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Surface and transport properties of Ni–Ti liquid alloys

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Abstract

Based on the phase diagram evidence of the existence of three intermetallic compounds, the phenomenon of compound formation in Ni–Ti liquid alloys has been analysed through the study of surface properties (surface tension and surface composition), dynamic properties (chemical diffusion) and microscopic functions (concentration fluctuations in the long-wavelength limit and chemical short range order parameter) in the frame of compound formation model (CFM).

Keywords: High temperature alloys; Surface and interfaces; Atomic scale structure; Shape memory; Thermodynamic modelling

1. Introduction

Ni–Ti alloys are principally used as shape memory materials [1–3] due to the martensitic and other metastable transformations of the NiTi compound. They are suitable as a binder phase of cermets with TiC, TiN and TiB_2 [4], or as constituents or subsystem of complex metallic glasses [5]. Together with Ni-based superalloys containing Ti they are of great importance for applications where aggressive thermal and mechanical conditions are predominant. Measurements of thermodynamic and thermophysical quantities on the alloys containing highly reactive titanium are difficult and usually is not possible to cover the whole range of composition and temperature. The Ni–Ti system is unique among Ti-systems in which the liquidus and solidus are precisely determined over the whole range of composition. The enthalpy of mixing [6–8], the Gibbs free energy of mixing and the activities [9–12] of liquid Ni–Ti alloys have been measured at temperatures ranging from 1740 to 2000 K. These data indicate negative deviation from the ideal mixing. The existence of two congruently melting intermetallic compounds, Ni_3Ti and NiTi, and $NiTi_2$, formed by a peritectic reaction [13], substantiate the exothermic mixing effects in this system. The asymmetric behaviour of its mixing properties is pronounced and can be partially deduced from the empirical factors such as size ratio ($V_{Ti}/V_{Ni} \approx 1.51$), valency difference (0, 1 or 2) [14] and electronegativity difference ($\approx$0.37) [15], but these factors are not sufficient to characterise the melt.

In order to understand the mixing behaviour in binary liquid alloys it is necessary to have the information on the energetics and the structure of melts as well as the ways how they are coupled. The nature of interactions and structural re-adjustement of the constituent atoms in liquid alloys can be deduced from the theoretical modelling of observable indicators, such as the thermodynamic and the thermophysical quantities [16–18]. On the other side, the atomic scale structural information can directly be evaluated from neutron and X-ray diffraction experiments. Although lacking these experimental data can be successfully described by the statistical thermodynamic approach of Bhatia and Thornton [19]. It takes into account the Darken stability function [20] as a part of the concentration–concentration structure factor in the long wavelength limit and gives the microscopic functions in terms of the thermodynamic functions of mixing.

Liquid binary systems characterised by the presence of one or more intermetallic compounds in the solid state exhibit a tendency to association of unlike constituent elements [21]. The effects of the chemical short range order phenomenon on the mixing properties of Ni–Ti melts are described by the compound formation model (CFM) [22,23]. Since the Ni_3Ti is the most stable intermetallic compound in the Ni–Ti system, it was taken as energetically favoured in our calculations [10,12]. In the present work the thermodynamic and thermophysical properties as well as the microscopic functions (concentration fluctuations in the long-wavelength limit and chemical short range order parameter) of liquid Ni–Ti alloys have been reproduced quantitatively

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by using the CFM. In particular, as concerns the thermophysical properties such as the surface tension, the diffusivity and the viscosity of liquid Ni–Ti alloys, a complete lack of experimental data was observed. Therefore, it is only possible to estimate the missing values by theoretical models.

