

Computer program for equilibrium calculation and diffusion simulation^①

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Abstract: A computer program called TKCALC(thermodynamic and kinetic calculation) has been successfully developed for the purpose of phase equilibrium calculation and diffusion simulation in ternary substitutional alloy systems. The program was subsequently applied to calculate the isothermal sections of the Fe-Cr-Ni system and predict the concentration profiles of two γ/γ' single-phase diffusion couples in the Ni-Cr-Al system. The results are in excellent agreement with THERMOCALC and DICTRA software packages. Detailed mathematical derivation of some important formulae involved is also elaborated.

Key words: diffusion; thermodynamics; kinetics; phase diagram

Document code: A

1 INTRODUCTION

The knowledge of thermodynamics and kinetics is of fundamental importance to the understanding of many processes in materials science, e.g. the homogenization annealing, the carburization and decarburization treatment of steels, the growth and dissolution behavior of second phases, the non-equilibrium solidification of alloys etc. Based upon the state-of-the-art CALPHAD(calculation of phase diagrams) method, two very general purpose software packages, namely THERMOCALC for thermodynamic calculation and DICTRA for numerical treatment of diffusion-controlled phase transformation in multicomponent systems, have already been well developed and extensively used worldwide. Although THERMOCALC and DICTRA are already sophisticated enough to tackle with most practical problems, we can not modify them to meet our own needs, therefore the purpose of the current paper is to develop a new computer program called TKCALC(thermodynamic and kinetic calculation) for calculation of thermodynamic equilibria and numerical solution of nonlinear diffusion equations in ternary substitutional alloy systems.

The program TKCALC also follows the basic ideas underlying the CALPHAD approach and the same assumptions are made by TKCALC as those made by DICTRA:

1) Only one-dimensional diffusion is considered, such as in the case of planar, cylindrical and spherical symmetry.

2) The same constant molar volume is assumed for each phase, so that the diffusion process induces no compositional stress field.

3) Simple vacancy-exchange mechanism for diffusion is adopted and vacancies are assumed to be in

thermal equilibrium everywhere.

4) The rate of phase transformation is controlled by volume diffusion to and from the phase interfaces.

5) Thermodynamic equilibrium can be established locally at the moving phase interface, and the moving direction and velocity of the interface are totally determined by the interfacial fluxes.

6) The effect of surface tension is negligible.

No more simplifications are made. The interdiffusion coefficients are allowed to be strongly composition and temperature dependent and the effects of magnetic ordering on phase equilibrium and lattice diffusion are also taken into full account.

Unfortunately, for a successful diffusion simulation, the complete and accurate set of thermodynamic and kinetic data of the system in question is prerequisite. Although the thermodynamic descriptions of many alloy systems are readily available in the SGTE solution database, kinetic databases are so far scarce. Luckily, due to their important industrial applications as austenitic stainless steel and nickel-based high-temperature oxidation and corrosion protection overlay coating for aerospace gas turbine engines respectively, the Fe-Cr-Ni and Ni-Cr-Al systems have been extensively investigated by various researchers^[1~15], both thermodynamically and kinetically, and they are taken as practical examples to demonstrate the problem-solving capability of TKCALC.

2 SOFTWARE DEVELOPMENT

Program TKCALC is coded entirely in C++ programming language using the state-of-the-art OOP(object-oriented programming) technique. A special point is also made of its 3-D graphics visualization capability, which is not yet implemented in graphics

① **Foundation item:** Project 59771037 supported by the National Natural Science Foundation of China

Received date: Jul. 1, 1999; **accepted date:** Nov. 1, 1999

post-processor of THERMO-CALC and DICTRA. TKCALC can run on any personal computer with a 80386 or better CPU, a math-coprocessor and a VGA graphics card, although the runtime performance still depends on the actual speed of computer.

3 THERMODYNAMIC MODELLING

The choice of appropriate thermodynamic model and the assessment of an accurate and consistent set of parameters for the model are not only crucial to phase diagram calculation, but also contributive to the interdiffusion coefficient matrix via the so-called thermodynamic factor, which virtually consists of the second-order partial derivatives of molar Gibbs free energy with respect to each composition variable.

