

# First-principles calculation of defects structure in b2 NiTi

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## Abstract

First-principles electronic structure calculations have been performed for defect structure in non-stoichiometric B2 NiTi. In order to determine the type of constitutional defects, the compositional dependence curves both of formation energies and of lattice parameters are obtained by the calculations employing super-cells in various sizes 16-atoms, 32-atoms and we have use the developed special quasi-random structures for random pseudo-binary  $A_{1-x}B_xC$  at compositions  $x = 0.25$  and  $0.5$ . According to our results, Ni anti-sites are the constitutional point defects in Ni-rich side B2 NiTi and Ti anti-sites present the minimum energy for the Ti-rich side so Ni an Ti anti-sites are the more stable defects of B2 NiTi. To investigate the thermal defect concentrations at finite temperatures, we adopted the Wagner-Schottky model using point defect formation enthalpies obtained from the SQS approaches. The present results suggest that the predominant thermal defects of NiTi are an exchange defects type. The calculated results show an agreement with the available theoretical and experimental data.

**Keywords:** constitutional defects; first principles calculations; SQS; super-cell.

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## 1. Introduction

The nitinol (NiTi) is widely used in the aeronautical, medical and seismological areas due to its shape memory effect [1-4]: the super-elasticity and the capacity to recover completely after large apparently plastic deformation (strains of the order 7-10% for NiTi-based alloys [5]). In the last few years, the scientific investigations for NiTi have been made extensively from the aspects of theory and experiment, including the structural properties [6-11], the phase stabilities [7,12-16], the elastic properties [13,17-20], the thermodynamics [14,21-23], the martensitic transformation path [12,13,15], etc. In order to design devices properly, basic researches on the fundamental physical properties are necessary. The thermodynamic properties, such as thermal equations of state (EOS), thermal expansivity, heat capacity and entropy under pressure and temperature can provide valuable information in understanding the phase diagram and dynamical response.

The central part of the NiTi phase diagrams is dominated by the high-melting B2 (CsCl-type) NiTi phase respectively [5, 6]. B2 structure have a large number of theoretical investigations in the electronic structure, the optical properties, the nature of inter-atomic interactions, and in the defects energies in the crystal structure performed within the last 20 years [7]. As it is well known, physical and mechanical properties are strongly affected by lattice defects, such as point defects and dislocations. Since the point defects are inherently introduced into alloy crystal at any temperatures and compositions, it is essential to explore these structures and behaviors in order to control the properties for practical applications [4, 6, 8, 9].

Over the past 20 years significant efforts have been devoted to developing computationally efficient approaches for calculating the properties of disordered alloy solid-solution phases within the predictive framework of electronic density-functional theory (DFT) (see, e.g., Ref. [24] and references there in). At present, the three most widely employed approaches for this purpose include: (i) the cluster expansion (CE) method [25-29], (ii) super-cells methods, including both conventional super-cells and special-quasirandom structures (SQS) [30-34], and (iii) approaches based on the coherent potential approximation (CPA) [35-37]. The latter two methods have found widespread application in calculations of the electronic structure of disordered alloys, and super-cells methods are also commonly employed to analyze local atomic structures and variations in bond lengths with chemical composition. A somewhat more demanding application of these first-principles-based methods involves calculation of the thermodynamic properties of solid solutions. For this purpose computational approaches must generally be capable of modeling effects on mixing energies and entropies resulting from varying degrees of configurational short-range-order (SRO) (i.e. correlations in the occupancies of neighboring atoms) and atomic displacements associated with elastic relaxations.

The goal of this paper is to determine the type of punctual defects in NiTi alloy, the compositional dependence curves of both formation energies and lattice parameters are obtained by the calculations employing super-cells in various sizes 16-atoms, 32-atoms and we have used the developed special quasi-random-structures for random pseudo-binary  $A_{1-x}B_xC$  at compositions  $x = 0.25$  and  $0.5$ . Our results have shown good agreement with theoretical investigations of T. Tokunaga et al. [13] and S.