2. Theory

2.1. The CFM and the QCA for regular solution: thermodynamic and surface properties

The CFM formalism related to a weak interaction approximation [22,23] has been successfully applied to the Ni–Ti system to describe the asymmetric behaviour of the mixing properties in the liquid state with respect to the A_3B stoichiometry [13]. In our previous work on the thermodynamic and the surface properties of liquid Bi–Pb alloys [24] many details related to the weak interaction approximation for the A_3B stoichiometry in the framework of the CFM have been reported. Thus, in the present work only the basic equations of this formalism are given. The generalised CFM formalism treats an alloy as a pseudoternary mixture of A atoms, B atoms and $A_\mu B_\nu$ (μ and ν are the small integers) group of atoms or clusters with the stoichiometry of the intermetallics present in the solid state, all in chemical equilibrium with one another [21–23,25,26]. The absence of clusters in the melt reduces the model to the quasi chemical approximation (QCA) for regular solutions [25,26]. Butler's concept of a layered interface structure [27] and the relationship between the component's activity in the bulk and the surface phase are basic hypotheses of both models. It should be pointed out that in the framework of the models mentioned above some parameters (i.e. the coordination number, Z, and the order energy parameters, W and ΔW_{ij}) are not concentration dependent. The value of Z is chosen from the structural data and the order energy parameters are determined from the thermodynamic data.

For all binary alloys in which intermetallic compounds with weak interactions are formed, the interaction energy parameters W/Zk_BT and $\Delta W_{ij}/Zk_BT$ should be less than unity. Using the standard thermodynamic relations and after some algebra the excess Gibbs energy of mixing, G_M^{xs} can be given by:

$$G_M^{xs} = Nk_BT\left[\left(\frac{W}{k_BT}\right)C(1-C) + \left(\frac{\Delta W_{AB}}{k_BT}\right)\Phi_{AB} + \left(\frac{\Delta W_{AA}}{k_BT}\right)\Phi_{AA}\left(\frac{\Delta W_{BB}}{k_BT}\right)\Phi_{BB}\right] \tag{1}$$

where N, k_B and T are the Avogadro's number, Boltzman's constant and the absolute temperature, respectively. C is the concentration of A and Φ_{ij} (i, j = A, B) are the concentration functions depending on μ and ν values. For $\mu = 3$, $\nu = 1$ (e.g. Ni_3Ti) these values are:

$$\begin{aligned}
\Phi_{AB} &= \tfrac{1}{5}C + \tfrac{2}{3}C^3 - C^4 - \tfrac{1}{5}C^5 + \tfrac{1}{3}C^6,\\
\Phi_{AA} &= -\tfrac{3}{20}C + \tfrac{2}{3}C^3 - \tfrac{3}{4}C^4 + \tfrac{2}{5}C^5 - \tfrac{1}{6}C^6,\\
\Phi_{BB} &= 0
\end{aligned} \tag{2}$$

Taking account the stoichiometry of A_3B, the expressions for the activity coefficients [28] and standard thermodynamic relations, the activities can be expressed as:

$$a_A = C\exp\left[\frac{W\phi + \Delta W_{AB}\phi_{AB} + \Delta W_{AA}\phi_{AA}}{k_BT}\right] \tag{3a}$$

$$a_B = (1-C)\exp\left[\frac{Wf + \Delta W_{AB}f_{AB} + \Delta W_{AA}f_{AA}}{k_BT}\right] \tag{3b}$$

where f, ϕ, ϕ_{ij} and f_{ij} (i, j = A, B) are the functions of bulk concentrations which for $\mu = 3$ and $\nu = 1$, take the form [28]:

$$\begin{aligned}
\phi &= (1-C)^2,\\
\phi_{AB} &= \tfrac{1}{5} + 2C^2 - \tfrac{16}{3}C^3 + 2C^4 + \tfrac{14}{5}C^5 - \tfrac{5}{3}C^6,\\
\phi_{AA} &= -\tfrac{3}{20} + 2C^2 - \tfrac{13}{3}C^3 + \tfrac{17}{4}C^4 - \tfrac{13}{5}C^5 + \tfrac{5}{6}C^6
\end{aligned} \tag{4a}$$

$$\begin{aligned}
f &= C^2, \qquad f_{AB} = -\tfrac{4}{3}C^3 + 3C^4 + \tfrac{4}{5}C^5 - \tfrac{5}{3}C^6,\\
f_{AA} &= -\tfrac{4}{3}C^3 + \tfrac{9}{4}C^4 - \tfrac{8}{5}C^5 + \tfrac{5}{6}C^6
\end{aligned} \tag{4b}$$

