Thermo-Calc and \( T-f_{S}-C_{L} \) coupling based method to determine solidification paths of alloys solidified under condition of Biot\( \leq 0.1 \)

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Abstract: A binary continuum model for dendritic solidification transport phenomena and corresponding numerical algorithm for the strong nonlinear coupling of \( T-f_{S}-C_{L} \) were extended to multicomponent alloys solidified under condition of Biot\( \leq 0.1 \). Based on the extended model/algorithm, a method considering heat transfer was proposed to predict the solidification paths and microsegregation of alloys solidified under the same condition. The new algorithm and method were closely coupled with the commercial Thermo-Calc package via its TQ6-interface codes for instantaneous determination of the related thermodynamic data at each calculation time step. The sample simulation performed on an Al−2Si−3Mg alloy system indicates the availability and reliability of the model/algorithm and the proposed method for predicting solidification paths and microsegregation. Computational and experimental investigations on an Al−5.17Cu−2.63Si ternary alloy were conducted, and a reasonable agreement between the computation and experiment was obtained.

Key words: thermo-calc; solidification transport; solidification paths; microsegregation

1 Introduction

Conventional alloy development, especially for multicomponent alloys such as the high speed tool alloys (Fe−C−Cr−W−Mo−V−Co) [1], is costly and time consuming because it involves casting and analyzing a series of specimens. Further more, most of the metallic industry alloys are multicomponent and solidified in a dendritic form with the formation of microsegregation and several kinds of secondary phases [2, 3]. The degree of the microsegregation and the types and amounts of the secondary phases may significantly impact the mechanical properties of the solidified alloy materials both at room and working temperatures [4, 5]. Therefore, accurate prediction of the solidification paths and microsegregation of multicomponent alloys under a given solidification condition is critical in optimizing the composition and processing parameters in new alloys development [6]. The analyses of solidification of multi-component alloys are much more difficult than binary alloys because of the lack of phase-diagram information [7]. Fortunately, the use of thermodynamic calculation tools, such as the Calphad approach [8], clearly appears to be the appropriate method for multi-component systems.

It is known from heat transfer knowledge that the Biot number is a dimensionless number used for non-steady-state heat transfer calculations [9]. It is defined as \( \text{Biot} = hl/k \), where \( h \) represents the heat transfer coefficient; \( l \) is the characteristic length which is commonly defined as the volume of the body divided by the surface area of the body and \( k \) is the thermal conductivity of the body. When the value of the Biot number is smaller than 0.1, the heat conduction inside the body is much faster than the heat convection away from its surface, and the temperature gradient inside the body is negligible [10].

In this work, a binary continuum model for dendritic solidification transport phenomena [11] and the corresponding numerical algorithm for the strong nonlinear coupling of \( T-f_{S}-C_{L} \) [12] were extended to multicomponent alloys solidified under a heat-transfer condition of Biot\( \leq 0.1 \). Based on the extended model or

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algorithm, a method was proposed for predicting the solidification paths and microsegregation of the alloys solidified under the condition of Biot≤0.1. The new algorithm and method were closely coupled with the commercial ThermoCalc package [13] via its TQ6-interface codes, for instantaneous determination of the related thermodynamic data at each calculation time step. This method can be used for predicting the alloy solidification behaviors of the thermal analysis cups used for the developments/analyses of the alloys [14], the suspended droplets [15], and especially the alloy specimens for DTA, DSC and single pan scanning calorimeter [16]. All the solidification cases mentioned above have a similar feature, i.e., the volumes of the alloy specimens are small [17] and can easily satisfy the heat-transfer condition of Biot≤0.1 (i.e. a simultaneously bulk solidification occurs).

2 Model description

A previously proposed continuum model for dendritic solidification phenomenon of binary alloys [11] was adopted and revised for multicomponent alloys, which can be described by the following governing equations.

1) Solidification heat energy transfer:
\[
\frac{\partial((\rho c_p)_{\text{m}} T)}{\partial t} + \nabla \cdot (f_L \rho_L \nabla v T) = \nabla \cdot (\lambda_m \nabla T) + \frac{\rho_b h b}{\partial t}
\]  
(1)

where \( \rho_m \) and \( \rho_b \) represent the density of the mushy zones, liquid phase and solid phase, respectively; \( c_{pm} \) and \( c_{pl} \) represent the specific heat capacity of the mushy zones, liquid phase and solid phase, respectively; \( \rho_b \) is the specific heat capacity of the alloy; \( \lambda_m \) represents the thermal conductivity of the mushy zones; \( t \) represents time and \( b \) represents the volume fraction of solid phase.

