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Statistical-thermodynamic description of the order–disorder transformation of $D0_{19}$-type phase in Ti–Al alloy

T.M. Radchenko [a,*], V.A. Tatarenko [a], H. Zapolsky [b], D. Blavette [b]

[a] *Department of Solid State Theory, Institute for Metal Physics, N.A.S. of Ukraine, 36 Acad. Vernadsky Blvd., 03680 Kyiv-142, Ukraine*
[b] *UMR 6634, CNRS, Faculte des Sciences et Techniques, Université de Rouen, 76801 Saint-Etienne du Rouvray Cedex, France*

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Abstract

Within the framework of the self-consistent field approximation and the static concentration waves approach, a statistical-thermodynamic description of $D0_{19}$-type superstructure in Ti–Al alloy is developed. A model of order–disorder phase transformation is applied for the non-stoichiometric intermetallic Ti_3Al phase. Interatomic-interaction parameters are estimated for both approximations. One model supposes temperature-independent interatomic-interaction parameters, while the other includes the temperature dependence of mixing energies. The partial phase diagrams (equilibrium compositions for the coexistent ordered α_2-phase and disordered α-phase) are evaluated for both cases.

Keywords: Intermetallics; Phase diagrams; Order–disorder phase transitions

1. Introduction

Over the past few years, intermetallic compounds based on Ti and Al have been the subject of research due to their potential for applications in the aerospace and automobile industries [1–4]. Due to their corrosion stability and strength, these intermetallic alloys attracted particular attention as suitable materials for high-temperature applications.

The structure of α_2-Ti_3Al phase is related to the $D0_{19}$-type superstructure [5–15], which can be derived from the hexagonal closed-packed (h.c.p.) solid solution (α-Ti–Al) by a diffusion controlled ordering of Ti and Al atoms. The first step in understanding the microstructure and the diffusion kinetics of the Ti–Al relaxation is the construction of a statistical-thermodynamic model and the estimation of the interatomic-interaction energy parameters of this system for arbitrary interatomic distances (i.e. outside the framework of the conventional Bragg–Williams approximation). In spite of some efforts [16], which have been made to describe the atomic-ordering reaction in Ti_3Al ($\alpha \rightarrow \alpha_2$), the statistical-thermodynamic description for non-stoichiometric h.c.p. phase has not been attempted. Only few experimental results and theoretical descriptions have been obtained [9,17–19] to describe the site occupation in Ti–Al alloys. Investigating symmetry of interchange energies, distribution functions for substitutional superstructures in h.c.p. lattices have been obtained in Ref. [20], but long-range order (LRO) parameters have not been calculated. The distribution functions for atoms in the $D0_{19}$-type superstructure given in [6,21,22] and the image of $D0_{19}$-type superstructure reported by [23] are wrong, in spite of the fact that coordinates of the atoms are correctly [23] indicated.

The present paper is devoted to the theoretical description of the phase transformation of the ordered intermetallic α_2-phase into the disordered α-phase and to the calculation of the interatomic-interaction parameters. The model is based on the self-consistent field (mean-field) approximation and the static concentration wave approach firstly proposed by Khachaturyan [24].

2. Statistical-thermodynamic model

The hexagonal closed-packed lattice is a complicated Ising lattice, which can be considered as two interpenetrating hexagonal Bravais sublattices displaced with respect to each other by the vector $\mathbf{h} = 2\mathbf{a}_1/3 + \mathbf{a}_2/3 + \mathbf{a}_3/2$, where $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are the unit vectors of the h.c.p. lattice along the [1 0 0], [0 1 0], [0 0 1]

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[*] Corresponding author. Tel.: +380 44 424 12 21; fax: +380 44 424 25 61.
E-mail address: taras.radchenko@gmail.com (T.M. Radchenko).