In the framework of the CFM the connection between the bulk and the surface properties has been established through the grand partition functions [22,25] providing a relation between bulk and surface compositions in terms of the surface tension, as [28]:

$$\sigma = \sigma_A + \frac{k_BT}{\alpha}\ln\frac{C^s}{C} + \frac{W}{\alpha}[p(f^s - f) - qf] + \sum_{i,j=A,B}\frac{\Delta W_{ij}}{\alpha}[p(f_{ij}^s - f_{ij}) - qf_{ij}] \tag{5a}$$

$$\sigma = \sigma_B + \frac{k_BT}{\alpha}\ln\frac{1-C^s}{1-C} + \frac{W}{\alpha}[p(\phi^s - \phi) - q\phi] + \sum_{i,j=A,B}\frac{\Delta W_{ij}}{\alpha}[p(\phi_{ij}^s - \phi_{ij}) - q\phi_{ij}] \tag{5b}$$

where σ_A and σ_B are the surface tensions of the components A and B, respectively. As in the case of G_M^{xs} (Eq. (1)), the expression for surface tension derived by the CFM formalism includes the concentration functions defined in (4a) and (4b). The functions ϕ_{ij}^s and f_{ij}^s can be calculated by Eqs. (4a) and (4b) substituting the bulk concentration C by the surface concentration C^s. p and q are the surface coordination fractions; for closed-packed structure the values of these parameters usually are taken as 1/2 and 1/4, respectively [25]. α is the mean surface area of the alloy, calculated by:

$$\alpha = \sum_i C_i\alpha_i \tag{6}$$

with the surface area of each atomic species, α_i, expressed in terms of the atomic volume V_i [14].

$$\alpha_i = 1.102N^{-2/3}V_i^{2/3} \tag{7}$$

The mixing behaviour of liquid binary alloys in which the formation of "complexes" does not take place can also be described by the Quasi Lattice Theory (QLT) [25]. The activity coefficients can be easily obtained by using the Fowler–Guggenheim method [29] and the surface tension for regular alloys can be expressed as:

$$\sigma = \sigma_A + \frac{k_B T(2-pZ)}{2\alpha}\ln\frac{C^s}{C} + \frac{Zk_B T}{2\alpha}\left[p\ln\frac{(\beta^s-1+2C^s)(1+\beta)}{(\beta-1+2C)(1+\beta^s)} - q\ln\frac{\beta-1+2C}{(1+\beta)C}\right] \tag{8a}$$

$$\sigma = \sigma_B + \frac{k_B T(2-pZ)}{2\alpha}\ln\frac{1-C^s}{1-C}\frac{Zk_B T}{2\alpha} \times \left[p\ln\frac{(\beta^s+1-2C^s)(1+\beta)}{(\beta+1-2C)(1+\beta^s)} - q\ln\frac{\beta+1-2C}{(1+\beta)(1-C)}\right] \tag{8b}$$

where the auxiliary variable β is defined by the order energy term, W.

$$\beta = \left[4C(1-C)\exp\left(\frac{2W}{Zk_B T}\right) + (1-2C)^2\right]^{1/2} \tag{9}$$

β^s is the function obtained from Eq. (9) by substituting the bulk concentration C by the surface concentration C^s.

2.2. Microscopic functions

The concentration–concentration structure factor in the long wavelength limit, $S_{cc}(0)$, is an important microscopic function [19] in describing the nature of mixing of liquid alloys such as chemical order and segregation. Once the Gibbs energy of mixing of the liquid phase, G_M, is known, $S_{cc}(0)$ can be expressed by G_M, or in terms of the activities, a_A and a_B, as:

$$S_{cc}(0) = RT\left(\frac{\partial^2 G_M}{\partial C_A^2}\right)^{-1}_{T,P,N} = C_B a_A\left(\frac{\partial a_A}{\partial C_A}\right)^{-1}_{T,P,N} = C_A a_B\left(\frac{\partial a_B}{\partial C_B}\right)^{-1}_{T,P,N} \tag{10}$$