2) Solidification species mass transfer for the \( n \)th component:
\[
\frac{\partial (\rho C_n)_{\text{m}}}{\partial t} + \nabla \cdot (f_L \rho_L \nabla C_{nl}) = \nabla \cdot (\lambda_m \nabla (f_L C_{nl}) + 
 \rho_b D_{bn} \nabla C_{nL})
\]  
(2)

where \( C_{pm} \), \( C_{pl} \) and \( C_{ps} \) represent the composition of the mushy zones, liquid phase and solid phase, respectively; \( D_{bn} \) and \( D_{bn} \) represent the diffusion coefficients of solute in liquid phase and solid phase, respectively.

3) L-S phase-change characteristic function for a specific multicomponent alloy:
\[
T_{L-S} = f(C_{nl}) \quad (n = 1, 2, \cdots, N)
\]  
(3)

4) Solidification mass conservation:
\[
\frac{\partial \rho_m}{\partial t} + \nabla \cdot (f_L \rho_L v) = 0
\]  
(4)

5) Momentum transfer for bulk/interdendritic liquid flow:
\[
\nabla \cdot (f_L \rho_L v) / \partial t + \nabla \cdot \{ \nabla (f_L \rho_L v) \cdot v \} = \nabla \cdot [ \mu \nabla (f_L v) ] - 
V(\nabla f_L P) + f_L \rho_L g - (\mu f_L^2 / K)v \quad (n = 1, 2, \cdots, N)
\]  
(5)

where \( T, C, f_L \) and \( v \) represent the macroscopic fields (on an ingot/casting length-scale) of temperature, composition, volumetric fraction and velocity vector of liquid phase in the solidification process of a multicomponent alloy, respectively; \( \mu \) represents the dynamic viscosity and \( K \) represents the permeability coefficient of mushy zones.

When Biot≤0.1 for an alloy specimen, the internal temperature distribution in the sample is assumed to be uniform, and the whole specimen can be treated as a close system [18]. Then the continuum transfer model of Eqs. (1)–(5) can be expressed as the following form for a ternary alloy specimen when neglecting the weak macroscopic liquid flow.

Heat transfer equation:
\[
(\rho C_p)_{\text{m}} \frac{\partial T}{\partial t} = \rho_b h b + h_r(T - T_r) S / V
\]  
(6)

where \( \rho \) is the density; \( h_b \) represents the equivalent heat transfer coefficient between the alloy specimen body and the environmental cooling medium; \( h_r \) is the latent heat of the alloy; \( V \) and \( S \) represent the volume and the surface area of the specimen investigated, respectively; \( T_r \) represents the room temperature and \( b \) is the volume of fraction solid phase in the alloy specimen.

The entire alloy specimen is isolated from the surrounding during cooling down, i.e. in a close solidification case, and then the solute mass balances can be expressed as:
\[
(\rho C_p)_{\text{m}} \frac{\partial C_n}{\partial t} = \int_0^b (\rho_b C_{ns} d \eta + f_L \rho_L C_{nl}) = \rho_0 C_{n0} \quad (n = 1, 2)
\]  
(7)

where \( C_{n0} \) and \( \rho_0 \) represent the initial composition and density of the liquid phase; \( \eta \) represents a volume fraction variable concentration within solidifying dendrites.

Equation (7) is equivalent to
\[
\nabla \cdot \mu \nabla (f_L v) = 0 \quad (n = 1, 2)
\]  
(8)

In the computation process, the liquidus temperature of the solidifying multicomponent alloy can be calculated by calling the related database COST2 and the interface program TQ6 of ThermoCalc software at each time step according to the corresponding liquid compositions \( C_{n+1} \) as:
\[
T_{L-S}^{n+1} = T_{L-S}^{n+1}(C_{n+1}) \quad (n = 1, 2)
\]  
(9)

where \( T_{L-S} \) represents the liquidus corresponding to the current composition.

3 Numerical procedure

It is known that the three variables of temperature,
solid fraction and liquid composition, i.e. \( T-f_{s}\)-\( C_{L} \), are strongly nonlinear coupled during solidification of the alloy, and a numerical method to solve this coupling is proposed with the consideration of any solid back diffusion (SBD) in a binary dendrite solidification problem [12]. This solution method could be extended to multicomponent alloys, and directly linked with a thermodynamics database COST2 and the interface program TQ6 of a Thermo-Calc software package [13].

