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# Evolution with temperature of point defects concentration in $Fe_2ZrX$ (X=V, Y, Tc, Ru): DFT and Wagner-Schottky modeling

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## Abstract

*The evolution with temperature of the point defect concentration in the cubic C15-$ZrFe_2$ Laves phase was investigated in the presence of several ternary additions X (X=V, Y, Tc, Ru). The heats of formation of the different point defects were carried out at 0K by means of DFT calculations. The Wagner-Schottky Model, based on substitutional and interstitial sublattices configuration within the canonical ensemble, was applied to investigate temperature effects on the defect concentration. The main results show a strong dependency of the C15-$Fe_2Zr$ stability on the point defect type. Energetically, the $Ru^{Fe}$ antisite is the most stable defect at low temperatures (0 K), whereas the $Va^{Fe}$, $Va^{Zr}$, and $Y^{Fe}$ are the least stable ones. At finite temperatures, it was found that antisites are the dominant constitutional defects on both sides of stoichiometry in the C15-$ZrFe_2$ compound.*

**Keywords:** Point Defect, Laves Phases, DFT, Wagner-Schottky Model.

## Introduction

Laves phases with topologically close-packed structures, are very attractive materials for high temperature structural applications [1]. They are also considered as superconducting materials and giant magnetostrictive materials, owing to their excellent physical and chemical properties [2]. However, the off-stoichiometry, that concerns about 25% of Laves phases, affects strongly the physical, mechanical and functional properties of these materials and therefore has a decisive impact on their performance in application [3,4]. In this context, vacancies and antisite defects, which are the main reasons of off-stoichiometry, assist the movement of Synchro-Shockly dislocations, thus facilitating the synchroshear deformation mechanism and modify the mechanical properties of Laves phases [2,5]. Moreover, vacancies play important role in diffusion of doping atoms and atomic self-diffusion in solid materials. In that way, point defects become an important topic in materials science that must be carefully investigated.

To date, several experimental and theoretical works have been done to study the point defects in Laves phases. Experimentally, antisites are found to be responsible for the off-stoichiometry observed in $Fe_2Nb$, $Cr_2Nb$ and $Co_2Nb$ compounds [5,6]. Whereas applying first-principles calculations, together with a statistical models, it was found that antisite defects are favored than vacancies on both sides of stoichiometry for $Mg_2Ca$ and $Zn_2Mg$ with C14 structure [3,4]. In addition, Zn2 vacancies are also favorable under moderate Mg-rich condition in $Zn_2Mg$ Laves phases [4]. Another theoretical study, found that Mn antisites are the most favorable defects broadening the homogeneity range of the $Mn_2Zr$ phase toward the Mn-rich side [7]. With C15 Laves structure, similar behaviors of point defects are evidenced. Namely, antisite defects on both sides of off-stoichiometry in the $Cu_2Mg$ Laves phase [2], $Co_2Zr$, $Cr_2Nb$ [8], $Co_2Zr$ [1] as well as several Cr-based Laves phases [9]. The effects of alloying elements are also investigated in some studies [2,8], nevertheless, the mechanismsof point defects formation and alloying elements effects on the overall trend of the point defects at lower and high temperatures are still poorly understood. In view of this, the present work aims at giving new insights on how finite temperature and alloying elements affect the intrinsic point defect behavior in the C15-$Fe_2ZrX$ system, with X being V, Y, Tc and Ru. Our choice of elements is motivated by the interesting results obtained by rabahi et al [10]. The relative stability of point defects in the C15-$Fe_2Zr$ compound is determined from the calculated formation enthalpies of point defects, obtained in the framework of DFT calculations. The statistical Wagner-Schottky model is applied to investigate effect of both temperature and X alloying elements on the point defects behavior in the C15-$ZrFe_2X$ Laves phase. The present paper is organized as follows. The technical details of the DFT calculations and the Wagner-Schottky model are presented in Sec. 2. The main results are discussed in Sec. 3. While concluding remarks are given in Sec. 4.