For most substitutional solution phases, the widely applicable Redlich-Kister-Muggianu extrapolation model is recommended, following which the molar Gibbs free energy of a solution phase in A-B-C ternary system can be readily estimated from the thermodynamic descriptions of its three boundary binary subsystems and is expressed as

$$G_m = \sum_{i=A}^C x_i ({}^\circ G_i + RT \ln x_i) + \sum_{i=A}^B \sum_{j>i}^C x_i x_j \left[\sum_{k=0}^{n_{ij}} L_{ij}^k (x_i - x_j)^k \right] + x_A x_B x_C \sum_{i=A}^C L_{ABC}^i x_i + \Delta G_m^{\text{mag}} \quad (1)$$

where x_i is the molar composition of component i , ${}^\circ G_i$ is the lattice stability of pure element i in the same crystal structure as the solution phase under consideration, L_{ij}^k are the binary interaction parameters of i - j binary system and L_{ABC}^i are ternary interaction parameters. This ternary excess term is added in order to get better fit to ternary experimental information. The last term ${}^\circ G_m^{\text{mag}}$ corresponds to the contribution to Gibbs free energy due to magnetic ordering. According to the Hillert-Jarl model^[7], which is a truncated series simplification of the phenomenological model originally proposed by Indén^[16], it is formulated as

$$\Delta G_m^{\text{mag}} = RT \ln(\beta + 1) f(\tau) \quad (2)$$

$$f(\tau) = \begin{cases} 1 - \frac{1}{A} \left[\frac{79}{140} \frac{\tau^1}{P} + \frac{474}{497} \left(\frac{1}{P} - 1 \right) \right] \cdot \left[\frac{\tau^2}{6} + \frac{\tau^3}{135} + \frac{\tau^5}{600} \right] & \text{for } \tau \leq 1 \\ - \frac{1}{A} \left[\frac{\tau^5}{10} + \frac{\tau^{15}}{315} + \frac{\tau^{25}}{1500} \right] & \text{for } \tau > 1 \end{cases}$$

where $\tau = \frac{T}{T_C}$ and $A = \frac{518}{1125} + \frac{11692}{15975} \left(\frac{1}{P} - 1 \right)$, β stands for the average magnetic moment per atom in Bohr magnetons and T_C stands for the critical temperature for magnetic ordering, i.e. the Curie temperature for ferromagnetic transition or Néel tempera-

ture for anti-ferromagnetic transition. All temperatures are in Kelvin. P is a structure dependent parameter, $P \approx 0.4$ for BCC and $P \approx 0.28$ for FCC. The magnetic contribution to enthalpy can then be evaluated using the Gibbs-Helmholtz equation:

$$\begin{aligned} \Delta H_m^{\text{mag}} &= - T^2 \frac{\partial}{\partial T} \left[\frac{\Delta G_m^{\text{mag}}}{T} \right] \\ &= - RT_C \ln(\beta + 1) g(\tau) \\ g(\tau) &= \tau^2 \frac{df(\tau)}{d\tau} = \begin{cases} \frac{1}{A} \left[\frac{79}{140} \frac{\tau^1}{P} - \frac{474}{497} \frac{\tau^4}{P} + \frac{\tau^0}{2} + \frac{\tau^0}{15} + \frac{\tau^6}{40} \right] & \text{for } \tau < 1 \\ \frac{1}{A} \left[\frac{\tau^4}{2} + \frac{\tau^{14}}{21} + \frac{\tau^{24}}{60} \right] & \text{for } \tau > 1 \end{cases} \quad (3) \end{aligned}$$

It is worth noting here that both β and T_C are generally composition dependent values and are usually expressed in the form of the generalized Redlich-Kister summation:

$$\Phi = \sum_{i=A}^C x_i \Phi_i + \sum_{i=A}^B \sum_{j>i}^C x_i x_j \left[\sum_{k=0}^{n_{ij}} \Phi_{ij}^k (x_i - x_j)^k \right] + x_A x_B x_C \sum_{i=A}^C \Phi_{ABC}^i x_i \quad (4)$$

where Φ denotes β or T_C . If the value of β or T_C calculated from the above expression becomes negative, it indicates that the alloy phase is anti-ferromagnetic rather than ferromagnetic. The true value of β or T_C can be obtained simply by dividing the negative value by an anti-ferromagnetic factor, which is -1.0 for BCC and -3.0 for FCC phase. Generally speaking, the surfaces of Φ and T_C are required to intersect with the zero value plane along exactly the same composition curve.