With $\mu = 3$ and $\nu = 1$, Eqs. (3a), (3b), (4a), (4b) and (10) give S_{cc} in the form:

$$S_{cc}(0) = \frac{(1-C)a_A}{\exp((W\phi + \Delta W_{AB}\phi_{AB} + \Delta W_{AA}\phi_{AA})/(k_B T))\left[1 + ((C)/(k_B T))(W\phi' + \Delta W_{AB}\phi'_{AB} + \Delta W_{AA}\phi'_{AA})\right]} = \frac{Ca_B}{\exp((Wf + \Delta W_{AB}f_{AB} + \Delta W_{AA}f_{AA})/(k_B T))\left[1 - ((1-C)/(k_B T))(Wf' + \Delta W_{AB}f'_{AB} + \Delta W_{AA}f'_{AA})\right]} \tag{11}$$

where ϕ', f', ϕ'_{ij} and f'_{ij} (i, j = A, B) are the first derivatives of the functions defined in (4a) and (4b) with respect to C ($=C_A$).For ideal mixing the energy parameters W and ΔW_{ij} become zero, and Eq. (11) reduces to:

$$S_{cc}(0, \text{id}) = C(1-C) \tag{12}$$

Owing to difficulties in diffraction experiments, the theoretical determination of $S_{cc}(0)$ is of great importance when the nature of atomic interactions in the melt has to be analysed. The mixing behaviour of liquid binary alloys can be deduced from the deviation of $S_{cc}(0)$ from the ideal value $S_{cc}(0, \text{id})$. The presence of chemical order is indicated when $S_{cc}(0) < S_{cc}(0, \text{id})$, on the contrary, if $S_{cc}(0) > S_{cc}(0, \text{id})$, the segregation and demixing in liquid alloys take place. In order to quantify the degree of order and segregation in the melt, another important microscopic function, known as Warren–Cowley short-range order parameter, α_1 [30,31] is used. α_1 is related to $S_{cc}(0)$ by:

$$\frac{S_{cc}(0)}{C(1-C)} = \frac{1+\alpha_1}{1-(Z-1)\alpha_1} \tag{13}$$

For equiatomic composition, the chemical short-range order (CSRO) parameter is found to be $-1 \le \alpha_1 \le 1$. The negative values of this parameter indicate ordering in the melt which is complete if $\alpha_1 = -1$. On the contrary, the positive values of α_1 indicate segregation, leading to complete phase separation if $\alpha_1 = 1$.

2.3. Diffusion

The mixing behaviour of two alloy forming molten metals can be analysed at the microscopic scale in terms of diffusion and viscosity. The formalism that relates diffusion and $S_{cc}(0)$ combines the Darken's thermodynamic equation for diffusion with the basic thermodynamic equations in the form [32]:

$$\frac{D_m}{D_{id}} = \frac{S_{CC}(0, \text{id})}{S_{CC}(0)} \tag{14}$$

where D_{id} is the intrinsic diffusion coefficient for an ideal mixture and D_m is the mutual diffusion coefficient, given as:

$$D_m = CD_B + (1-C)D_A \tag{15}$$

with D_A and D_B being the self-diffusion coefficients of pure components A and B, respectively. According to Eq. (14) $S_{cc}(0) < S_{cc}(0, \text{id})$ typical of compound forming alloys implies $D_m > D_{id}$. A peak on the diffusivity curve, D_m/D_{id} versus C suggests the presence of maximum chemical order in molten alloy system as well as the composition of the most probable associates formed in the liquid phase [21]. The relationship between $S_{cc}(0)$ and the diffusivity expressed by the ratio of the mutual and self-diffusion coefficients, D_m/D_{id}, indicates the mixing behaviour of alloys, i.e. the tendency to compound formation or phase separation for $D_m/D_{id} > 1$ and $D_m/D_{id} < 1$, respectively.