## 2. Computational Details

### *2.1 DFT calculations*

The present study calculations were performed basing on the density functional theory (DFT) using pseudopotential method as implemented in the Quantum-Espresso [11]. The many-body problem of interacting electrons and nuclei was treated using a series of one-electron equations, the so-called Kohn-Sham (KS) equations [12,13]. The generalized gradient approximation (GGA) of Perdew et al (PBE) to the local density approximation, was taken to include the exchange-correlation energy [14] and ultrasoft pseudopotentials of Vanderbilt were used [15]. A kinetic energy cut-off of 40 Ry and a well converged value of the k-point mesh over the Brillouin zone were considered, Namely, 6 6 6 for the C15 supercell. All structures were allowed to fully relax using Broyden- Fletcher-Goldforb-Shanno (BFGS) scheme [16] until the total energy has converged to less than $10^5$ eV/atom. The maximum force has converged to lower than 0.004 eV/Å.

### *2.2 Wagner-Schottky model*

Deviations from the ideal stoichiometric compositions are always accommodated by the creation of constitutional point defects (e.g. vacancies, antisites, ternary substitutional or interstitial atoms) on one or both sublattices. Thermal defects are also activated at finite temperature in addition to the constitutional ones, in order to maintain the overall composition of the alloy. To allow the use of the Wagner-Schottky model, two assumptions must be considered. (i) The defect concentrations are sufficiently dilute i.e gaz of non-interacting (isolated) atoms and point defects. (ii) At constant pressure, the internal energy, volume, and vibrational entropy of the crystal are linear functions of the number of atoms or vacancies in the different sublattices.We consider a canonical ensemble containing a fixed number of atoms, $N_{at}$, and the total number of lattice sites $N_s$ may thus vary when vacancies are present, consequently, it is more convenient to describe the distribution of alloy components between the sublattices in terms of atomic concentrations defined with respect to the total number of atoms $N_{at}$. The atomic concentration of species Iin sublattice m is defined as:

$$x_i^m = \frac{N_i^m}{N_{at}} \tag{1}$$

Where $N_i^m$ is the number of species i on the sublattice m with i={A, B, Va} and m={α, β}. The ordered C15-AB$_2$ structure can be divided into two sublattices: the α sublattice, normally occupied by A atoms, and the β sublattice, normally occupied by B atoms, therefore, the number of A atoms $N_A = N_A^\alpha + N_A^\beta$, and the number of B atoms $N_B = N_B^\alpha + N_B^\beta$ are fixed. The number of vacancies in the alloy $N_{Va}$ as well as the number of lattice sites may vary. In this case, the equilibrium state of the alloy at temperature T and pressure P is determined by the minimization of the Gibbs free energy G, or, equivalently, of its excess value ΔG defined relative to some standard states and normalized per atom.

$$\Delta G = \Delta H - T\Delta S \tag{2}$$

Where ΔH is the enthalpy (or heat) of alloy formation and ΔS is the entropy. According to this model, the formation enthalpy (per atom) of alloy is a linear function of the point defect concentrations.

$$\Delta H = \Delta H_0^f + \sum_d H_d x_d \tag{3}$$

where $x_d$ is the atomic concentration of defects of type *d* defined as the total number of defects divided by the total number of atoms in the system, with d={vacancies, antisites}. $H_d$ is the formation enthalpy of isolated point defects of type d in stoichiometric structure. $\Delta H_0^f$ is the formation enthalpy of the fully ordered stoichiometric alloy. Here, the effects of vibrational entropy are neglected and only the configurational entropy is taken into account.

$$\Delta S = k_B ln\left(\prod_m \frac{N_s^m!}{\left(\prod_i N_i^m!\right)}\right) \tag{4}$$

where $k_B$ is Boltzmann's constant and $N_s^m$ is the total number of sites on the m sublattice. When considering the substitutional atoms, the entropy (per atom) of alloy can be written as:

$$\Delta S \;= k_B\left(1 + x_{Va}^{sub}\right)\left(\frac{2}{3} ln(2) + ln\left(\frac{1+x_{Va}^{sub}}{3}\right)\right) - k_B \sum_i \sum_j x_j^i ln\left(x_j^i\right) \tag{5}$$

where i={α, β} and j={A, B, X, Va}.