Given the expression of molar Gibbs free energy, the partial molar Gibbs energy, i.e., the chemical potential of component i can be conveniently derived by using the following standard relationship:

$$\begin{aligned} G_i = \mu_i &= \frac{\partial}{\partial n_i} [(n_A + n_B + n_C) G_m(x_A, x_B, x_C)] \\ &= G_m + \frac{\partial G_m}{\partial x_i} - \sum_{j=A}^C x_j \frac{\partial G_m}{\partial x_j}, \quad i = A, B, C \quad (5) \end{aligned}$$

where x_i is the molar composition of component i and $x_i = n_i / (n_A + n_B + n_C)$, n_i stands for the number of moles of component present in the phase.

The thermodynamic equilibrium can then be calculated by means of equalizing the chemical potentials of each component in all phases participating in equilibrium. Additional conditions may need to be arbitrarily specified if the freedom of the system is nonzero according to the Gibbs phase rule under isothermal and isobaric conditions:

$$F = C - P \quad (b)$$

where F means the degree of freedom of system, C denotes the total number of components and P denotes the total number of phases present in system.

The resultant set of nonlinear equations must be solved numerically using some standard algorithms, such as the widely used Newton-Rapson iteration method or the simplex method. However, it must be noted here that for phases with sublattices, if any of the components occupies more than one sublattice at the same time, then the above mentioned strategy for phase diagram calculation will no longer be applicable. To save the situation, a more general and direct equilibrium conditions proposed by Hillert^[17] and implemented in THERMO-CALC system, which corresponds to the constrained minimization of the total Gibbs free energy of the whole system by means of the Lagrange Multiplier method, should be employed instead.

4 KINETICS MODELLING

According to the Fick-Onsager law, which is a phenomenological extension of Fick's first law to multicomponent systems, for a ternary system A-B-C, the interdiffusional flux of component i in a laboratory-fixed frame of reference can be generally expressed as

$$\tilde{J}_i = - \frac{1}{V_m} \sum_{j=A}^B \tilde{D}_{ij}^C \nabla x_j, \quad i = A, B \quad (7)$$

where \tilde{D}_{ij}^C constitutes the 2×2 interdiffusion coefficient matrix, ∇x_j is the molar composition gradient of component j and V_m is the molar volume and is assumed to be independent of composition. By default, component C is chosen as solvent, i.e. the dependent component, other components can also be chosen as solvent and we get the following general relationships for a ternary system:

$$\begin{aligned} \tilde{D}_{ij}^k &= - \tilde{D}_{ik}^j, \quad \tilde{D}_{ij}^k \tilde{D}_{ii}^k = \tilde{D}_{ii}^j \\ \tilde{D}_{ij}^k &= \tilde{D}_{kk}^i - \tilde{D}_{jj}^k, \quad i \neq j \neq k \end{aligned} \quad (8)$$

Following the formalism proposed by Andersson and Ågren^[18], which is derived based on the assumption of simple vacancy-exchange mechanism for diffusion, for a ternary substitutional solution phase, the full interdiffusion coefficient matrix in the laboratory-fixed frame of reference can be evaluated as

$$\tilde{D}_{ij}^C = x_i M_i \frac{\partial \mu_i}{\partial x_j} - x_i \sum_{k=A}^C x_k M_k \frac{\partial \mu_k}{\partial x_j}, \quad i = A, j = B \quad (9)$$

where M_k represents the atomic mobility of component k and is purely kinetic, x_i and μ_i are the molar composition and chemical potential of component i respectively, and $\frac{\partial \mu_i}{\partial x_j}$ is the so-called thermodynamic factor and is purely thermodynamic.