An explicit finite difference scheme is used to obtain the numerical solution of the strongly coupled alloy solidification problem. Omitting the latent heat term temporarily, Eq. (6) can be expressed as:

\[
\frac{\partial T}{\partial t} = \frac{2h_{e}}{(\rho c_{p})_{m} R} (T - T_{R})
\]

where \( R \) is the radius of the alloy specimen.

Discretizing Eq. (10) and assuming \((\rho_{S}c_{PS})^y = (\rho_{C}c_{nP})\) and \((\rho_{L}c_{PL})^y = (\rho_{C}c_{nL})^y\) in a time interval \( \Delta t \), the numerical equation for calculating the temperature \( T^{i+1} \) at time \( t^{i+1} \) can be calculated as:

\[
T^{i+1} = \frac{(T_{0} + T_{1}) - \frac{S}{V} \Delta t^{i+1/2} \theta_{L}^{i+1/2}}{T_{0} + T_{1} + \frac{S}{V} \Delta t^{i+1} \theta_{L}^{i+1/2}}
\]

where

\[
T_{0} = (f_{s}\rho_{S}c_{PS} + f_{L}\rho_{L}c_{PL})
\]

\[
T_{1} = (\rho_{S}c_{PS} - \rho_{L}c_{PL})^{y+1} \Delta t_{L}^{i+1} + T_{0}
\]

The species mass formulation of Eq. (8) may represent a general microsegregation model when taking a differential form but in a mixture-averaged or statistical-average sense. According to the micro/ macrosegregation modeling proposed in Refs. [19, 20], Equation (8) can be rewritten for a closed single-phase \( \alpha(Al) \), the multicomponent solidification

\[
\theta_{L} = \frac{[1 + \beta_{L}]k_{n}f_{S}^{2}/f_{L}^{2} (n = 1, 2)}
\]

which represent the sensibility of interdendritic liquid-concentration to the SBD-behaviors and the Fourier diffusion number with a dendrite-geometry modification for the \( n \)-th-solute, respectively. Where \( R_{c} \) represents the solidification shrinkage; \( \beta_{L} \) represents the solute partition coefficients and the solid diffusion coefficients for the \( n \)th solute, respectively.

Now, the solidification of a typical ternary eutectic solidification-path is taken as example, i.e. \( 0 \leq f_{S}(\alpha) \rightarrow f_{S}(\beta_{2E}) \rightarrow f_{S}(\beta_{3E}) \leq 1.0 \), and the corresponding liquid concentrations can be calculated by the following equations for each corresponding solidification stage (the subscripts 2E and 3E represent binary and ternary eutectic solidification, respectively).

In the stage of single-solution solidification, e.g.

\[
\theta_{n} = \frac{C_{n}^{i+1}}{C_{n}^{i}} = \frac{f_{S}(\alpha)}{f_{S}(\beta_{2E})}
\]

\[
\theta_{n} = \frac{C_{n}^{i+1}}{C_{n}^{i}} = \frac{f_{S}(\alpha) + f_{S}(\beta_{2E}) + f_{S}(\beta_{3E})}{f_{S}(\alpha) + f_{S}(\beta_{2E}) + f_{S}(\beta_{3E})}
\]

(11)

(12)

In this general microsegregation model of Eq. (12), the unified SBD-parameters for the \( n \)-th-solute can be expressed as:

\[
\phi_{n} = \frac{\theta_{n} \phi_{n}}{(1 + \theta_{n}) \phi_{n}} \quad (n = 1, 2)
\]

(13)

where the non-dimensional parameters of \( \phi_{n} \) and \( \theta_{n} \) can be written accordingly as:

\[
\phi_{n} = \frac{[D_{S}(T) / R_{c}] \mathcal{A}_{2N}}{(n = 1, 2)}
\]

(14)

and

\[
\theta_{n} = \frac{[1 + \beta_{n}]k_{n}f_{S}^{2}/f_{L}^{2} (n = 1, 2)}
\]
where parameters $\Phi_{n(2E)}$, $\varphi_{n(2E)}$, $\theta_{n(2E)}$, $k_{n(2E)}$ and $D_{nS(2E)}$ of the two phases eutectic solidification stage have the same meanings with $\Phi_n$, $\varphi_n$, $\theta_n$, $k_n$ and $D_{nS}$ of the single-solution solidification, respectively. The symbols of $f_{S(\tau_{2E}))}$ and $f_{S_{(2E))}}$ denote the critical solid-fractions at which the solidification transitions of $f_{S(\tau_{2E}))}$ and $f_{S_{(2E))}}$ occur, respectively.