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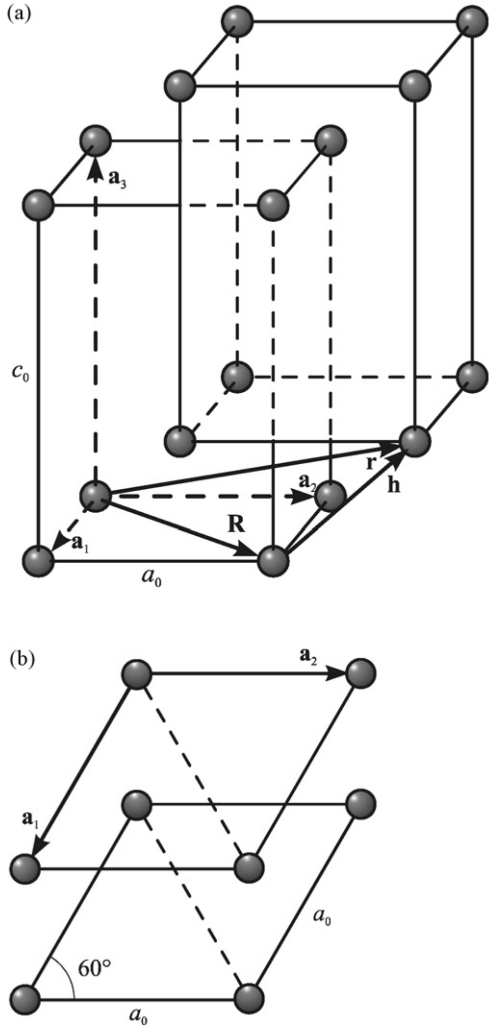

Fig. 1. Hexagonal close-packed lattice: perspective view (a) and top view (b).

directions, in the oblique system of coordinates (see Fig. 1). Each crystal lattice site $\mathbf{r}$ can be described by two vectors $\mathbf{R}$ and $\mathbf{h}_p$ ($\mathbf{r} = \mathbf{R} + \mathbf{h}_p$) [24]. Vector $\mathbf{R}$ refers to the unit-cell's origin position, $\mathbf{h}_p$ denotes the distance of a given site with respect to the unit-cell's origin, and p denotes the sublattice.

In the self-consistent field model, the configurational part of the free energy of the h.c.p. binary A–B alloy based on the complicated Ising lattice can be written as [24]:

$$F = \frac{1}{2}\sum_{p,q=1}^{2}\sum_{\mathbf{R},\mathbf{R}'} w_{pq}(\mathbf{R}-\mathbf{R}')P_p(\mathbf{R})P_q(\mathbf{R}') + k_{\mathrm{B}}T\sum_{q=1}^{2}\sum_{\mathbf{R}}[P_q(\mathbf{R})\ln P_q(\mathbf{R}) + (1-P_q(\mathbf{R}))\ln(1-P_q(\mathbf{R}))], \qquad (1)$$

where the indexes p and q denote the sublattices (p, $q = 1$, 2). k_{B} is the Boltzmann constant and T is the absolute temperature. The single-site occupation-probability functions $P_p(\mathbf{R})$ ($P_q(\mathbf{R})$) represent the probability of finding a B atom at the site of the pth (qth) sublattice within the cell with the origin $\mathbf{R}$. In the last equation, the summation is carried out over all unit-cells ($\mathbf{R}$, $\mathbf{R}'$) and all sublattices, i.e. over all Ising lattice sites. For a binary solid solution, $w_{pq}(\mathbf{R}-\mathbf{R}')$ defines the interchange energy [24], which known also as mixing energy:

$$w_{pq}(\mathbf{R}-\mathbf{R}') = W_{pq}^{AA}(\mathbf{R}-\mathbf{R}') + W_{pq}^{BB}(\mathbf{R}-\mathbf{R}') - 2W_{pq}^{AB}(\mathbf{R}-\mathbf{R}'). \qquad (2)$$

Here, W_{pq}^{AA}, W_{pq}^{BB}, W_{pq}^{AB} are the pairwise interaction energies of A–A, B–B, A–B pairs of atoms of the unit-cells separated by a distance $|\mathbf{R}-\mathbf{R}'|$. The radius-vector $\mathbf{R}$ is related to the basic vectors as $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ with $|\mathbf{a}_1| = |\mathbf{a}_2| = a_0$ and $|\mathbf{a}_3| = c_0$. n_1, n_2, n_3 are the integer 'coordinates' of the unit-cell positions in the oblique system of coordinates of the h.c.p. lattice (see Figs. 1 and 2). Experimental values of the Ti_3Al lattice parameters are $a_0 = 0.289$ nm and $c_0 = 0.464$ nm [7], therefore the radii of the first four coordination shells are as follows: $r_1 = 0.286$ nm, $r_2 = 0.289$ nm, $r_3 = 0.406$ nm and $r_4 = 0.464$ nm (Fig. 2).