3. Results and discussion

In order to understand the mixing behaviour of the liquid Ni–Ti system, the phase diagram [13] and various thermodynamic functions have been analysed [6–9]. The Ni–Ti phase diagram indicates the presence of three intermetallic phases in the solid state [10–12]. The optimised data set related to the excess Gibbs energy of mixing, $G_{\rm M}^{\rm xs}$ of liquid Ni–Ti phase [12] together with experimental data on the activity [9] and the enthalpy of mixing [6–8] are taken as input data for the calculations of order energy parameters. A normalised form of the Gibbs free energy of mixing of liquid Ni–Ti alloys, expressed as $G_{\rm M}/RT$ is shown in Fig. 1. The experimental data [9] and the theoretical results [12] calculated at $T = 1873$ K exhibit minima of about −1.901 and −2.149, at $C_{\rm Ti} = 0.4$ and 0.43, respectively, indicating that the tendency of compound formation in the Ni–Ti liquid phase is not strong. The same can be concluded from the activity data [9] (Fig. 1). The enthalpy of mixing measured at different temperatures ranging from 1740 to 2000 K [6–8] exhibits the same asymmetry (Fig. 2). The displacement of the expected compositional location of the $\rm Ni_3Ti$ from $C_{\rm Ti} = 0.25$ to 0.4 can probably be attributed to the simultaneous formation of a compound of stoichiometry NiTi, as it was observed in the case of Au–Sn liquid alloys [33]. Unfortunately, in the present formulation of the CFM the effects of the second intermetallic can not be taken into account. The computed values of the order energy parameters in units of $k_{\rm B}T$ at 1873 K are $W = -2.54$, $W_{\rm AB} = -6.25$, $W_{\rm AA} = 1.06$ and $W_{\rm BB} = 0.0$, while at 1973 K they are $W = -2.43$, $W_{\rm AB} = -5.48$, $W_{\rm AA} = 0.93$ and $W_{\rm BB} = 0.0$. In all calculations the coordination number, Z, in the liquid phase was taken as 10 [25,26].

3.1. Surface properties: surface tension and surface segregation

Regular alloys usually mean symmetry of their mixing properties and microscopic functions around the equiatomic composition as well as a similar size of their constituent atoms. On the contrary, in the case of the compound forming alloys and in particular in strongly interacting systems, a pronounced asymmetry of all properties over the concentration range takes place, even when the constituent species do not differ greatly in size. The QCA for regular solution describes correctly the mixing behaviour of regular alloys, while it can be applied to the compound forming alloys only as the first approximation. The CFM reproduces fairly well the thermodynamic and the thermophysical quantities as well as the microscopic functions of that class of liquid alloys. The effect of short range order on their surface properties was usually estimated from the difference in the corresponding property obtained by the two models [33]. In this paper, the surface properties of liquid Ni–Ti alloys at 1873 K were considered in the framework of CFM and QCA. The surface segregation calculated by the CFM is obtained by Eqs. (5a) and (5b), while in the case of the QCA for the regular solution the same is obtained by Eqs. (8a) and (8b). The calculated values suggest the segregation of Ti for concentrations of $C_{\rm Ti} > 0.32$ (Fig. 3). At variance with the “normal” behaviour, up to $C_{\rm Ti} < 0.32$ (Ni-rich alloys), the results obtained by both models indicate the segregation of Ni. The presence of associates or clusters in the liquid phase as represented by the CFM slightly decreases the segregation of Ti and increases that of Ni, the maximum difference being found at compositions that correspond to the NiTi and the $\rm Ni_3Ti$ intermetallic compound, respectively.

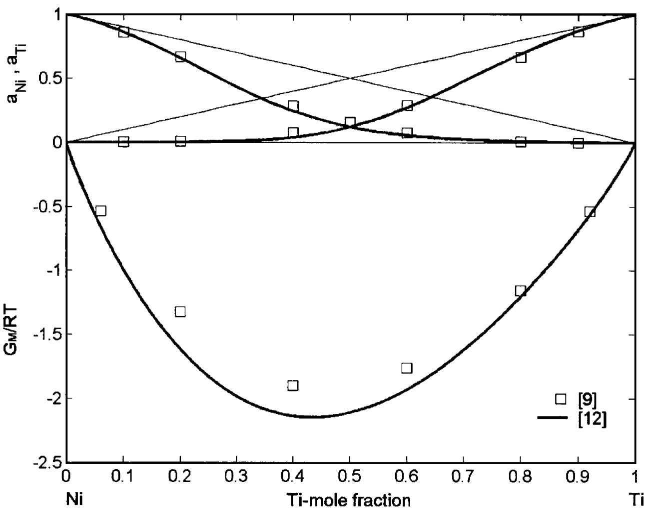

Fig. 1. Concentration dependence of Gibbs free energy of mixing ($G_{\rm M}/RT$) and activity coefficients ($a_{\rm Ni}$ and $a_{\rm Ti}$) of liquid Ni–Ti alloys at 1873 K. (—) Calculated [12] and (□) experimental [9].