Matsumoto et al. [14], also show a good rapprochement with the experimental results of O.J. Kleppa. [8] and C. Jia et al. [9]. To investigate the thermal defect concentrations at finite temperatures, we have adopted the Wagner-Schottky model using point defect formation enthalpies obtained from SQS approach. The calculated results show an agreement with the available theoretical and experimental data.

## 2. Computational Methodology

### 2.1. Super-cell (mean field)

The super-cell (MF) approach has been widely used in the literature to study defects in materials [36-29]. Such an approach is usually carried out by introducing one defect in a given super-cell to study the point defects in terms of first-principles calculations.

In this work, we have used two super-cells; a 16-atom  $2 \times 2 \times 2$  cubic B2 and a 32-atom one [37], each one contains one single point defect (Ni or Ti vacancy, Ni or Ti anti-site) per super-cell. In the 16-atom super-cell, the periodically arranged point defects form a simple cubic (SC) lattice with a lattice parameter of  $2\alpha$ , while the point defects in the 32-atom super-cell form a face centered cubic (FCC) lattice with a lattice parameter of  $4\alpha$ , where  $\alpha$  is the B2 lattice parameter.

The formation enthalpies of  $\Delta H(Ti_{1-x}Ni_x)$  alloys can be calculated from the following equation:

$$\Delta H(Ti_{1-x}Ni_x) = E(Ti_{1-x}Ni_x) - (1-x)E(Ti) - xE(Ni) \quad (1)$$

Where:

$E(Ti)$ ,  $E(Ni)$  and  $E(Ti_{1-x}Ni_x)$  : are the first-principles calculated total energies (per atom) of the constituent pure elements Ti or Ni and the corresponding alloy, respectively.

$x$  : is the molar composition of Ni in the alloy.

Simple Hexagonal (HCP-A3) Ti and Ni were used as reference states in equation (2).

The formation enthalpies of point defects in the super-cell approach are obtained by:

First we start from the equation of enthalpy [27]:

$$H = \lim_{N_{at} \rightarrow \infty} \frac{\Delta H}{N_{at}} \quad (2)$$

Where:

$\Delta H$  : The minimum enthalpy of the entire system.

$N_{at}$  : Number total of atoms.

In general case, it is more natural to use the atomic concentration, where the vacancy concentration can reach 10 at.%. So:

$$H_d = \lim_{N_{at} \rightarrow \infty} \frac{\Delta H}{N_{at}} = \frac{\partial \Delta H}{\partial n_d} = \frac{\partial \Delta H}{\partial x_d} \quad (3)$$

Second by means of finite differencing, as follows [27, 31, 32]:

$$H_d = \frac{\partial \Delta H}{\partial x_d} = \frac{\Delta H_d - \Delta H_{NiTi}}{x_d} \quad (4)$$

Where:

$\Delta H_d$ : is the formation enthalpy (per atom) of a 16-atom (32-atom) B2 NiTi super-cell containing one point defect of type d.

$\Delta H_{NiTi}$  : is the formation enthalpy of perfectly ordered B2 NiTi.

For 16-atom super-cells:  $\begin{cases} x_d = 1/16 \text{ for anti - sites.} \\ x_d = 1/15 \text{ for vacancies.} \end{cases}$

For the 32-atom super-cells:  $\begin{cases} x_d = 1/32 \text{ for anti - sites.} \\ x_d = 1/31 \text{ for vacancies.} \end{cases}$

### 2.2. Special quasi-random structure (SQS)

The SQS specially designs small-unit-cell periodic structure with only a few (16-32) atoms per unit cell, which closely mimic the most relevant local pair and multi-site correlation functions of the random substitutional alloys for more details, see references [30,31].