For the h.c.p. lattice, interchange-energy matrix is [5,6,20,24]:

$$\left\|\tilde{w}_{pq}(\mathbf{k})\right\| = \begin{pmatrix} \tilde{w}_{11}(\mathbf{k}) & \tilde{w}_{12}(\mathbf{k}) \\ \tilde{w}_{12}^{*}(\mathbf{k}) & \tilde{w}_{11}(\mathbf{k}) \end{pmatrix},$$

where

$$\tilde{w}_{pq}(\mathbf{k}) = \sum_{\mathbf{R}} w_{pq}(\mathbf{R}-\mathbf{R}')\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}, \qquad (3)$$

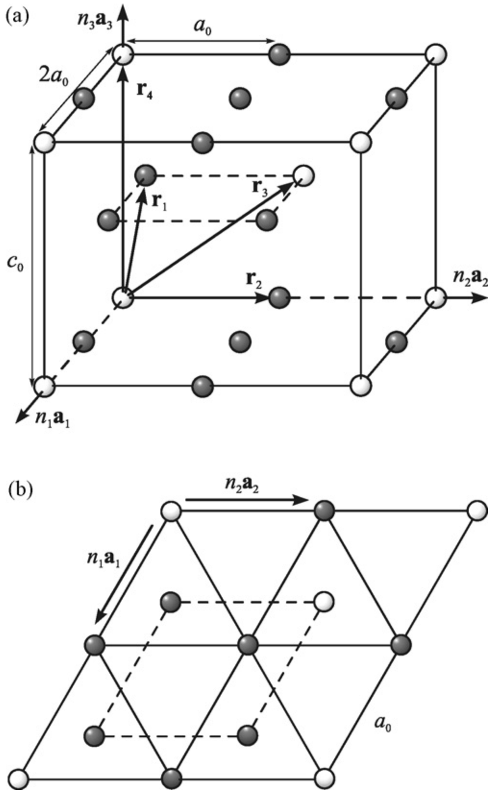

Fig. 2. Unit-cell of $D0_{19}$-type Ti_3Al superstructure: perspective view (a) and top view (b). White balls are Al atoms and dark balls are Ti atoms.

$\mathbf{k}=(k_1, k_2, k_3)$ is a wave vector, $\tilde{w}^*_{12}(\mathbf{k})$ is the complex conjugate to $\tilde{w}_{12}(\mathbf{k})$. The $D0_{19}$-type superstructure (Fig. 2) is generated by the superlattice wave vectors [5,6,20,24] $\mathbf{k}_1 = \pi\mathbf{a}^*_1 = (\frac{1}{2}, 0, 0)$, $\mathbf{k}_2 = \pi\mathbf{a}^*_2 = (0, \frac{1}{2}, 0)$, $\mathbf{k}_3 = \pi(\mathbf{a}^*_1 + \mathbf{a}^*_2) = (\frac{1}{2}, \frac{1}{2}, 0)$; $\mathbf{a}^*_1$ and $\mathbf{a}^*_2$ are the basic reciprocal lattice vectors of the h.c.p. lattice along the directions [1 0 0] and [0 1 0], respectively. The interchange-energy matrix has two eigenvalues:

$$\lambda_1(\mathbf{k}) = \tilde{w}_{11}(\mathbf{k}) + |\tilde{w}_{12}(\mathbf{k})|, \qquad \lambda_2(\mathbf{k}) = \tilde{w}_{11}(\mathbf{k}) - |\tilde{w}_{12}(\mathbf{k})|. \tag{4}$$

