

Direct Calculation of Ferrite Number from Thermodynamic and Kinetic Models

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Introduction

In recent years, new and improved models for Ferrite Number (FN) prediction have been developed using neural network analyses (1-4). These have been shown to be significantly more accurate than conventional constitution diagrams when predicting FN and, in addition, they have the necessary flexibility to account for complex, non-linear effects. In the most recent model, cooling rate has also been included as a variable in the model (3,4). However, both constitution diagrams and neural network FN predictive models have been developed with the use of experimental databases that are subject to a range of experimental errors that can be quite significant and can lead to poor data. For example, measurement of FN can be inaccurate when samples are small or when making optical microscopy measurements that are then converted to FN (3). When trying to include cooling rate effects, which are well known to have a significant impact, evaluation of the cooling rate is a problem (3). Finally, weld composition analyses have inherent inaccuracies and, furthermore, critical elemental compositions are often not evaluated.

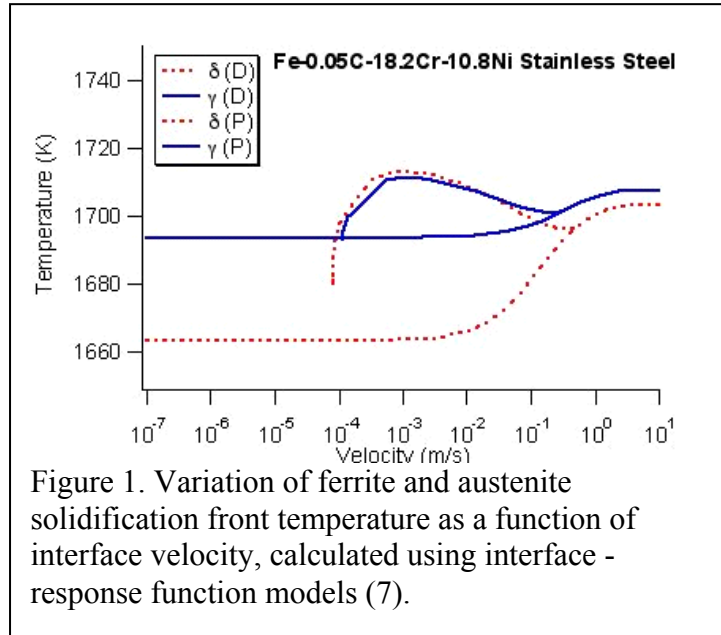
In parallel with the development of new FN predictive tools, major advances have been made with regard to the application of computational thermodynamics to analyze phase stability in complex multi-component alloy systems. In addition, computational thermodynamics can be coupled with kinetic models to follow the diffusion-controlled transformations that take place in stainless steels during and after solidification and lead to the final ferrite levels at room temperature. In this paper, these tools have been applied to study the feasibility of predicting FN in stainless steel welds by direct computation.

The submitted manuscript has been authored by a contractor of the U.S. Government, under contract No. DE-AC05-00OR22725. Accordingly, the U.S. Government retains a non-exclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

Procedure and Results

Computational thermodynamics software will be used to identify the solidification behavior and phase stability in several stainless steel alloys. The software is capable of taking into account all of the alloying elements present in the complex, multi-component steel welds. These calculations will then be integrated with two different kinetics models

to determine the amount of ferrite present at room temperature after solidification and cooling. The first model is that described by Koseki et al (5) in which the solidification and solid-state transformation is modeled in a wedge-shaped representative section. The second model uses the commercial Dictra code (6) for modeling one-dimensional



diffusion-controlled transformation behavior. Both calculations take the cooling rate into account and therefore they will be used to consider a range of cooling rate conditions. A third model will be used to provide the basis for choosing the solidification mode. This model will be used to predict when the solidification mode is likely to change from equilibrium primary phase solidification to non-equilibrium solidification as a function of the growth velocity. This type of calculation is necessary because it is well documented that the mode of solidification in stainless steels can change at high growth rates from primary ferrite formation to primary austenite formation. An example of the results from this model for an Fe-0.05C-18.2Cr-10.8Ni stainless steel is shown in Figure 1, where the solidification front temperature for both planar (P) and dendritic (D) morphologies and for ferritic (δ) and austenitic (γ) growth is plotted as a function of growth velocity. The phase that has a higher front temperature is the predicted primary solidification phase. The figure shows that at higher growth rates ($> 10^{-2}$ m/s), non-equilibrium austenite solidification replaces the equilibrium ferrite solidification.

The results will be compared with experimental measurements as well as predictions using the conventional constitution diagrams and the newer neural network models. Conclusions will be drawn as to the accuracy of direct calculations. Furthermore, the feasibility of using such calculations to supplement experimental data to provide a more robust, consistent, and accurate database for future model development will be assessed.

Acknowledgment

A part of this research was sponsored by the Division of Materials Sciences and Engineering, U. S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

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