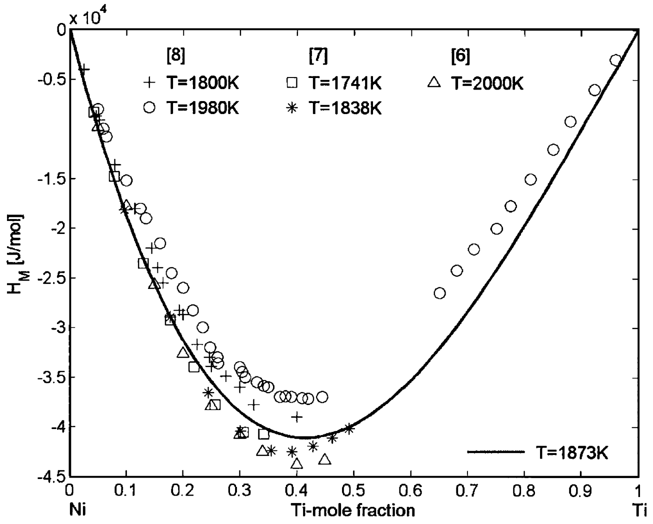

Fig. 2. Concentration dependence of enthalpy of mixing ($H_{\rm M}/RT$) in liquid Ni–Ti alloys calculated at 1873 K (—) together with the experimental data (+, ○) [8], (□, *) [7] and (Δ) [6].

Numerous theoretical and experimental literature data on binary liquid alloys show that the component having lower surface tension value always segregates. An exception is represented by the theoretical study on Cu–Ni liquid alloys, as reported by Prasad and Singh [34] and experimentally confirmed by Sakurai et al. [35]. These authors reported the “unexpected” segregation of Ni in the Cu-rich part of the system. Up to now, the exact mechanism of this inversion is not yet established. According to [35], one possible mechanism of the observed

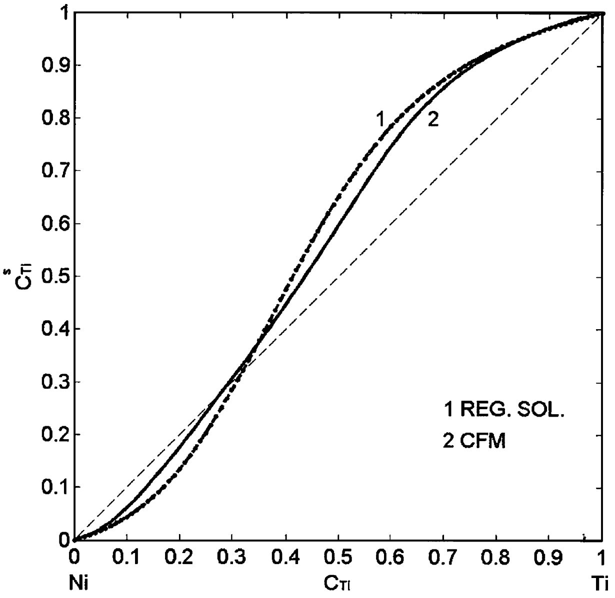

Fig. 3. Surface composition (C^{s}_{Ti}) vs. bulk composition (C_{Ti}) in liquid Ni–Ti alloys calculated by the QCA (curve 1) and by the CFM (curve 2) at 1873 K.

crossover is the increase of the regular solution parameter at the surface due to bond relaxation that may lead to phase separation in the surface layer. A similar explanation was given by Prasad and Singh [34], underlying the possibility that the order energy parameters of the bulk could be different (less negative) from that in the surface phase. For the sake of simplicity, in the framework of the CFM both interaction energies are taken as invariants of the system, and for almost all binary alloys this approach can be successfully applied. To reveal the exact mechanisms of this inversion phenomenon further investigations are needed.