Using definition (3), one can obtain expressions for the elements of the interchange-energy matrix (3):

$$\begin{aligned}\tilde{w}_{11}(\mathbf{k}) = {}& w_2(\mathrm{e}^{2\pi \mathrm{i}k_1} + \mathrm{e}^{2\pi \mathrm{i}k_2} + \mathrm{e}^{-2\pi \mathrm{i}k_1} + \mathrm{e}^{-2\pi \mathrm{i}k_2} + \mathrm{e}^{2\pi \mathrm{i}(k_1+k_2)} \\ &+ \mathrm{e}^{-2\pi \mathrm{i}(k_1+k_2)}) + w_4(\mathrm{e}^{2\pi \mathrm{i}k_3} + \mathrm{e}^{-2\pi \mathrm{i}k_3}) + \cdots,\end{aligned} \tag{5}$$

$$\begin{aligned}\tilde{w}_{12}(\mathbf{k}) = {}& w_1(1 + \mathrm{e}^{-2\pi \mathrm{i}k_3} + \mathrm{e}^{-2\pi \mathrm{i}k_1} + \mathrm{e}^{-2\pi \mathrm{i}(k_1+k_3)} \\ &+ \mathrm{e}^{-2\pi \mathrm{i}(k_1+k_2)} + \mathrm{e}^{-2\pi \mathrm{i}(k_1+k_2+k_3)}) \\ &+ w_3(\mathrm{e}^{2\pi \mathrm{i}k_2} + \mathrm{e}^{2\pi \mathrm{i}(k_2-k_3)} + \mathrm{e}^{-2\pi \mathrm{i}k_2} + \mathrm{e}^{-2\pi \mathrm{i}(k_2+k_3)} \\ &+ \mathrm{e}^{-2\pi \mathrm{i}(2k_1+k_2)} + \mathrm{e}^{-2\pi \mathrm{i}(2k_1+k_2+k_3)}) + \cdots\end{aligned} \tag{6}$$

Here, w_1, w_2, w_3, w_4 are the interchange energies for the 1st, 2nd, 3rd, 4th coordination shell with the radii r_1, r_2, r_3, r_4 shown in Fig. 2.

Within the framework of the static concentration waves approach [24], the atoms' distribution function, $P_q(\mathbf{R})$, can be represented as a superposition of static concentration waves (as Fourier series):

$$\begin{aligned}P_q(\mathbf{R}) = c + \frac{1}{2}\sum_{s}\sum_{\sigma=1}^{2}\eta_{s,\sigma}\sum_{j_s}(\gamma_{s,\sigma}(j_s)v_\sigma(q, \mathbf{k}_{j_s})\,\mathrm{e}^{\mathrm{i}\mathbf{k}_{j_s}\cdot\mathbf{R}} \\ + \gamma^*_{s,\sigma}(j_s)v^*_\sigma(q, \mathbf{k}_{j_s})\,\mathrm{e}^{-\mathrm{i}\mathbf{k}_{j_s}\cdot\mathbf{R}}),\end{aligned} \tag{7}$$

where c is a relative concentration of B atoms in the $A_{1-c}B_c$ alloy and $v_\sigma(q, \mathbf{k})\exp(\mathrm{i}\mathbf{k}_{js}\cdot\mathbf{R})$ is a static concentration wave. In formula (7), $v_\sigma(q, \mathbf{k})$ is a unit 'polarization vector' of the wave, $\mathbf{k}_{js}$ is a wave vector, σ is a 'polarization number'. The variable $\eta_{s,\sigma}$ represents the LRO parameter, which is equal to 0 and 1 in the disordered and completely ordered states, respectively. The coefficients $\gamma_{s,\sigma}(j_s)$ determine the symmetry of the occupation probabilities $P_q(\mathbf{R})$, j_s denotes the wave vectors in the first Brillouin zone of the star s. The star s is a set of wave vectors $\mathbf{k}_{js}$, which can be obtained from the one wave vector by the applying to it all operations of the symmetry group of the disordered solid solution. In formula (7), the summation is carried out over all vectors $\{j_s\}$ of the star s. We can describe the atomic distribution in the binary alloy by the one distribution function because of $P^A_q(\mathbf{R}) + P^B_q(\mathbf{R}) \equiv 1$.

