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THERMODYNAMIC CALCULATIONS AND PRECIPITATION SIMULATIONS OF HSLA STEELS

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Abstract

For more than thirty years, CALPHAD based tools have been successfully applied within the steel industry. Such tools are useful from an alloy design perspective and as a way of improving understanding of existing steels and process optimization. This presentation focuses on the thermodynamic modeling and precipitation simulation of high strength, low alloy (HSLA) steels. Thermodynamic calculations using Thermo-Calc can be used to predict the underlying thermodynamics of multicomponent alloys of industrial importance; phase equilibrium and phase transformation information by taking into account compositional and temperature variations, e.g., the effect of an alloying element on the austenite to ferrite transformation temperature; segregation during solidification; driving force for nucleation; stability of precipitates; etc. Additionally, precipitation plays an important role in industrial steels, especially for strengthening HSLA steels. The precipitation kinetics of alloy carbides, i.e., NbC, is simulated using TC-PRISMA, a computational tool that is integrated with Thermo-Calc and DICTRA together with additional interface property data. Properties such as interfacial energies between matrix and precipitate phases can be estimated by using an approximation model which has been implemented in TC-PRISMA.

Introduction

In materials science and engineering, the capturing of 'process-structures-properties-performance' relationships has always been the focus. The properties of materials are dependent on the microstructure which in turn can be varied by changing the chemical composition, processing route etc. The CALPHAD (CALculation of PHAse Diagram) method [1] fundamentally links the phases that form, and thus the microstructure to the materials compositions and processing variants. It thus has been successfully employed in understanding the microstructures under a process production and in materials selection for a given application. For more than 30 years, the CALPHAD method has been used within the industry for various alloys, i.e., Fe-based, Ni-based, Al-based, Mg-based alloys etc. Notably, the CALPHAD method has been successfully applied to improve the understanding of nearly every stage of the life cycle of steels, ranging from alloy design, extraction, casting, forging, heat treatment, joining, corrosion etc., all the way to waste and recycling [2].

High-strength low-alloy (HSLA) steel, or microalloyed steels, differs from other steels in that it is not made to meet a specific chemical composition but rather to meet specific mechanical properties, i.e., provide better mechanical properties and/or greater resistance to atmospheric corrosion than conventional carbon steels. The common microalloying elements used in HSLA steels today are

vanadium (V), niobium (Nb) and to a lesser extent, titanium (Ti). Compared to vanadium, niobium is a more effective grain refiner. Niobium also increases yield strength by precipitation hardening. The magnitude of the increase depends on the size and amount of precipitated niobium carbides. A combination of precipitation strengthening and ferrite grain refinement makes Nb an effective strengthening agent. Microalloying additions of Nb are thus of great importance for the industrial fabrication of HSLA steel. The present work focuses on the thermodynamic modeling and precipitation simulation of Nb-microalloyed high-strength low-alloy steels.

Thermodynamic calculations

In CALPHAD modeling, each phase in the system is described with an appropriate thermodynamic model based on its crystal structure, physical and chemical properties. The thermodynamic model describes the Gibbs free energy as a function of temperature, pressure and composition. The adjustable model parameters in the expressions of the model are evaluated by optimizing the fit of the model to all available thermodynamic and phase equilibria data. Critically evaluated descriptions of low order systems, e.g., binary and ternary systems, can be combined to make extrapolations/predictions to higher order systems.

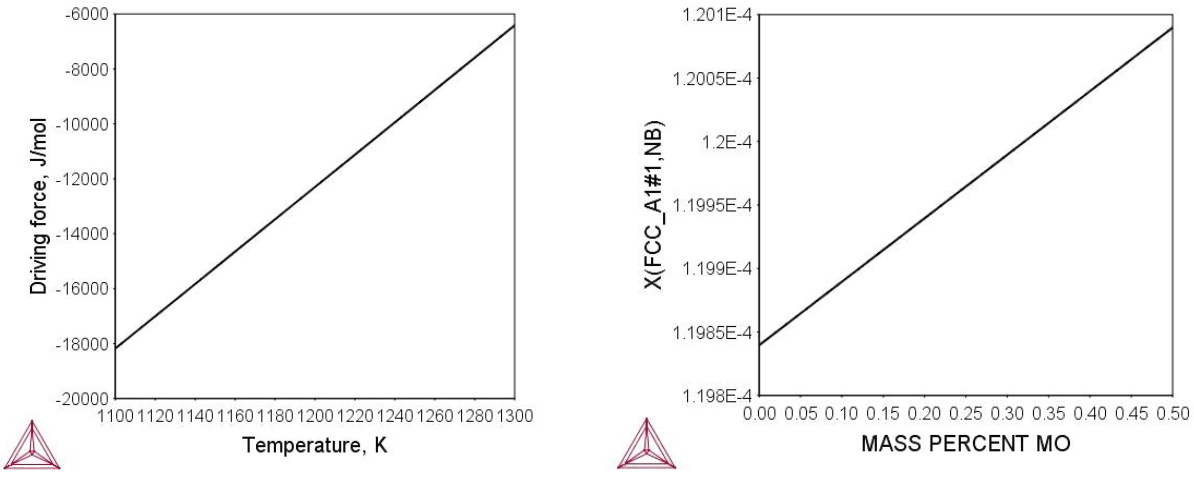

Figure 1 (a) Calculated driving force of formation of NbC in austenite for Fe-0.045Nb-0.11C-0.26Si-1.1Mn (wt.%) steel; (b) Calculated effect of Mo to the solubility of Nb in austenite for a line pipe steel (Fe-0.02Nb-0.08C-1.8Mn-0.06V-0.02Mo, wt.%) steel.

