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Research Article

Thermodynamic calculation of Iron Phases with Thermo Calc Software

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Abstract:

Thermodynamic calculation of iron phases in alloys is crucial for understanding and optimizing their mechanical properties. This study focuses on predicting the iron phases in an alloy with the chemical composition of 0.45% Carbon, 0.15% Silicon, 0.60% Manganese, 0.40% Nickel, and 0.30% Chromium using Thermo-Calc software. Thermo-Calc is a powerful computational tool that facilitates the thermodynamic and phase equilibrium analysis of complex materials. By leveraging this software, we can simulate the microstructural evolution and phase transformations that occur during thermal processing. This research aims to provide a detailed thermodynamic assessment of the specified alloy composition, highlighting the stability and distribution of various iron phases such as ferrite, austenite, and carbides. The findings will contribute to a deeper understanding of the alloy's behaviour under different thermal conditions, offering insights for future alloy design and processing optimization. The experimental results obtained through Thermo-Calc simulations will be compared with available theoretical and empirical data to validate the accuracy and reliability of the predictions. This study underscores the importance of computational tools in advancing material science and engineering by enabling precise phase predictions and enhancing alloy performance.

1. Introduction

Thermodynamic calculations of iron phases in alloys are essential for predicting and optimizing their mechanical properties. Understanding the distribution and stability of various phases, such as ferrite, austenite, and carbides, is fundamental for tailoring the microstructural evolution of these materials.

Advances in computational tools, such as Thermo-Calc software, have revolutionized the field of material science by enabling precise thermodynamic and phase equilibrium analyses.

This study focuses on the thermodynamic evaluation of an alloy with the chemical composition of 0.45% Carbon, 0.15% Silicon, 0.60% Manganese, 0.40% Nickel, and 0.30% Chromium.

The chosen composition is representative of medium-carbon steels, widely used in engineering applications due to their excellent balance of strength and toughness. The investigation employs Thermo-Calc software to simulate the phase transformations and microstructural changes that occur during thermal processing.

The primary goal of this research is to provide a comprehensive assessment of the thermodynamic behavior of the alloy under varying temperature conditions.

By identifying the phases present in the iron-carbon phase diagram and analyzing their stability, this study aims to offer valuable insights into the alloy's behavior and potential optimization strategies for industrial applications. Furthermore, the results obtained from Thermo-Calc simulations will be validated through comparisons with theoretical and empirical data to ensure accuracy and reliability [1-5].

This research highlights the growing importance of computational tools in material science and underscores their potential in advancing the design and processing of high-performance alloys.

2. Material and Methods

2.1 Thermodynamic Calculation -Thermo-Calc

Thermo-Calc software was employed for thermodynamic and phase equilibrium analysis of the specified alloy. The process began with the input of the alloy's chemical composition, which was defined as 0.45 % Carbon, 0.15 % Silicon, 0.60% Manganese, 0.40 % Nickel, and 0.30 % Chromium, with iron as the base element. The TCL (Thermodynamic and Phase Diagram Database for Steels) database was selected for the simulations, as it provides accurate thermodynamic descriptions of iron-carbon alloys and their associated phases. Using the "Equilibrium Calculation" module, phase diagrams were generated for the alloy system under equilibrium conditions, covering a temperature range from 0 °C to 1600 °C to account for all relevant phase transformations. Additionally, the volume fraction of various phases was calculated as a function of temperature to predict the stability and distribution of phases, including ferrite (BCC), austenite (FCC), graphite, and cementite. Finally, the calculated results were validated by comparing them with established phase diagrams and empirical data to ensure consistency and reliability [6-13].

3. Results and Discussions

The thermodynamic calculations reveal the evolution of iron phases as a function of temperature and carbon content. The primary phases identified include ferrite (BCC_A2), austenite (FCC_A1), cementite (Fe_3 C), and graphite. Ferrite, a body-centered cubic (BCC) phase, is stable at lower carbon contents and temperatures, appearing below 912°C and reappearing during cooling at even lower temperatures. Austenite, characterized by a face-centered cubic (FCC) structure, is stable at intermediate temperatures and carbon contents, forming above 912°C and transitioning into ferrite or cementite during cooling. Cementite, an iron carbide phase, forms at higher carbon contents and lower temperatures, playing a critical role in determining the mechanical properties of steel. At elevated temperatures and higher carbon concentrations, graphite formation is observed, which is essential for applications involving cast iron. The phase diagram Figure 1 shows equilibrium phases as a function of carbon content and temperature. Notable observations include the dominance of the liquid phase above 1400 °C, which transitions into a mixture of liquid and austenite (FCC) upon cooling. The FCC region persists down to 912 °C, where it transforms into ferrite (BCC) at lower carbon contents. The eutectoid point, located at approximately 0.76% carbon, marks the decomposition of FCC into BCC and cementite