Applying the static concentration wave method for the $D0_{19}$-type superstructure, we obtain

$$\begin{aligned}\begin{pmatrix} P_1(\mathbf{R}) \\ P_2(\mathbf{R}) \end{pmatrix} = c\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{4}\eta\Bigg[&\xi_1\begin{pmatrix} 1 \\ 1 \end{pmatrix}\cos(\pi n_1) \\ &+ \xi_2\begin{pmatrix} 1 \\ -1 \end{pmatrix}\cos(\pi n_2) \\ &+ \xi_3\begin{pmatrix} 1 \\ -1 \end{pmatrix}\cos[\pi(n_1+n_2)]\Bigg],\end{aligned} \tag{8}$$

where $\xi_1 = \xi_2 = \xi_3 = 1$, $\xi_1 = -\xi_2 = -\xi_3 = 1$, $-\xi_1 = \xi_2 = -\xi_3 = 1$ or $-\xi_1 = -\xi_2 = \xi_3 = 1$. The function (8) assumes two values, $c - \eta/4$ and $c + 3\eta/4$, on all crystal lattice sites. Substituting expression (8) into the formula (1), we have the configurational free energy of $D0_{19}$-type ordered phase per atom as a function of temperature, concentration and the LRO parameter:

$$\begin{aligned}F_{\mathrm{ord}} = {}& \frac{c^2\lambda_1(\mathbf{0})}{2} + \frac{3\eta^2\lambda_2(\mathbf{k}_1)}{32} + \frac{k_\mathrm{B}T}{4} \\ &\times\left[\left(c + \frac{3\eta}{4}\right)\ln\left(c + \frac{3\eta}{4}\right) + \left(1 - c - \frac{3\eta}{4}\right)\right. \\ &\times\ln\left(1 - c - \frac{3\eta}{4}\right) + 3\left(c - \frac{\eta}{4}\right)\ln\left(c - \frac{\eta}{4}\right) \\ &\left. + 3\left(1 - c + \frac{\eta}{4}\right)\ln\left(1 - c + \frac{\eta}{4}\right)\right].\end{aligned} \tag{9}$$

The configurational free energy (per atom) of the disordered phase ($\eta \equiv 0$) is

$$F_{\mathrm{disord}} = \frac{c^2\lambda_1(\mathbf{0})}{2} + k_\mathrm{B}T[c\ln c + (1 - c)\ln(1 - c)]. \tag{10}$$

To determine the equilibrium fields of the ordered (α_2) and disordered (α) phases, which is a part of the phase diagram of the system Ti–Al, we need to determine the interaction energy parameters, $\lambda_1(\mathbf{0})$ and $\lambda_2(\mathbf{k}_1)$, which enter into the free energy expressions. These energy values can be obtained from the radiation (X-ray or thermal neutrons) scattering data. However, these measurements apparently have not been done for Ti–Al alloys. Therefore, we chose the strategy of fitting energy parameters to experimental phase diagram [25].

3. Calculated results

According to the experimental phase diagram [25] there is a concentration–temperature range, where the equilibrium state of Ti–Al corresponds to an ordered intermetallic state (i.e. $D0_{19}$-type α_2-phase). By the decreasing the Al concentration or/and increasing the temperature, this ordered phase becomes unstable, and the disordered α-phase appears.

To calculate the equilibrium LRO parameter, we have to minimise the configurational free energy, F, with respect to the η. For $c = 1/4$, such a procedure performed at different temperatures gives branch A–B–C in Fig. 3. On the other hand, the equilibrium order parameter must satisfy the following condition for F being a minimum with respect to η:

$$\frac{\eta}{\tau} = \ln\frac{(c - \eta/4)(1 - c - 3\eta/4)}{(c + 3\eta/4)(1 - c + \eta/4)}, \tag{11}$$

where $\tau = k_\mathrm{B}T/|\lambda_2(\mathbf{k}_1)|$ is a reduced temperature. Eq. (11) has no simple analytic solution, but one can solve it numerically.

