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Polynomial regression and interpolation of thermodynamic data in Al–Si–Mg–Fe system

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ABSTRACT

A numerical technique for constructing thermodynamic databases has been proposed. This technique offers accurate calculations of solidification temperature, phase fractions, and solute concentrations of specific alloys in quaternary systems. The thermodynamic data is extracted by calling the TQ-interface (Thermodynamic Calculation Interface) from Thermo-Calc software, and modeled through efficient computational approaches such as polynomial regression and interpolation. This method is described in three parts. First, the applicability of regression functions is demonstrated on the Al–Si binary phase diagram. Second, the way of combining polynomial regression and interpolation is applied to model the Al–Si–Mg ternary system. Finally, the A356 alloy, which belongs to the Al–Si–Mg–Fe system, is modeled by a series of sub-ternary systems using regression and interpolation. The valid accuracy of the method is demonstrated by comparing the present results with those calculated using Thermo-Calc software. The application of the TQ-interface to solidification processes in Scheil and lever-rule models is also included. The results indicate that this method can offer accurate thermodynamic parameters for the A356 alloy in Al–Si–Mg–Fe system and reduce CPU time significantly when applied to solidification simulation. Several problems and the corresponding strategies for high order functions, unsmooth variations of thermodynamic information and partition coefficients are discussed to improve this method. This technique can also be applied to other specific alloys with small variations of thermodynamic variables in quaternary systems.

1. Introduction

Solidification simulations of commercial aluminum and iron alloys play an important role in manufacturing of automobile, aerospace and architecture materials due to their ability to predict macrosegregation, dendritic growth and mechanical properties [1–4]. During recent years, the CALculation of PHAse Diagrams (CALPHAD) method has been proved to be a powerful tool in making accurate predictions of the phase equilibria transition in solidification processes. It is possible to calculate solidification processes in detail by coupling CALPHAD software with different solidification models [5–8]. However, the large physical memory it takes when performing repetitive calculations for complex phase equilibria makes it less efficient to simulate the solidification processes on multicomponent alloy systems with macroscopic models [9].

Several techniques for addressing this issue via indirect coupling of phase equilibrium data with Thermo-Calc software have been developed. Dore et al. [10] proposed a mapping technique, in which the phase equilibrium data of Al–Si–Mg system was combined with CALPHAD calculations. Equilibrium information at each time step during the solidification simulation was obtained for the corresponding composition condition via bilinear interpolation. Du et al. [11,12] applied this method to multicomponent Al–Cu–Mg alloys, making the content data stored in a tabulation file. While many researchers employed regression method only for the calculation of thermodynamic information of alloys with set composition [9,13–16], this technique has been adopted to calculating liquid phase fractions and solute concentrations in multicomponent systems. Notably, Ludwig et al. [17] proposed a model which contains a non-linear system of equations of interpenetration continua to simulate solidification process while coupled with a thermodynamic program. Zhao et al. [18] developed a regression model to compute solute partition coefficients and applied it to solidification simulations for the Al–Cu–Si alloys.

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In this work, the authors aim to simplify the thermodynamic descriptions by using parameterized phase diagrams to enable multicomponent solidification simulations in complex macrosegregation simulations. A software package has been developed to extract phase diagram data from the thermodynamic database and store the information in a tabulation file. Both the data structure used and the method of parameterization of the thermodynamic phase diagram are analyzed. Thermodynamic calculations are performed by applying the TQ-interface from Thermo-Calc [19,20], which is linked to the software by using a shared library. The proposed computational strategy is a combination of polynomial regression and interpolation [21,22] due to their much less time-consuming than the Gibbs minimization computations [9,18]. While previous works [10–12,18] using mapping techniques and regressions have successfully modeled the solidification of ternary systems with reduced computational time, literature information on data reduction for quaternary systems is still scarce. Therefore, the A356 alloy of Al–Si–Mg–Fe quaternary system with an established thermodynamic database was employed as an example to gain a thorough understanding of the capability of the present data reduction method in modeling the solidification process in this type of systems.

2. Models

2.1. Numerical model for describing phase diagrams

The numerical model used in the present work is based on polynomial fitting with an incorporated bilinear interpolation [21,22]. This method is much less computationally-intensive than the minimizing of the Gibbs energy functions, which results in a significantly smaller physical memory. The regression modeling is performed by using Matlab 7.0 software [23], which can both analyze data and fit various regression functions such as polynomial functions, power functions and exponential functions. The COST2 thermodynamic database [24] was used as a data source. For simplicity, only the liquid, fcc, diamond and β-Al_5FeSi phases of the A356 alloy in the Al–Si–Mg–Fe system were considered during the simulation.