Further simplifications can be made by introducing the Gibbs-Duhem relationship:

$$\sum_{i=A}^C x_i \frac{\partial \mu_i}{\partial x_j} = 0, \quad i = A, j = B \quad (10)$$

and we get:

$$\tilde{D}_{ij}^C = x_i M_i \frac{\partial \mu_i}{\partial x_j} - x_i \sum_{k=A}^B x_k (M_k - M_C) \frac{\partial \mu_k}{\partial x_j}, \quad i = A, j = B \quad (11)$$

The temperature and composition dependence of atomic mobility taking account of the effect of paramagnetic to ferromagnetic transition is modeled by Björn Jönsson^[3] as follows:

$$M_i = \frac{1}{RT} \text{EXP} \left[\frac{\mathcal{Q}_i^p}{R} + \Lambda \alpha \xi - \frac{Q_i^p}{RT} (1 + \alpha \xi) \right] \quad (12)$$

where $\xi = \frac{\Delta H_m^{\text{mag}}(T)}{\Delta H_m^{\text{mag}}(O)}$, ΔH_m^{mag} is the magnetic enthalpy and can be calculated using Eqn.(3), Q_i^p is the activation energy, \mathcal{Q}_i^p is a quantity introduced by Björn Jönsson in order to get better fit to the experimental diffusivity data, which is defined as $\mathcal{Q}_i^p = R \ln(M_i^p)$, M_i^p is the pre-exponential or frequency factor, the superscript p here refers to the paramagnetic state of the phase in which the magnetic moments are totally disordered, R is gas constant and temperature T is in Kelvin. For BCC phase, $\Lambda \approx 6$ and $\alpha = 0.3$, for FCC phase, $\alpha = 0$, i.e. the magnetic ordering is assumed to have no effect on atomic mobility. Again, both \mathcal{Q}_i^p and Q_i^p are generally functions of alloy composition and are also expressed as the generalized Redlich-Kister summation, i.e. Eqn.(4). ξ is a quantity describing the degree of magnetic ordering and it depends both on temperature and composition in a more complex way.

Finally, the multicomponent diffusion equation can be derived from the continuity equation which is given as

$$\frac{1}{V_m} \frac{\partial x_i}{\partial t} = - \frac{1}{Z^{m-1}} \frac{\partial}{\partial Z} [Z^{m-1} \tilde{J}_i], \quad i = A, B \quad (13)$$

where Z represents distance perpendicular to the diffusion couple interface, m represents the number of dimensions of the diffusion couple, $m=1$ for planar symmetry, $m=2$ for cylindrical symmetry and $m=3$ for spherical symmetry. Eliminate the constant molar volume V_m and assume the simple planar case, i.e. let $m=1$, we get

$$\begin{cases} \frac{\partial x_A}{\partial t} = \frac{\partial}{\partial Z} \left[\tilde{D}_{AA}^C \frac{\partial x_A}{\partial Z} \right] + \frac{\partial}{\partial Z} \left[\tilde{D}_{AB}^C \frac{\partial x_B}{\partial Z} \right] \\ \frac{\partial x_B}{\partial t} = \frac{\partial}{\partial Z} \left[\tilde{D}_{BA}^C \frac{\partial x_A}{\partial Z} \right] + \frac{\partial}{\partial Z} \left[\tilde{D}_{BB}^C \frac{\partial x_B}{\partial Z} \right] \end{cases} \quad (14)$$

where \tilde{D}_{AA}^C and \tilde{D}_{BB}^C are the main interdiffusion coefficients, which represent the effect of the concentration gradient of a given component on its own interdiffusional flux, and \tilde{D}_{AB}^C and \tilde{D}_{BA}^C are the off-diagonal or cross-effect interdiffusion coefficients which are usually neglected due to their relatively small values.

Since the interdiffusion coefficients may be

strongly dependent upon composition, Eqn.(14) is in general a set of coupled nonlinear partial differential equations and has to be solved numerically. In DIC-TRA software package, a numerical method developed by Agren^[19], which is based on the well-known Galerkin method, i.e. the finite-element method, is used to solve the coupled diffusion equations. While in TKCALC program, these partial differential equations together with appropriate boundary conditions are first discretized using the equidistant finite-difference approximation taking full account of the composition dependence of the four interdiffusion coefficients as follows:

$$\left. \frac{\partial}{\partial Z} \left[D \frac{\partial x_i}{\partial Z} \right] \right|_{(Z,t)} =$$