In the process of the ternary eutectic solidification, the liquid concentrations for the both two solutes have to keep constant according to Gibbs phase rule, i.e.,

$$C_{nL}^{\text{eq}} = C_{n(3E)} (n = 1, 2) \quad (23)$$

As Eq. (11) is derived without considering latent heat temporarily, the temperature $T^{i+1}$ calculated by Eq. (11) only represents the decreased value due to the heat loss by conduction/convection in the time interval $\Delta t^{i+1} = t^{i+1} - t^i$. According to the temperature-compensation method [21], the solidification temperature at time $t^{i+1}$ is the liquidus temperature $T_{\text{Liq}}^{i+1}$, while the latent heat released by the solid phase formed in $\Delta t^{i+1}$ is equal to the heat capacity of the temperature difference between the liquidus temperature and the temperature calculated by Eq. (11), i.e. $(T_{\text{Liq}}^{i+1} - T^{i+1})$. Based on the principle of heat energy balance and the assumption of local thermodynamic equilibrium solidification, the numerical formula for the solid fraction increase in the time interval $\Delta t^{i+1}$ can be derived as:

$$\Delta S_S^{i+1} = \left[ f_{S\text{ps}}c_{ps} + f_{L\text{ps}}c_{pl} \right] \left( T_{\text{Liq}}^{i+1} - T^{i+1} \right) / \rho_S h \quad (24)$$

Although the solid fraction $\Delta S_S^{i+1}$ of time $t^{i+1}$ can be calculated by Eq. (24), it can be seen from Eqs. (11), (16) and (17) that, the calculation of $T^{i+1}$ and $C_{nL}^{i+1}$ needs the value of $\Delta S_S^{i+1}$. As mentioned above, the solid fraction increase $\Delta S_S^{i+1}$, the temperature $T^{i+1}$ and the liquid composition $c_{nL}^{i+1}$ are strongly coupled and there must be a local balance among them at time $t^{i+1}$, which means they need to be solved at the same time. Based on the above argument, the following iteration procedure directly coupled with a thermodynamics database COST2 and the interface program TQ6 of Thermo-Calc software package is proposed to obtain the solution to the $T-f_S-C_l$ coupling.

1) The initial value of $\Delta S_S^{i+1}$ is set equal to zero ( $F_1 = \Delta S_S^{i+1} = 0$ ) and the approximation of $T^{i+1}$ is calculated using Eq. (11).

2) The approximations of $T^{i+1}$, $C_{1L}^{i+1}$ and $C_{2L}^{i+1}$ are used as the initial values of temperature and compositions at time $t^{i+1}$ ($T_1 = T^{i+1}$, $C_{B1} = C_{1L}^{i+1}$ and $C_{C1} = C_{2L}^{i+1}$, respectively), the approximate compositions of $C_{1L}^{i+1}$ and $C_{2L}^{i+1}$ are calculated using Eqs. (16) and (17).  

3) The approximate compositions of $C_{1L}^{i+1}$ and $C_{2L}^{i+1}$ are used, and the TQ6-interface program and the related database COST2 of Thermo-Calc are called to calculate the liquidus temperature $T_{\text{Liq}}^{i+1}$ and other thermodynamic parameters such as the solute partition coefficient.

4) The approximation of solidification increase $\Delta S_S^{i+1}$ is calculated by Eq. (24) and the average is taken $F_1 = 0.5(\Delta S_S^{i+1} + F_1)$.

5) The new approximation of $T^{i+1}$ is calculated with new initial values of $F_1$ using Eq. (11), $C_{B1} = C_{1L}^{i+1}$ and $C_{C1} = C_{2L}^{i+1}$, $T_1 = 0.5(T_1 + T^{i+1})$.

6) With the new initial values of $T_1$, $F_1$, $C_{B1}$ and $C_{C1}$, the new initial approximations of $C_{1L}^{i+1}$ and $C_{2L}^{i+1}$ are calculated by Eqs.(16) and (17), and $C_{B1} = 0.5(C_{B1} + C_{1L})$ and $C_{C1} = 0.5(C_{C1} + C_{2L})$ are taken;