Surface tension data on pure Ni [36] and Ti [37] were taken from the literature. For liquid Ti, surface tension data [37] are extrapolated from the Ti-melting point to 1873 K. Once the surface composition, C^{s}_{i}, is known, the surface tension of binary liquid alloys can be calculated by inserting these values into one of the equations, Eqs. (5a) and (5b) or Eqs. (8a) and (8b), for compound forming alloys or for regular alloys, respectively. The clustering effects on the surface tension and surface segregation are reciprocal, and thus the surface tension isotherm obtained by the CFM is higher than that calculated by the QCA (Fig. 4), in agreement with the previous considerations related to the segregation on the surface of Ni–Ti melts (Fig. 3).

The surface tension isotherms of the Ni–Ti system computed at 1873 K are shown in Fig. 4 together with some marginal experimental data reported by [4]. Both isotherms exhibit extremely high deviation from the ideal solution in the composition range between the two intermetallic compounds, NiTi and Ni_3Ti. As concerns the experimental surface tension data on liquid Ni–Ti alloys, there are only the data reported by Eremenko and Nizhenko [4]. These authors measured the surface tension of Ni-rich alloys containing up to 2.59 at.% Ti at 1823 K (Fig. 4). Due to the high reactivity of Ti in the presence of even small amount of oxygen they had great experimental difficulties, and after experiments their samples were covered by a quite visible film of oxide [4]. Accordingly, these experimental data can not be considered as reliable, and it was impossible to make a comparison with our theoretical results.

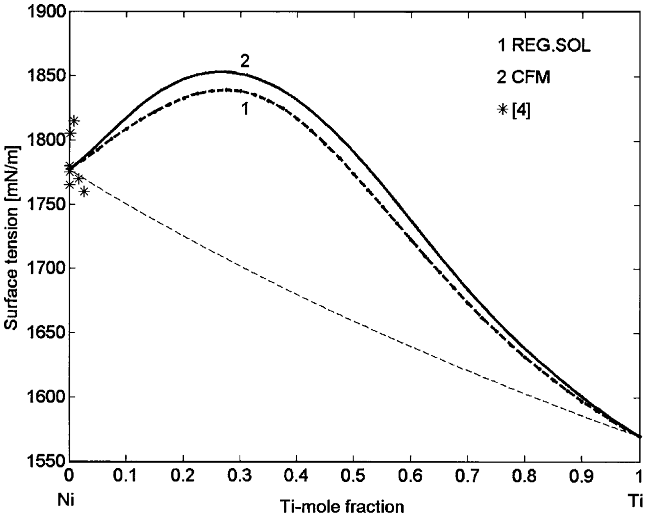

Fig. 4. Surface tension of liquid Ni–Ti alloys calculated at 1873 K (1, the QCA; 2, the CFM; - - -, the ideal solution model), (*) experimental data measured at 1823 K [4].

3.2. Microscopic functions: concentration fluctuations in the long-wavelength limit and chemical short-range order parameter

The ordering phenomena in the Ni–Ti system have been analysed by concentration fluctuations in the long-wavelength limit, $S_{cc}(0)$, and the CSRO parameter, α_1, as functions of the bulk compositions. $S_{cc}(0)$ was calculated by Eq. (11). Its deviation from the ideal values, $S_{cc}(0, \text{id})$ is used as an indicator to determine the mixing tendency in binary alloys expressed in terms of ordering or segregation. The variation of $S_{cc}(0)$ with composition shown in Fig. 5 clearly indicates a tendency of