$$D_{Z+\frac{\Delta Z}{2},t} \frac{x_i(Z+\Delta Z,t) - x_i(Z,t)}{\Delta Z^2} -$$

$$D_{Z-\frac{\Delta Z}{2},t} \frac{x_i(Z,t) - x_i(Z-\Delta Z,t)}{\Delta Z^2}$$

$$D_{Z\pm\frac{\Delta Z}{2},t} = \frac{D(x_A(Z,t), x_B(Z,t))}{2} +$$

$$\frac{D(x_A(Z\pm\Delta Z,t), x_B(Z\pm\Delta Z,t))}{2}$$

or

$$D_{Z\pm\frac{\Delta Z}{2},t} = D \left[\frac{x_A(Z,t), x_A(Z\pm\Delta Z,t)}{2}, \right.$$

$$\left. \frac{x_B(Z,t) + x_B(Z\pm\Delta Z,t)}{2} \right] \quad (15)$$

where $i = A, B$; ΔZ is the distance between two adjacent grid points; $D = D(x_A, x_B)$ is a general function of two variables, which stands for D_{AA}^C , D_{AB}^C , D_{BA}^C or D_{BB}^C .

If we further assume that the interdiffusion coefficients are of constant values, then we get:

$$D \frac{\partial^2 x_i}{\partial Z^2} \Big|_{(Z,t)} = \frac{\partial}{\partial Z} \left[D \frac{\partial x_i}{\partial Z} \right] \Big|_{(Z,t)}$$

$$= \frac{x_i(Z-\Delta Z,t) - 2x_i(Z,t) + x_i(Z+\Delta Z,t)}{D^{-1} \Delta Z^2} +$$

$$\frac{x_i(Z+\Delta Z,t)}{D^{-1} \Delta Z^2}$$

$$i = A, B \quad (16)$$

which is simplified finite difference approximation widely used in Ref.[11~14] for diffusion simulation.

In order to ensure superior numerical accuracy as well as stability, e.g. very large time increments can be used in order to significantly reduce the total computing time required without sacrificing much precision or causing numerical instability problems, in TKCALC program, the Crank-Nicholson implicit method is subsequently employed to solve the finite difference equations, i.e. Eqn.(15), which can be easily derived from the trapezoidal rule for numerical integration as follows:

$$x_i(Z,t+\Delta t) - x_i(Z,t) = \int_{Z,t}^{Z,t+\Delta t} \frac{\partial x_i}{\partial t} dt =$$

$$\frac{\Delta t}{2} \left[\frac{\partial x_i}{\partial t} \Big|_{(Z,t)} + \frac{\partial x_i}{\partial t} \Big|_{(Z,t+\Delta t)} \right], \quad i = A, B \quad (17)$$

where Δt denotes small time increment.

5 THERMODYNAMIC CALCULATION OF Fe-Cr-Ni

Owing to its great commercial importance as the basis for austenitic stainless steel, the Fe-Cr-Ni system has been assessed and reassessed by several researchers^[7-10] with special attention paid to the modeling of the effects of alloying on the ferromagnetic properties of α -BCC phase. In the current calculation, the thermodynamic parameters of FCC and BCC phases in Fe-Cr-Ni system are directly taken from the SGTE solution database and are listed in Table 1.

The isothermal section of the Fe-Cr-Ni system at 1373 K is then calculated by using TKCALC program and THERMO-CALC software package simultaneously, and the results are presented in Fig.1. The