Thermodynamic calculations using Thermo-Calc can show what phases could form at varying operation temperatures and different alloy compositions both under equilibrium and non-equilibrium conditions. It is also possible to see the influence of an element on the phase stabilities and solubilities of different elements, and the amounts of precipitates and their compositions as a function of temperature or alloy composition. Moreover, phase transformation temperature, driving force of formation for nucleation, equilibrium and non-equilibrium solidification, especially segregation during solidification, etc. can be obtained as well. Figure 1(a) illustrates the calculated driving force of formation of NbC in austenite for an Fe-0.045Nb- 0.11C-0.26Si-1.1Mn (wt.%) steel. The driving force of NbC increases with increasing temperature. The calculated effect of Mo to the solubility of Nb in austenite for a line pipe steel

(Fe-0.02Nb-0.08C-1.8Mn-0.06V-0.02Mo, wt.%) is shown in Fig. 1(b). As can be seen, Mo in microalloyed steels increases the solubility of Nb in austenite, thereby enhancing the precipitation of NbC in the ferrite. This increases the precipitation-strengthening effect of NbC. Both calculations are performed using Thermo-Calc software with the TCFE7 thermodynamic database.

Precipitation simulation

Precipitation is a solid state phase transformation process which has been exploited to improve the strength and toughness of various alloys for centuries. TC-PRISMA is a general computational tool for simulating kinetics of diffusion controlled multi-particle precipitation process. With TC-PRISMA, the kinetics of concurrent nucleation, growth/dissolution and coarsening of dispersed precipitates can be simulated by calculating the evolution of the probability distribution of the particle number densities, or particle size distribution (PSD). TC-PRISMA is developed based on the Langer-Schwartz theory [3] and the Kampmann-Wagner numerical approach [4]. More details can be found in ref. [5]. TC-PRISMA relies on CALPHAD based software tools, such as Thermo-Calc and DICTRA [6], and databases to provide necessary bulk thermodynamic and kinetic data for phases in multicomponent systems. In addition, properties such as interfacial energies between matrix and precipitate phases can be estimated by using an approximation model which has been implemented in TC-PRISMA.

Table 1 Chemical composition of Nb-microalloyed steels used in the simulations (wt.%).

Alloy	Fe	Nb	C	Si	Mn
#1	Balance	0.045	0.11	0.26	1.1
#2	Balance	0.04	0.0058	—	—
#3	Balance	0.079	0.011	—	—

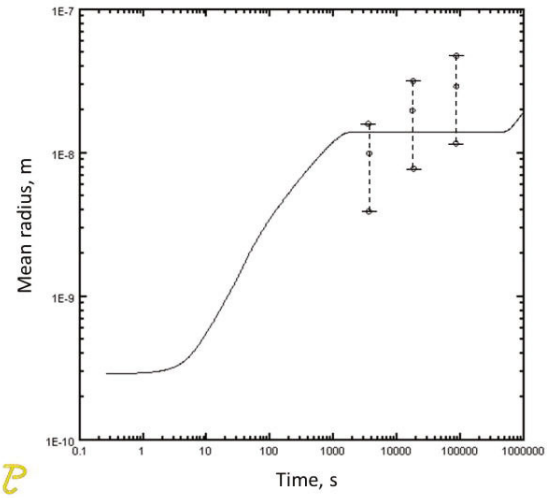

Fig. 2 Modeled precipitation kinetics of NbC in austenite at 1173 K for steel #1 (Fe-0.045Nb-0.11C-0.26Si-1.1Mn, wt.%). Experimental data from Akamatsu et al. [7] are marked as circles. Dash lines are error bars.