The equilibrium concentrations of point defects can now be obtained through a minimization of the Gibbs free energy of the system ΔG, which together with mass-balance constraints leads to the following set of non-linear equations:

$$\frac{3\,x_A^{\beta}x_{Va}^{\alpha}}{x_{Va}^{\beta}\left(2-3x_B^{\alpha}-3x_X^{\alpha}+2x_{Va}^{\beta}-x_{Va}^{\alpha}\right)}=exp\left[-\frac{H_A^{\beta}+H_{Va}^{\alpha}-H_{Va}^{\beta}}{k_BT}\right] \tag{6a}$$

$$\frac{3\,x_B^{\alpha}\,x_{Va}^{\beta}}{x_{Va}^{\alpha}\left(1-3x_A^{\beta}-3x_X^{\beta}-2x_{Va}^{\beta}+x_{Va}^{\alpha}\right)}=exp\left[-\frac{H_B^{\alpha}+H_{Va}^{\beta}-H_{Va}^{\alpha}}{k_BT}\right] \tag{6b}$$

$$\frac{x_X^{\beta}x_{Va}^{\alpha}}{x_{Va}^{\beta}x_X^{\alpha}}=exp\left[-\frac{H_X^{\beta}-H_X^{\alpha}-H_{Va}^{\beta}+H_{Va}^{\alpha}}{k_BT}\right] \tag{6c}$$

$$\frac{27x_{Va}^{\beta}(x_{Va}^{\alpha})^2}{4\left(1+x_{Va}^{\beta}+x_{Va}^{\alpha}\right)^3}=exp\left[-\frac{H_{Va}^{\beta}+2H_{Va}^{\alpha}}{k_BT}\right] \tag{6d}$$

$$x_A=x_A^{\beta}+\frac{1}{3}\left(2+2x_{Va}^{\beta}-3x_B^{\alpha}-3x_X^{\alpha}-x_{Va}^{\alpha}\right) \tag{6e}$$

$$x_X=x_X^{\alpha}+x_X^{\beta} \tag{6f}$$

At any given total alloy composition and temperature, a numerical solution of Eqs. (6) can give us the equilibrium concentrations of point defects.

## 3. Resultsand Discussion

### *3.1 Point defects in C15 $Fe_2ZrX$ at 0K*

In ref [17], the stability and magnetic properties of the clean $Fe_2Zr$ Laves phase were investigated. At the stoichiometric composition, Rabahi et al [17], found that this material is more stable in the C15 Laves structure with the ferromagnetic state. However, presents an extended homogeneity range, between about 34 and 27-28 at % [18]which is always attributed to the point defects creation. Consequently, the first part of this work is devoted to the energetic and behavior of the point defects in C15-$Fe_2Zr$ Laves phase. To this purpose, several compositions were considered for the defected materials, including one of the following six defects: Fe vacancy, Zr Vacancy, Fe antisite, Zr antisite, ternary X substitutional atom for Fe or Zr. Since Laves phases present topologically close packed structure, there are no interstitial sites with a size comparable to that of the component atoms, therefore interstitial defects were excluded. For each composition, the Heats of formation, volume variations and total magnetization were predicted and the results are given in the Table 1. As it can be seen, the stability of the C15-$Fe_2Zr$ compound is affected by the point defects creation, remarkably, $Ru^{Fe}$ defect increases the stability of the system, while opposite effect is found when vacancies $Va^{Fe}$, $Va^{Zr}$ and $Y^{Fe}$ antisite are created. Comparatively, the remaining defects slightly destabilize the C15-$Fe_2Zr$ material.

The magnetic properties and total volume are also found to be affected by point defects creation. Fe and Zr vacancies, as well as Zr antisite reduce the unit cell volume, while the Fe antisite induces the opposite effect. For the substitutional X elements, it is found that Ru, V, and Tc increase the volume only when they replace Fe, whereas the case of Y is rather singular, a volume expansion is noticed whatever the nature of the site replaced by Y, these results are explained by size effects as already discussed in ref [10], in addition, the total magnetization obtained for the different configurations is slightly affected and fluctuating around 1.6 $\mu_B$ /Fe atom, which is related to the magneto-volume effects.