Table 1 Thermodynamic data for Fe-Cr-Ni system

α ferrite (BCC)	γ austenite (FCC)
$^{\circ}G_{Ni}^{BCC} - ^{\circ}G_{Ni}^{FCC} = 8715.084 - 3.556 T (298.15 < T < 3000 \text{ K})$	$^{\circ}G_{Cr}^{FCC} - ^{\circ}G_{Cr}^{BCC} = 7284 + 0.163 T$
$L_{Cr,Fe}^{BCC} = 20500 - 9.68 T$	$^{\circ}G_{Fe}^{FCC} - ^{\circ}G_{Fe}^{BCC} = -1462.4 + 8.282 T - 1.15 T \ln T +$ $6.4 \times 10^{-4} T^2 \quad (298.15 < T < 1811 \text{ K})$
$L_{Cr,Ni}^{BCC} = 17170 - 11.82 T + (34418 - 11.858 T)(x_{Cr} - x_{Ni})$	$L_{Cr,Fe}^{FCC} = 10833 - 7.477 T + 1410(x_{Cr} - x_{Fe})$
$L_{Fe,Ni}^{BCC} = -95663 - 1.28 T + (1789.03 - 1.929 T)(x_{Fe} - x_{Ni})$	$L_{Cr,Ni}^{FCC} = 8030 - 12.88 T + (33080 - 16.036 T)(x_{Cr} - x_{Ni})$
$L_{Cr,Fe,Ni}^{BCC} = -2673 + 2.042 T$	$L_{Fe,Ni}^{FCC} = -12054.355 + 3.274 T + (11082.132 -$ $4.45 T)(x_{Fe} - x_{Ni}) - 725.805(x_{Fe} - x_{Ni})^2$
$T_C^{BCC} = -311.5 x_{Cr} + 1043 x_{Fe} + 575 x_{Ni} + x_{Cr} x_{Fe} [1650 +$ $550(x_{Cr} - x_{Fe})] + x_{Cr} x_{Ni} [2373 + 617(x_{Cr} - x_{Ni})]$	$L_{Fe,Cr,Ni}^{FCC} = 16580 - 9.783 T$
$\beta^{BCC} = -0.01 x_{Cr} + 2.22 x_{Fe} + 0.85 x_{Ni} - 0.85 x_{Cr} x_{Fe}$ $+ 4 x_{Cr} x_{Ni}$	$T_C^{FCC} = -1109 x_{Cr} - 201 x_{Fe} + 633 x_{Ni} - 3605 x_{Cr} x_{Ni} +$ $x_{Fe} x_{Ni} [2133 - 682(x_{Fe} - x_{Ni})]$
	$\beta^{FCC} = -2.46 x_{Cr} - 2.1 x_{Fe} + 0.52 x_{Ni} - 1.91 x_{Cr} x_{Ni} + x_{Fe} x_{Ni}$ $[9.55 + 7.23(x_{Fe} - x_{Ni}) + 5.93(x_{Fe} - x_{Ni})^2 +$ $6.18(x_{Fe} - x_{Ni})^3]$

Note: All parameters listed above are in international standard units, the default valid temperature range is $298.15 < T < 6000 \text{ K}$, unless the range is explicitly indicated.