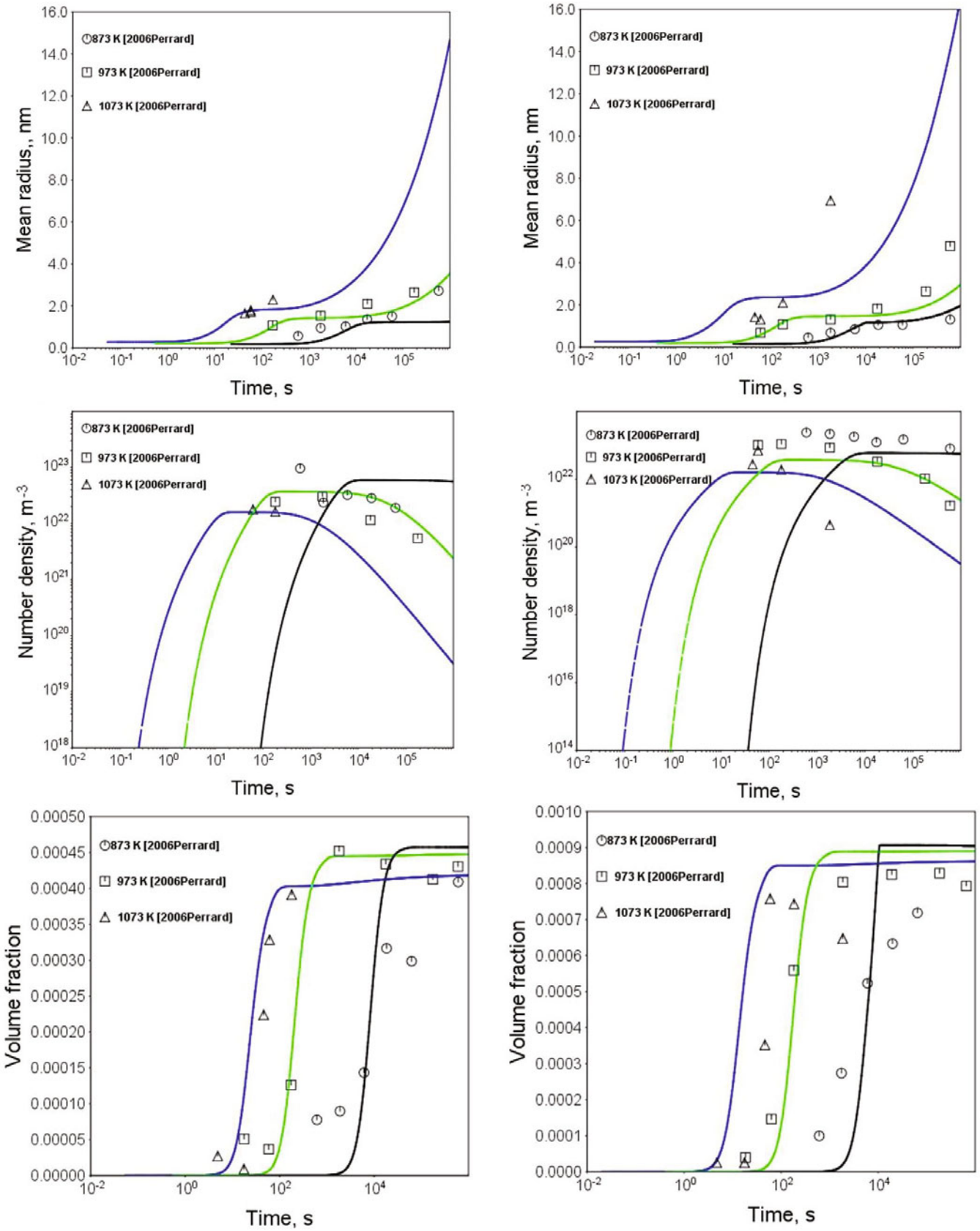

Fig. 3 Simulated precipitation kinetics of NbC in ferrite at 873 K, 973 K and 1073 K, left: for steel #2; right: for steel #3. Experimental data are from Perrard et al. [8].

Figure 2 and Fig. 3 demonstrate the applications of using TC-PRISMA (version 2015a) for the simulation of precipitation kinetics of NbC for HSLA steels. The databases used in the simulations are TCFE7 for the thermodynamic data and MOBFE2 for the mobility data. Chemical compositions of Nb-microalloyed steels used in the simulations are listed in Table 1. Figure 2 shows the simulated NbC precipitation in austenite of an Nb-added micro-alloyed steel (steel #1: Fe-0.045Nb-0.11C-0.26Si- 1.1Mn) at 1173 K. Experimental data from Akamatsu et al. [7] are superimposed for comparison. Interfacial energy used for simulation is 0.26 J/m^2. The modeled mean radius of NbC precipitate shows a good agreement with the reported values within experimental uncertainty. Figure 3 presents the comparison between experiment [8] and simulated precipitation of NbC on dislocations in ferrite between 873 K to 1073 K for steel #2 (Fe-0.105Nb-0.009C) and steel #3 (Fe-0.049Nb-0.011C). The dislocation density used in the simulation is taken directly from the experimentally measured value $2*10^{14}$ m^{-2}. Experimental mean radius, number density and volume fraction are well described by the present modeling.

Summary

In the present work, thermodynamic calculations of nucleation driving force and effect of micro-alloying element on the solubility of Nb in austenite were performed. Precipitation kinetics of NbC for several Nb-microalloyed steels was studied using the precipitation simulation software TC-PRISMA. Results were compared with experimental measurements. Reasonable agreement between simulation and experiment suggests that thermodynamic and kinetic modeling software such as Thermo-Calc and TC-PRISMA are computational tools that can be readily used for the prediction of the effect of process and composition parameters on the microstructure of materials.

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