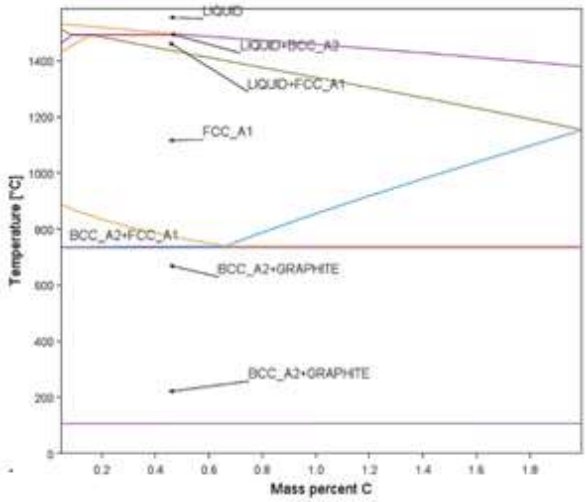

Figure 1. *Thermodynamic calculation of phase diagram of Fe-C alloy*

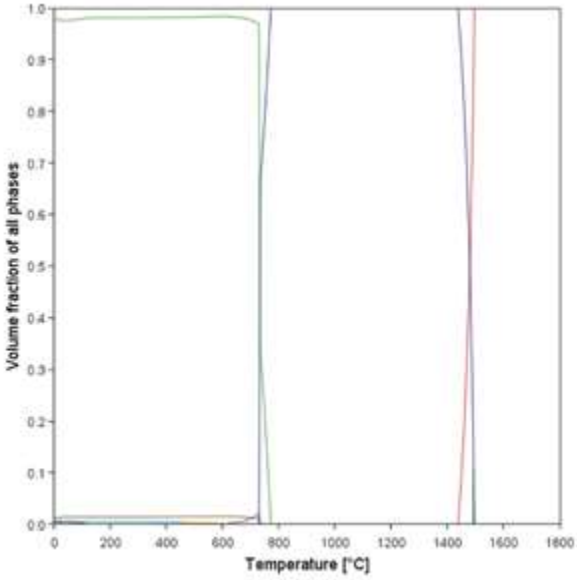

Figure 2. *Thermodynamic calculation of phase fraction*

(Fe_3 C) upon cooling below 727 °C. Additionally, graphite formation is favored at higher carbon contents and elevated temperatures, indicating its stability in cast iron compositions. The volume fraction plot figure 2 further illustrates the temperature-dependent distribution of phases. At high temperatures (~1400 °C), the liquid phase is predominant, followed by a sharp decline as austenite (FCC) forms during cooling. Austenite remains dominant until approximately 912 °C, where a transition to ferrite (BCC) and cementite occurs. Below 727 °C, the cementite fraction increases significantly, corresponding to the eutectoid transformation. The presence of graphite at elevated carbon levels is evident, with its fraction

increasing at lower temperatures, highlighting its relevance in cast iron behaviour.
These findings underscore the importance of phase stability and transformations in influencing the alloy's mechanical properties and processing behavior.

4. Conclusions

This study utilized Thermo-Calc software to perform a thermodynamic assessment of an alloy with 0.45 % Carbon, 0.15 % Silicon, 0.60 % Manganese, 0.40 % Nickel, and 0.30 % Chromium. The results revealed the stability and distribution of key phases, including ferrite, austenite, cementite, and graphite, under varying thermal conditions. The generated phase diagrams and volume fraction plots provide a comprehensive understanding of the alloy's behavior during thermal processing.
By validating the computational predictions with theoretical data, this research underscores the reliability of Thermo-Calc as a tool for advancing material design and optimization.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper
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