In this work, we have used SQS-4 ( $A_{0.5}B_{0.5}C$ ) and SQS-16 ( $A_{0.75}B_{0.25}C$ ) proposed by Jiang et al. [31] where the generated structures are: Ni anti-site ( $Ti_{0.5}Ni_{0.5}Ni$ ), Ti vacuum ( $Ti_{0.5}Va_{0.5}Ni$ ), Ti anti-site ( $Ni_{0.5}Ti_{0.5}Ti$ ), and Ni vacuum ( $Ni_{0.5}Va_{0.5}Ti$ ) in the SQS-4 structure Ni anti-site ( $Ti_{0.75}Ni_{0.25}Ni$ ), Ti vacuum ( $Ti_{0.75}Va_{0.25}Ni$ ), Ti anti-site ( $Ni_{0.75}Ti_{0.25}Ti$ ), and Ni vacuum ( $Ni_{0.75}Va_{0.25}Ti$ ) in the SQS-16 structure.

In the SQS approach, for each of the four branches in Figures (1), the formation enthalpies of isolated point defects in stoichiometric B2 NiTi are obtained by fitting the calculated formation enthalpies to a quadratic function of alloy composition in the following form [30]:

$$\Delta H(\chi) = \Delta H_{NiTi} + c_1\chi + c_2^2\chi \quad (5)$$

Where:  $\chi = |x_{Ni} - 0.5|$  is the absolute deviation from stoichiometry.

$\Delta H_{NiTi}$ : is the formation enthalpy of the ordered stoichiometric B2 NiTi, which is a linear function of the composition, where the coefficient  $c_i$  represents the tangent and is directly related to the defect formation enthalpies  $H_d$ ; since the atomic concentration of defect d is  $\chi$  for anti-sites and  $2\chi$  for vacancies, we have  $H_d = c_1$  for anti-sites and  $H_d = \frac{c_1}{2}$  for vacancies.

The interactions between point defects of the same type were considered in the SQS calculations, as indicated by the nonlinear quadratic term in equation (3). Where the physical means of  $c_2$  coefficient is that two branches in Figures (1) may cross each other at certain composition and in this case a reversal of the stable constitutional point defects may occur [30]. Such a case is theoretical since the crossover composition is outside of the stable composition range of B2 NiTi.

### 2.3. Defect structure at finite temperature

While studying the point defect structure of B2 TiNi, it is assumed that those point defects are sufficiently dilute, which allows us to adopt the Wagner-Schottky model (a gas of non-interacting point defects on well-defined sublattices) [34,35-55] to calculate the point defect concentrations as a function of alloy composition and temperature. Instead of using a grand-canonical ensemble (i.e. a fixed number of lattice sites with varying number of atoms), we consider a canonical ensemble containing a fixed number of Ti and Ni atoms, thus the total number of lattice sites may vary when vacancies are present. In this case, it is more convenient to use the atomic concentration rather than the site fraction. The atomic concentration of species  $i$  on sublattice  $\alpha$  is defined as:

$$x_{i(\alpha)} = \frac{n_{i(\alpha)}}{N_{atom}} \quad (4)$$

Where:

$N_{atom}$ : is the total number of atoms (excluding vacancies).

$n_{i(\alpha)}$ : is the number of species  $i$  on the sublattice  $\alpha$  with  $i = \{\text{Ni}, \text{Ti}, \text{Va}\}$  and  $\alpha = \{\text{Ni}, \text{Ti}\}$ , Va denotes vacancy.

According to the Wagner-Schottky model, the formation enthalpy (per atom) of a B2 NiTi alloy is a linear function of the point defect concentration:

$$\Delta H = \Delta H_{\text{NiTi}} + \sum_{\alpha} H_d x_d \quad (5)$$

Where:

$x_d$ : is the atomic concentration of defects of type  $d$  with  $d = \{\text{Va}_{\text{Ni}}, \text{Va}_{\text{Ti}}, \text{Ti}_{\text{Ni}}, \text{Ni}_{\text{Ti}}\}$ .