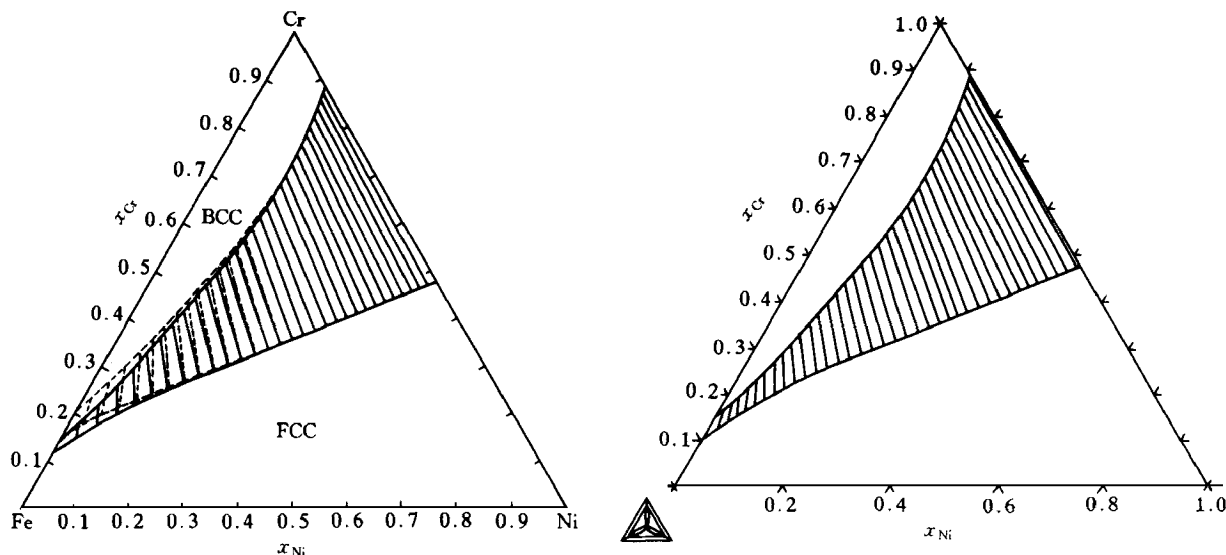


Fig.1 Calculated isothermal sections of Fe-Cr-Ni at 1373 K
(a) — TKALC; (b) — THERMOCALC

dashed lines in Fig.1(a) represent calculation neglecting the magnetic contribution, while the solid lines represent calculation taking into account the magnetic effect. Very good agreement is reached between the two programs as can be seen. It is also observed that the ferromagnetic transition of α -BCC phase has a non-negligible effect on phase equilibrium in the Fe-Cr-Ni system, especially when near the iron-rich corner or when the temperature is very low, whereas the effect of magnetic ordering in FCC phase is trivial.

6 SIMULATION OF SINGLE-PHASE DIFFUSION IN Ni-Cr-Al

In the current simulation, the optimized set of thermodynamic parameters of FCC phase in the Ni-Cr-Al system is directly retrieved from the SGTE solution database, and the atomic mobility data are obtained from the assessment work by Engström and Ågren^[2], which are all listed in Table 2. The lattice stability data are not presented here since they are not needed for the current simulation.

The concentration profiles of two ν/ν diffusion couples in the Ni-Cr-Al system after 100 and 10 000 h of annealing at 1200 °C are then predicted by using TKALC program and DICTRA software package simultaneously. Each diffusion couple is 2 mm/2 mm in thickness, and their nominal alloy compositions are in Ref.[3]. The final simulated concentration profiles are presented in Fig.2. Dashed lines indicate the original diffusion couple interface, solid lines are calculated by TKALC program and triangles represent calculations by DICTRA. Again, excellent agreement between the two programs is observed.

Table 2 Thermodynamic and kinetic data of FCC phase in Ni-Cr-Al

α FCC	
$L_{Al,Cr}^{FCC} = -63800 - 5T + 8(x_{Al} - x_{Cr}) - 4000(x_{Al} - x_{Cr})^2$	
$L_{Al,Cr}^{FCC} = -154590.84 + 9.929T + (31030.09 - 43.888T)(x_{Al} - x_{Ni})$	
$L_{Cr,Ni}^{FCC} = 8030 - 12.88T + (33080 - 16.036)(x_{Cr} - x_{Ni})$	
$T_C^{FCC} = -1109x_{Cr} + 633x_{Ni} - 3605x_{Cr}x_{Ni}$	
$\beta^{FCC} = -2.46x_{Cr} + 0.52x_{Ni} - 1.91x_{Cr}x_{Ni}$	
$\phi_{Al}^{FCC} = -72.1188x_{Al} - 82x_{Cr} - 59.8265x_{Ni} - 91.2x_{Al}x_{Ni}$	
$Q_{Al}^{FCC} = 142000x_{Al} + 235000x_{Cr} + 284000x_{Ni} - 335000x_{Al}x_{Cr} + 53200x_{Cr}x_{Ni} + 41300x_{Al}x_{Ni}$	
$\phi_{Cr}^{FCC} = -3.71066x_{Al} - 82x_{Cr} - 64.4x_{Ni}$	
$Q_{Cr}^{FCC} = 261700x_{Al} + 235000x_{Cr} + 284000x_{Ni} - 487000x_{Al}x_{Cr} + 68000x_{Cr}x_{Ni} + 118000x_{Al}x_{Ni}$	
$\phi_{Ni}^{FCC} = -64.261x_{Al} - 82x_{Cr} - 69.8x_{Ni} + 65.5x_{Al}x_{Ni}$	
$Q_{Ni}^{FCC} = 145900x_{Al} + 235000x_{Cr} + 287000x_{Ni} - 211000x_{Al}x_{Cr} + 81000x_{Cr}x_{Ni} + 113000x_{Al}x_{Ni}$	

Note: All parameters listed above are in international standard units, the default valid temperature range is $298.15 < T < 6000$ K, unless the range is explicitly indicated.