7) All the following conditions are judged if they are true:

$$\frac{|F_1 - \Delta S_S^{i+1}|}{F_1} \leq \varepsilon_F, \quad \frac{|T_1 - T^{i+1}|}{T_1} \leq \varepsilon_T,$$

$$\frac{|C_{B1} - C_{1L}^{i+1}|}{C_{B1}} \leq \varepsilon_{B1}, \quad \frac{|C_{C1} - C_{2L}^{i+1}|}{C_{C1}} \leq \varepsilon_{C1}$$

where $\varepsilon_F$, $\varepsilon_T$, $\varepsilon_{B1}$ and $\varepsilon_{C1}$ are the predefined convergence accuracies for the iterations of the solid fraction, temperature and compositions of solutes B and C, respectively. If the conditions are not true, the liquidus temperature $T_{\text{Liq}}^{i+1}$ is calculated using $C_{B1}$ and $C_{C1}$ via calling Thermo-Calc and steps 4)–7) are repeated until all the above accurate conditions are satisfied.

4 Sample calculations of Al–2Si–3Mg alloy

To investigate the feasibility of the model and algorithm coupled with the ThermoCalc databases, sample calculations are carried out on an Al–2Si–3Mg alloy. The solidification paths and $T-f_S$ curves are calculated under five assumed solidification conditions with the legends of lever-rule, $h_s=20$ (unit: W/(m$^2$K)) and similarly hereinafter, $f_s^0=476.46$ and 476.46$^{\circ}$C, $h_s=200$ and Scheil model. These legends represent the limiting solidification case of fully equilibriums in both the solid and liquid phases, and in a relative real solidification mode, as described/calculated by Eqs. (6)–(24), with the heat transfer coefficient $h_s$ values of 20, 476.46$^{\circ}$C and 200, and in another limiting case of complete non-solidification for both solute Si and Mg, respectively. Under the third condition, the heat transport coefficient is obtained by fitting the inversely calculated data of heat transfer coefficient for the sand mold to power function form which is the same to that in Ref. [22].
Figure 1(a) shows the calculated solidification paths and Fig. 1(b) shows the temperature vs solid fraction curve of Al−2Si−3Mg alloy under the assumed different solidification conditions. It can be seen from Fig. 1(a) that the solidification path of the Scheil model is \((L\rightarrow\alpha)\rightarrow(L\rightarrow\alpha+\text{Si})\rightarrow(L\rightarrow\alpha+\text{Si+Mg}_2\text{Si})\), while the solidification paths under the other four conditions finished on the binary trough \((L\rightarrow\alpha)\rightarrow(L\rightarrow\alpha+\text{Si})\). It can be also seen from the temperature vs solid fraction \((T−f_s)\) curve shown in Fig. 1(b) that only the solidification path of Scheil model reaches the ternary eutectic point and with the volume fractions of 21.69% and 5.77% form binary and ternary eutectic phases, respectively. Under other conditions of Lever-rule, \(h_e=20\), \(h_e=476.46^{0.45}\) and \(h_e=200\), the solidification paths end on the binary eutectic trough at temperatures of 581.40, 580.06, 578.38 and 571.73 °C, respectively, and with the binary eutectic formed volume fraction of 23.13%, 24.87%, 26.13% and 26.80%, respectively. It can be seen that the influence of heat transfer coefficient on the solidification path is obviously. For the present Al−Si−Mg alloy, the greater the heat coefficient is, the closer the solidification path is to the predicted results by Scheil model. On the contrary, the solidification path is closer to the lever-rule model.

5 Experimental verification

5.1 Experimental process and results

To further investigate the reliability of the present model and algorithm, a solidification experiment of Al−Cu−Si ternary alloy is carried out. The experimental material of Al−5.17Cu−2.63Si was prepared with pure Al(99.7%), Al−49.2Cu and Al−12.7Si master alloys by ingot metallurgy in a graphite crucible in a resistance furnace. The alloy composition was analyzed chemically using samples taken from different locations of the specimens. The mold was made of sodium silicate sand. The dimensions of the specimen are shown in Fig. 2. In the pouring and solidification processes, the cooling curves were recorded using calibrated K-type thermocouples, which were linked to a PC-computer controlled data-acquisition module of ECON series (Data Translation, Inc., USA).

It can be seen from Fig. 3(a) that the solidification of the alloy experiences three stages including single phase solidification, binary eutectic solidification and the final ternary eutectic solidification, respectively. Figure 4 shows the BSE image of the solidified specimen (near the thermocouples, see Fig. 2) captured by a Hitachi S−4700 scanning electron microscope (SEM). As marked on the BSE image, the gray area is \(\alpha\) (Al), the light gray area is Si phase of the divorced binary eutectic, and the rest is ternary eutectic including \(\alpha\) (Al), Si and \(\theta\) phases. The image was used for measurements of the amounts of phases formed in each solidification stage.