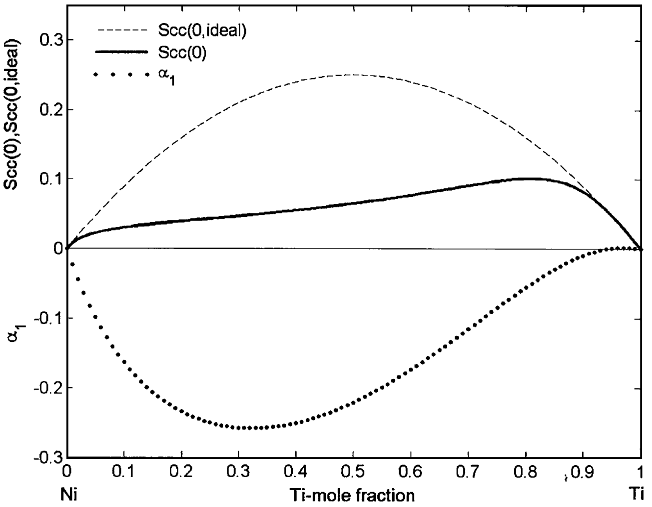

Fig. 5. Concentration fluctuations in the long-wavelength limit ($S_{CC}(0)$, $S_{CC}(0, \text{id})$) and chemical short-range order parameter (α_1) vs. bulk composition (C_{Ti}) in liquid Ni–Ti alloys calculated at 1873 K.

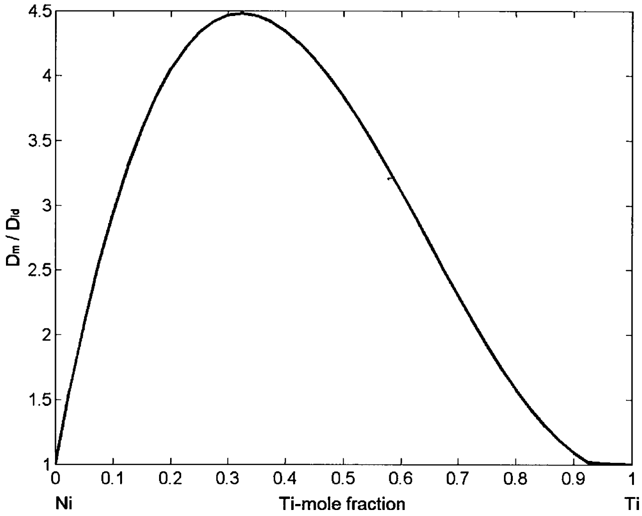

Fig. 6. Diffusivity (D_m/D_{id}) in liquid Ni–Ti alloys vs. bulk composition (C_{Ti}) at 1873 K.

heterocoordination, i.e. a preference of unlike atoms as nearest neighbours over the concentration range. The maximum deviation $|S_{cc}(0)–S_{cc}(0, id)|$ can be used as an indicator of the possible stoichiometric composition of the chemical clusters in the liquid phase [16,21]. Applying this criterion, the maximum compound forming tendency appears in the composition range between Ni_3Ti and NiTi.

The negative values of α_1 substantiate that this alloy system belongs to the compound forming alloy group. The position of their maximum values reproduces fairly well the most probable cluster stoichiometry of Ni_3Ti (Fig. 5).

3.3. *Diffusivity*

The calculated diffusivity for liquid Ni–Ti alloys yield values of $D_m/D_{id} > 1$ over the whole concentration range indicating a compound forming tendency. The calculations reproduce fairly well the maximum compound forming tendency with $D_m/D_{id} \approx 4.5$ at $C_{Ti} \approx 0.32$, which is slightly shifted from the composition Ni_3Ti (Fig. 6).

4. Conclusions

The QCA and the CFM have been used to study the thermodynamic and the thermophysical properties of liquid Ni–Ti alloys, namely surface tension and diffusivity. Surface properties of Ni–Ti liquid alloys were predicted by the CFM and QCA indicating the segregation of Ti for $C_{Ti} > 0.32$, while Ni-segregation was observed for Ni-rich alloys. Although a similar segregation behaviour was observed in the case of Cu–Ni liquid alloys, up to now an adequate theoretical description is not available. The thermodynamic properties of liquid Ni–Ti alloys exhibit negative deviations from Raoult's law and, as expected, the calculated surface tension isotherms deviate positively. Thermodynamic, surface and transport properties together with the microscopic functions (concentration fluctuations in the long-wavelength limit and chemical short range order parameter) indicate a compound forming tendency in this system. The lack of the data on thermophysical properties makes it impossible to compare the obtained theoretical results.

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