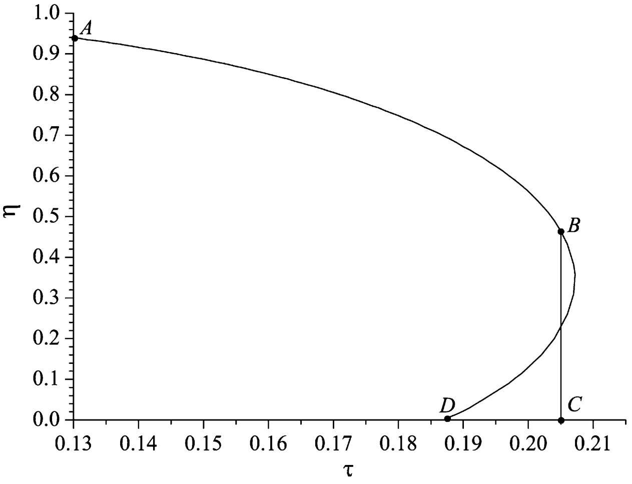

Fig. 3. Equilibrium long-range order parameter, η, vs. reduced temperature, τ, for the $D0_{19}$-type superstructure.

The solution, for a given c, has the form shown in Fig. 3 (branch A–B–D).

If we know the equilibrium LRO parameter, we can calculate configurational free energy as a function of temperature and concentration. The equilibrium compositions for the coexistence of the ordered intermetallic α_2-phase and disordered α-phase can be determined numerically by the common tangent construction. In this case, the values of $\lambda_1(\mathbf{0})$ and $\lambda_2(\mathbf{k}_1)$ in expressions (9) and (10) are the fitting parameters which have to be estimated. Using this procedure combined with the least-squares method, the phase relationships were computed for two assumptions (Fig. 4). The first approximation yields the temperature-independent eigenvalues of the interchange-energy matrix ($\lambda_1(\mathbf{0}) \approx 462.36$ meV/atom, $\lambda_2(\mathbf{k}_1) \approx -555.91$ meV/atom) relevant to the whole temperature range 600–1000 °C. The second gives temperature-dependent values ($\lambda_1(\mathbf{0}) = \lambda_1(\mathbf{0}, T)$, $\lambda_2(\mathbf{k}_1) = \lambda_2(\mathbf{k}_1, T)$). The temperature dependences of $\lambda_1(\mathbf{0}, T)$ and $\lambda_2(\mathbf{k}_1, T)$ are shown in Fig. 5.

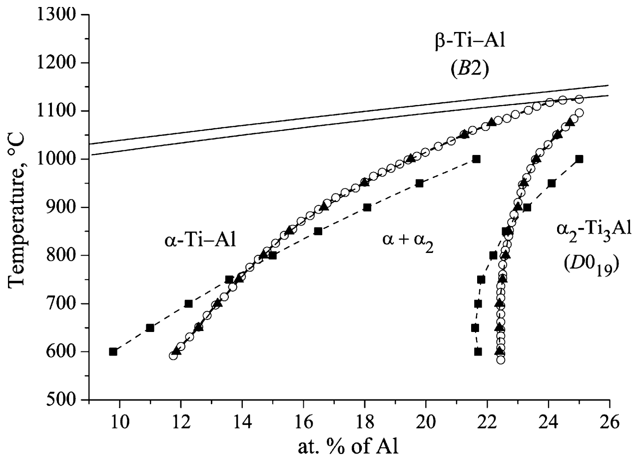

Fig. 4. Calculated and experimental phase diagrams of Ti–Al alloy: model with temperature-independent interatomic-interaction parameters (■), model with temperature-dependent ones (▲) and experiment (○) [25].

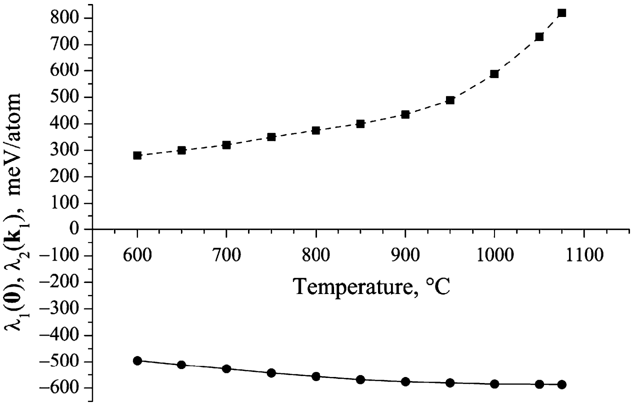

Fig. 5. Temperature dependence of interatomic-interaction parameters, $\lambda_1(\mathbf{0})$ (■) and $\lambda_2(\mathbf{k}_1)$ (●), for h.c.p. Ti–Al.