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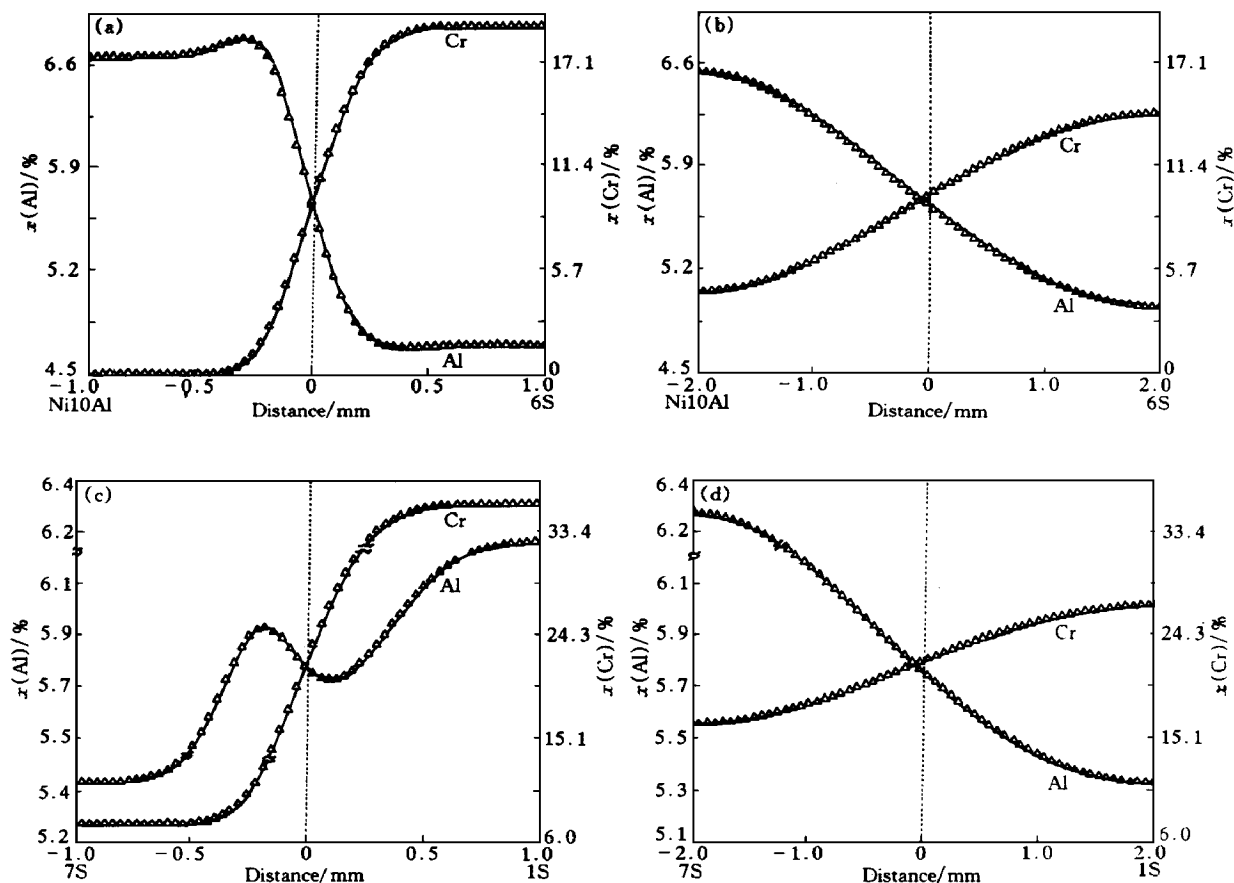


Fig.2 Simulated concentration profiles of two ν/ν diffusion couples in Ni-Cr-Al system after being annealed at 1 200 °C for various periods of time
(a) —Ni10Al/6S, 100 h;(b) —Ni10Al/6S, 10 000 h;(c) —7S/1S, 100 h;(d) —7S/1S, 10 000 h

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(Edited by HUANG Jin song)