The function of the equivalent heat transfer coefficient between the casting and mold is determined using an inverse calculation technique [23, 24] via the present simulation program. In the inverse calculation process, the interface heat transfer coefficient is adjusted to insure the simulated cooling curves coincide with the measured values. Figure 3(a) also shows the comparison
5.2 Results and discussion

The thermal conductivity of Al alloy is normally $k=100–300$ W/(m·K) [10], the heat transfer coefficient and characteristic length of the specimen in this work are $h_e=30–250$ W/(m²·K) (see Fig.3(b)) and $l=15–17.5$ mm. According to the equation of $\text{Biot} = \frac{hl}{k}$, the Biot number in the present study is $\text{Biot}=0.0015–0.04375<0.1$. Therefore, the model/algorithm and method proposed above are applicable to calculate the solidification paths and microsegregation of the specimen.

Figures 5(a) and (b) show the calculated solidification path and the temperature vs solid fraction curve of the specimen, including the calculation results for the two limit models of lever-rule (i.e. $Q_{Cu} = Q_{Si} = 1$) and Scheil model (i.e. $Q_{Cu} = Q_{Si} = 1$). It can be seen from Fig. 5(a) that the solidification path of the alloy runs down the liquidus surface from initial composition until the binary trough of $L\rightarrow \alpha + Si$, and reaches the ternary eutectic point of $L\rightarrow \alpha + Si + \theta$ at the end of the solidification for all the three cases, i.e. the present solidification path is $(L\rightarrow \alpha)\rightarrow (L\rightarrow \alpha + Si)\rightarrow (L\rightarrow \alpha + Si + \theta)$ which is the same with the experimental results. From the temperature vs solid fraction curves shown in Fig. 5(b), it can be seen that the solidification path of the
specimen meets the binary trough at 541.2 °C with volume fraction of 77.85% formed as the primary phase, and reaches the ternary eutectic point at 512.1 °C with volume fraction of 9.09% formed as ternary eutectic \((\alpha + \text{Si} + \theta)\) and the remainder is the binary eutectic \((\alpha + \text{Si})\).

Quantitative analysis of the microstructure is carried out using an image analysis software (Image-Pro Plus 6.0). As the atomic number of Al and Si is neighboring, it is difficult to accurately distinguish \(\alpha(\text{Al})\) and Si-phase by the analysis software because of the almost same contrast in the BSE image. In the present work, the image-fractions for the primary phases (\(\alpha\)) and binary eutectic \((\alpha + \text{Si})\) are counted together as a combined phase of \((\alpha + \text{Si})\), and the remainder is ternary eutectic \((\alpha + \text{Si} + \theta)\). Figure 6 shows the comparison of volume fractions for the different phases between the calculated and measured results. It can be seen that the calculated results for the present experimental conditions are reasonably agreeable to the measured results.

![Graph showing comparison of volume fractions](image)

**Fig. 6** Comparison of volume fractions of phases between calculated and measured results of different solidification stages of Al−5.17Cu−2.63Si alloy solidified in sand mold.

It can be seen from the above sample calculations and experiment that the present model and algorithm for the prediction of the solidification paths and microsegregation of alloys solidified under the condition of Biot≤0.1 are feasible and reliable. This method can be used for the analysis of any alloy solidified under the condition of Biot≤0.1 in principle. As the volumes of the specimens of DTA, DSC and SPTA are small and can easily satisfy the condition of Biot≤0.1, the present technique may be used for providing additional information for the solidification paths and microsegregation of an alloy for new alloy developments instead of an experimental investigation.

### 6 Conclusions

1) A binary continuum model for dendritic solidification transport phenomena and the corresponding numerical algorithm for the strong nonlinear coupling of \(T-f_{s}-C_{l}\) are extended to a multicomponent alloys solidified under the condition of Biot≤0.1. Based on the extended model and algorithm, a method considering heat transfer is proposed to predict the solidification paths and microsegregation of alloys solidified under the same condition.

2) The new algorithm and method are closely coupled with the commercial Thermo-Calc package via its TQ6-interface codes, for instantaneous determination of the related thermodynamic data at each calculation time step.

3) The availability and reliability of the proposed multicomponent/multiphase model and algorithm for predicting the solidification paths and microsegregation are demonstrated by sample calculations with Al−2Si−3Mg specimens solidified under different heat transfer conditions, and by comparing the results between computations and the corresponding experimental investigations with Al−5.17Cu−2.63Si ternary alloy.

### References