$\Delta H_{\text{NiTi}}$ : is the formation enthalpy of the fully-ordered stoichiometric B2 NiTi.

$H_d$ : is the formation enthalpy of isolated point defects of type  $d$  in stoichiometric B2 NiTi, which will be obtained in the present study through first-principles calculations.

In considering the effects of finite temperatures, the effects of vibrational entropies will be neglected and the configurational entropy (per atom) will be treated using the following mean-field approximation [11]:

$$S = k_B (1 + x_{\text{Va}_{\text{Ni}}} + x_{\text{Va}_{\text{Ti}}}) \ln \left( \frac{1 + x_{\text{Va}_{\text{Ni}}} + x_{\text{Va}_{\text{Ti}}}}{2} \right) - k_B \sum_i \sum_{\alpha} x_{i\alpha} \ln(x_{i\alpha}) \quad (6)$$

Where the summation goes over  $i = \{\text{Ni}, \text{Ti}, \text{Va}\}$  and  $\alpha = \{\text{Ni}, \text{Ti}\}$ .  $k_B$  is the Boltzmann's constant.

The equilibrium concentrations of point defects can now be obtained through a minimization of the Gibbs free energy of the system, i.e.  $\Delta G = \Delta H - TS$ , which with the mass-balance constraints leads to the following set of nonlinear equations [31]:

$$\frac{2x_{\text{Va}_{\text{Ni}}} x_{\text{Co}_{\text{Ti}}}}{x_{\text{Va}_{\text{Ti}}} (1 - 2x_{\text{Ti}_{\text{Ni}}} - x_{\text{Va}_{\text{Ni}}} + x_{\text{Va}_{\text{Ti}}})} = \exp \left[ - \frac{H_{\text{Ni}_{\text{Ti}}} - H_{\text{Va}_{\text{Ti}}} + H_{\text{Va}_{\text{Ni}}}}{k_B T} \right] \quad (7a)$$

$$\frac{2x_{\text{Va}_{\text{Ti}}} x_{\text{Ti}_{\text{Ni}}}}{x_{\text{Va}_{\text{Ni}}} (1 - 2x_{\text{Ni}_{\text{Ti}}} + x_{\text{Va}_{\text{Ni}}} - x_{\text{Va}_{\text{Ti}}})} = \exp \left[ - \frac{H_{\text{X}_{\text{Ni}}} + H_{\text{Va}_{\text{Ti}}} - H_{\text{Va}_{\text{Ni}}}}{k_B T} \right] \quad (7b)$$

$$\frac{4x_{\text{Va}_{\text{Ni}}} x_{\text{Va}_{\text{Ti}}}}{(1 + x_{\text{Va}_{\text{Ti}}} + x_{\text{Va}_{\text{Ni}}})^2} = \exp \left[ - \frac{H_{\text{Va}_{\text{Ni}}} + H_{\text{Va}_{\text{Ti}}}}{k_B T} \right] \quad (7c)$$

$$\frac{1}{2} (1 - 2x_{\text{Ni}_{\text{Ti}}} + 2x_{\text{Ti}_{\text{Ni}}} + x_{\text{Va}_{\text{Ni}}} - x_{\text{Va}_{\text{Ti}}}) = x_{\text{Ti}} \quad (7d)$$

Where

$x_x$ : is the total mole fraction of  $X = (\text{Ni}, \text{Ti})$  in the alloy.

A numerical solution of Equations (7a) - (7d) can thus give us the equilibrium concentrations of all point defects at a given alloy composition and temperature.

