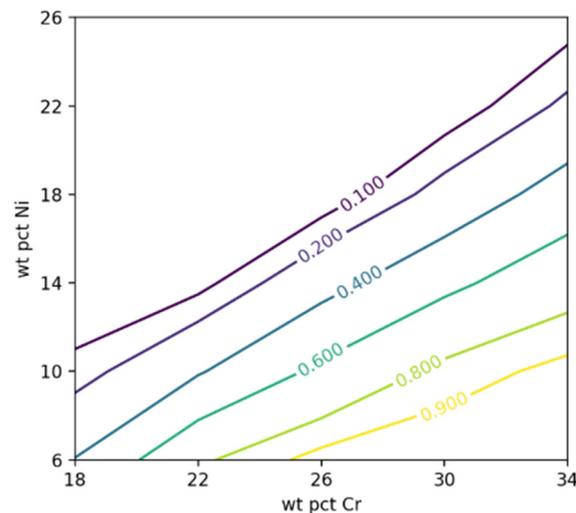


Figure 6. ICME-predicted “Schaeffler diagram”.

4. Conclusions

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

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