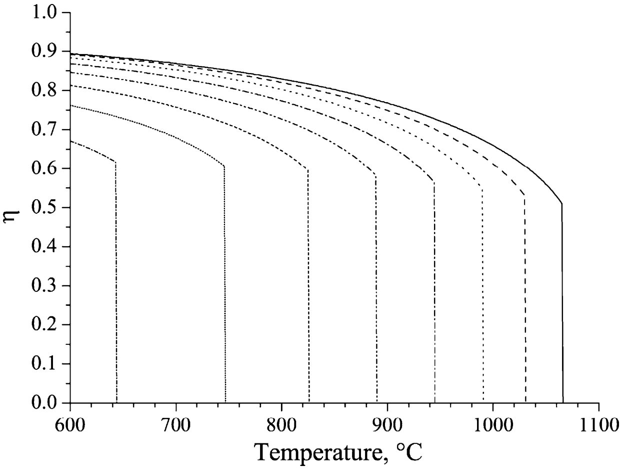

Fig. 6. Equilibrium long-range order parameter, η, vs. temperature in the non-stoichiometric $D0_{19}$-type phases with compositions $Ti_{0.84}Al_{0.16}$ (–·–), $Ti_{0.83}Al_{0.17}$ (···), $Ti_{0.82}Al_{0.18}$ (- - -), $Ti_{0.81}Al_{0.19}$ (–··–), $Ti_{0.80}Al_{0.20}$ (—·—), $Ti_{0.79}Al_{0.21}$ (· · ·), $Ti_{0.78}Al_{0.22}$ (– – –) and $Ti_{0.77}Al_{0.23}$ (—).

The calculations were not extended above $T = 1075$ °C, since at higher temperatures the Ti_3Al-type phase already coexists with the b.c.c. β-phase.

Using the $\lambda_2(\mathbf{k}_1)$ values the temperature dependence of LRO parameters in non-stoichiometric Ti_3Al was calculated (Fig. 6). Figs. 3 and 6 demonstrate that the order–disorder phase transformation of $D0_{19}$-type superstructures into the disordered α-Ti–Al solid solution is a first-order phase transition.

4. Summary and conclusions

The study deals with a semi-phenomenological description of the order–disorder phase transformation of ordered Ti_3Al into the h.c.p. solid solution. The atomic configurations of the ordered state are described by single-site occupation-probability functions which have been calculated for the $D0_{19}$-type superstructure. The description is also applied to the phase transformation to the α-Ti–Al solid solution using both the self-consistent field approximation and the method of static concentration waves.

By the computing the partial equilibrium Ti–Al phase diagram, interatomic-interaction parameters were evaluated. For the model with temperature-dependent interatomic-interaction parameters, the computed phase boundaries almost coincide with the experimental findings. For the model with temperature-independent interatomic-interaction parameters, there is a less agreement.

A change of lattice parameters, a_0 and c_0, with both temperature and composition results in the change of interatomic-interaction energies which implicitly dependent on T and c. In particular, the thermal expansion, the temperature dependence of elasticity, and the softening of oscillatory modes are responsible for the temperature dependence of $\lambda_1(\mathbf{0})$ and $\lambda_2(\mathbf{k}_1)$.

The order–disorder transformation of the intermetallic α_2-phase into the disordered α-phase is a first-order phase transition.

The findings eliminate the disagreement in the literature as regards the atomic distribution functions for the $D0_{19}$-type superstructure. This work is the first step of the investigation of kinetics relaxation of non-equilibrium h.c.p. Ti–Al alloys. The results obtained for the interatomic-interaction parameters will be used in the Önsager-type microscopic diffusion equations to study the kinetics of precipitation in the ordered intermetallic phases.

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