### 2.4. Ab-initio calculation

In the present work, calculations were performed using the projected augmented wave (PAW) pseudo-potentials [53, 54] with the generalized gradient approximation as implemented by Perdew, Burke and Erzhenfest (GGA-PBE) [55]. A plane wave cut-off energy of 350 eV is used. K-point meshes are compiled using the fully automatic scheme [56], which generates centered Monkhorst-Pack [57] grids, where the numbers of subdivisions  $N_1$ ,  $N_2$  and  $N_3$  along reciprocal lattice vectors  $b_1$ ,  $b_2$  and  $b_3$ , respectively, are given by:

$$N_i = \max(1, l|b_i| + 0.5), \quad i = 1, 2, 3 \quad (8)$$

Where  $l|b_i|$  is the norm of the reciprocal lattice vector  $b_i$ . According to Kresse et al. [36], useful values for the length  $l$  vary between 10 (large gap insulators) and 100 (d-metals). In this work, it was found that  $l = 50$  is sufficient to achieve convergence to a precision less than 1 meV/atom for the B2 NiTi. In addition to Monkhorst-Pack k-point meshes, Brillouin-zone integrations are performed using the Methfessel-Paxton technique with the smearing parameter of 0.1 eV. All calculations were performed

using the “Accurate” setting within VASP, and all the degrees of crystal structures freedom were allowed to relax, including cell shape, volume and atom positions with a preconditioned conjugated gradient (CG) algorithm with the default VASP's convergence criteria. Finally, relaxed structures are examined using SGROUP program [38]; all the results structures maintain the initial space-group.

### 3. Results

Figure (1) presents the formation energy of NiTi including constitutional defect as a function of Ni composition. Figure (1) shows the formation energies of the B2 NiTi as a function of composition, simulated with a 16-atom and a 32-atom super-cell (MF), compared to the formation energies obtained using the SQS approach. Figure (1) shows that our calculations using super-cell and SQS approaches are in good agreement, specifically in the Ti-rich side. In Ni-rich side of B2 NiTi, the calculated alloy formation enthalpies using super-cell and SQS approaches agree with each other and give the same prediction of the ascending order of the formation energies. As a note, the Super-cell results converge to SQS results whenever the cell is larger, but sometimes the super-cell approach fails when determining the formation enthalpy in high defect concentration. It's for that we count really more on the SQS results to continue the different steps in this work.

In general figure (1) shows that in the Ni-rich side of B2 NiTi, the Ni anti-sites atoms are more stable than the Ti vacancies, which indicates that the Ni anti-sites atoms are introduced as constitutional defects. On the other hand, in the Ti-rich side of B2 NiTi, the Ti anti-sites are slightly more stable than the Ni vacancies defect. So as a result, the Ti anti-sites and Ni anti-sites are the constitutional defects of B2 NiTi.

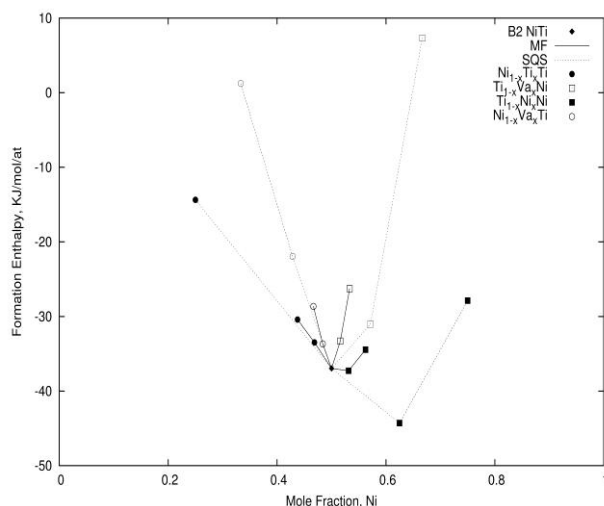


Figure 1. Comparison between the first-principle super-cell (MF) and the special quasi-random structures calculations (SQS) of formation enthalpies of NiTi as a function of composition.