2.1.1. Binary and ternary systems

In the Al–Si binary system (Fig. 1a), the TQ-interface coupled with COST2 database was used to calculate the α-liquidus and α-solidus points as well as the temperature as a function of Si weight fraction, as shown in Fig. 1b

$$T = F_1(w_{\mathrm{Si}}) \tag{1}$$

The polynomials of liquidus and solidus temperature in Fig. 1b are expressed in the forms of [21]

$$T^{L,bin} = \sum_{i=1}^{n+1} a_i w_{\mathrm{Si}}^{i-1} = a_1 + a_2 w_{\mathrm{Si}} + a_3 w_{\mathrm{Si}}^2 + \cdots + a_{k+1} w_{\mathrm{Si}}^n \tag{2a}$$

$$T^{S,bin} = \sum_{j=1}^{n+1} b_j w_{\mathrm{Si}}^{j-1} = b_1 + b_2 w_{\mathrm{Si}} + b_3 w_{\mathrm{Si}}^2 + \cdots + b_{k+1} w_{\mathrm{Si}}^n \tag{2b}$$

where $T^{L,bin}$ and $T^{S,bin}$ are the liquidus and solidus temperatures, respectively; w_{Si} is the composition of the mixture in terms of the Si weight fraction; a_i and b_j are coefficients ($i,j=1,2,\ldots,n+1$); and k is the degree. Eqs. (2a) and (2b) are obtained using a polynomial regression and the degree n is determined by the coefficient of determination R^2 [21].

In Fig. 1b, the fitting functions of liquidus and solidus pass every liquidus and solidus points, respectively. A eutectic line is added to determine the L+α region. The weight percentages of each phase in the L+α region can be described using the lever-rule [25], which is a simple arithmetic calculation of the weight percentage of liquid and solid phases with respect to composition; hence a simple digital model to describe the phase equilibrium of in the Al-rich side of the Al–Si phase diagram during the solidification can be constructed.

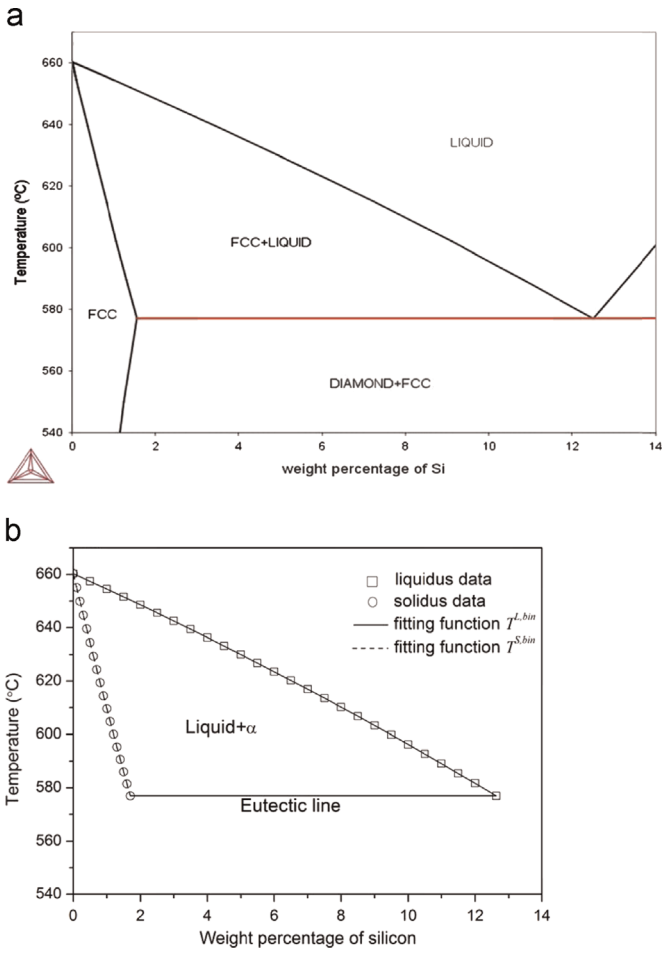

Fig. 1. (a) Al–Si binary phase diagram calculated by database COST2 of Thermo-Calc software; (b) schematic diagram of digital liquidus and solidus in Al corner: the data points calculated by a program coupling TQ-interface and COST2, as well as the fitting functions passing all the data points are shown.

In the Al–Si–Mg ternary eutectic system, the liquidus temperature is a function of Si and Mg weight fraction:

$$T = F_2(w_{\mathrm{Si}}, w_{\mathrm{Mg}}) \tag{3}$$

The α-liquidus data points corresponding to compositions in Al corner obtained by Thermo-calc software are shown in Fig. 2a. The α-liquidus surface is described with the following function [21]:

$$T^{L,ter} = a_0 + a_1 w_{\mathrm{Si}} + a_2 w_{\mathrm{Mg}} + a_3 w_{\mathrm{Si}}^2 + a_4 w_{\mathrm{Si}} w_{\mathrm{Mg}} + a_5 w_{\mathrm{Mg}}^2 \tag{4}$$

where $T^{L,ter}$ is the liquidus temperature in the ternary system; w_{Si} and w_{Mg} are the weight fractions of the Si and Mg, respectively; and a_0–a_5 are coefficients.

Eq. (4) is a second-order polynomial function and it can be changed into an i-degree ($i=1,2,3,\ldots$) function, while still being based on the value of the coefficient of determination R^2 [21]. The α-liquidus surface calculated by this fitting function is shown in Fig. 2b. Comparing with Fig. 2a, it can be seen that the function not only represents the original liquidus points, but also contains irrelevant data. To handle this problem, it is necessary to include