The calculated lattice parameter using the SQS and super-cell (MF) approaches of B2 NiTi is shown in figure (2). These results are consistent with the experimental and logical data. Figure (2) shows a little difference between the experimental [8,13] and our calculated lattice parameter where the atomic parameter decreases with the increasing of vacancies so figure (2) proofs that in both sides of B2 NiTi the predominant defects are the anti-sites.

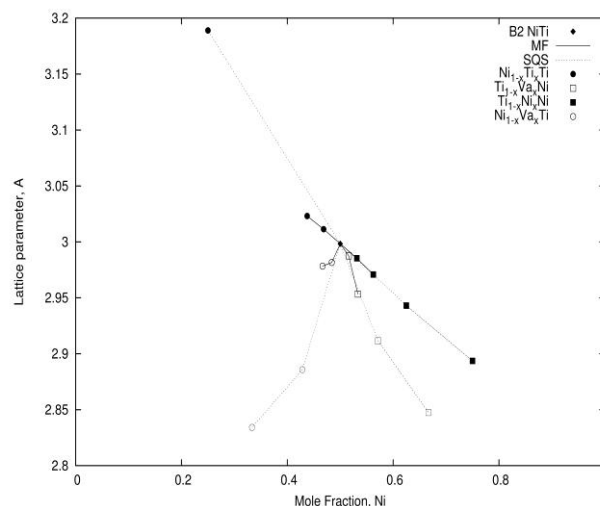


Figure 2. Comparison between the first-principle super-cell (MF) and the special quasi-random structures calculations (SQS) observed equilibrium lattice parameter.

At  $T = 1583$  K and zero external pressure, the calculated atomic concentrations of thermal defects  $x_i$  in NiTi are shown in figure (3) as a function of composition. The main defects in Ni-rich side are Ni anti-sites atoms, and in Ti-rich side NiTi are Ti anti-sites. It is useful to substitute constitutional defects that are present at ground state  $T = 0$  K, to separate thermal defect which appear at a finite temperature ( $T = 1583$ ). It can be observed that the dominant thermal defects in intermediate phase B2 NiTi are an exchange type where the Ni anti-sites and Ti anti-sites do a permutation at the passage of the stoichiometric NiTi and each Ni anti-site take the place of one Ti anti-site which are the constituents of an exchange defect type.

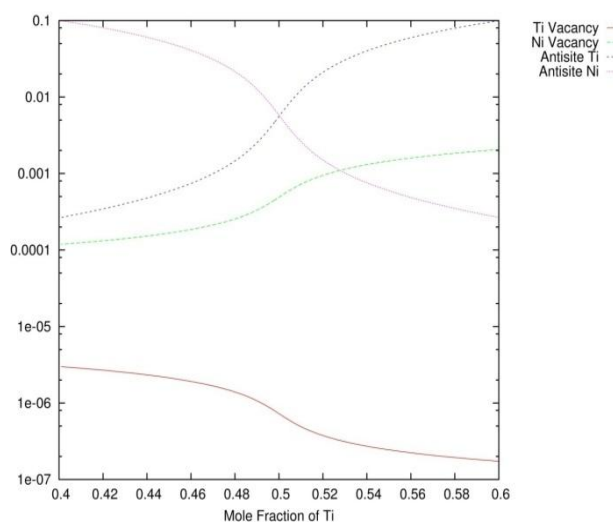


Figure 3. Equilibrium defect concentration in B2 NiTi at  $T = 1583$  K as function of composition

#### 4. Conclusion

In this study, we have obtained the formation enthalpies of isolated point defects in stoichiometric B2 NiTi by means of super-cell in a various size and SQS approaches at different concentrations. The present work shows that Ti anti-sites and Ni anti-sites are the constitutional point defects in Ti-rich and Ni-rich B2 NiTi, respectively. Using the Wagner-Schottky model, we have also calculated the thermal defect concentrations at finite temperatures. Our results suggest that the predominant thermal defects in B2 NiTi are an exchange defects type.

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