In the Table 2, the heats of formation of punctual defects predicted at 0 K in the C15-$Fe_2ZrX$ compound are reported. At this temperature, the punctual defects are only governed by their formation enthalpies and the stable ones, are considered as constitutional defects. The deviation toward Zr-rich $Fe_2Zr$ side could be caused either by Zr antisites and/or Fe vacancies. Similarly, the deviation toward Fe-rich $Fe_2Zr$ could be accommodated either by Fe antisites or Zr vacancies. From Table 2, it can be seen that $H_{VaZr} > H_{FeZr}$ and $H_{VaFe} > H_{ZrFe}$. Therefore, it could be concluded that antisites are the dominant constitutional defects in both side of stoichiometry in C15-$ZrFe_2$ compound. Moreover, all the formation enthalpies values are positives except the anti-site $Ru^{Fe}$. This means that the creation of defects in the compound C15-$Fe_2ZrX$ is an endothermic reaction which requires a supply of external energy. The Table 2 shows that Fe and Zr vacancies as well as $Y^{Fe}$, $Tc^{Zr}$, and $Zr^{Fe}$ anti-sites are the least favorable. While $Ru^{Fe}$, $Tc^{Fe}$ and $V^{Fe}$ anti-sitesare the most favorable. In addition, the Ru and Tc atoms mark a strong preference to Fe site. While, the Y atom prefers the Zr site. The Vanadium V element slightly prefers the Fe site. This behavior of X elements is attributed to the size and electronic effects as already discussed in the work of L. Rabahi et al [10].

### *3.2 Point defects in C15 $Fe_2ZrX$ at finite temperature*

Using the heats of formation values given in the Table 2, the equilibrium point defects are obtained by solving the set of equations 6(a-f) at a given temperature and alloy composition. It is well known that the Wagner-Schottky model, applied in this work is only valid at intermediate and high temperatures. For this reason, several temperatures are considered as a first step, and convergence is reached from 1373 K (for the $Fe_2Zr$ system) and 1673 K (for the $Fe_2ZrX$ system). Consequently, three temperatures were considered, namely 1373, 1673 and 2073 K, in order to include both temperature and alloy composition effects on the point defects behavior in the C15 $Fe_2Zr$ and C15 $Fe_2ZrX$ systems. As it can be seen (from Figure 1), the point defect structure in the off-stoichiometric $Fe_2Zr$ is very complex, and the concentrations exhibit a brutal change when the alloy composition vary from Zr-rich to Fe-rich side. This fact reflects the strong correspondence between the point defect and its local chemical environment. The Fe and Zr anti-site are found to be the dominant defects in C15-$ZrFe_2$ even at high temperatures, while the vacancies, and more particularly, $Va^{Fe}$ are the less activated ones, and the less affected by Zr concentration, meaning that, deviation from ideal stoichiometry in the C15-$ZrFe_2$ is only governed by Fe and Zr anti-sites. This result is similar to the general tendency of point defects in C15 Laves phases found in previous studies [1,2,5,7,8], and could be easily explained by geometrical rules. The smallest Fe atom is apt to replaces larger Zr atom to form anti-site defect on the Zr sublattice [5], however, it is rare for large atom to replace small atom to form the anti-site defect in small atom sublattice. So, according to previous studies, the formation of this kind of defects is feasible in Laves phases with atomic size ratio smaller than the ideal ratio 1.225 [18]. Thus the formation of anti-site defect $Zr^{Fe}$ is possible in the C15-$Fe_2Zr$, since the atomic sizes of the Fe and Zr atoms are respectively 1.60 A° and 1.39A°, and the atomic size ratio is about 1.15, less than the ideal atomic radii ratio in Laves phases. Moreover, comparing the results obtained at different temperatures, it is found that all the defect concentrations are found to be increased with temperature. This fact is attributed to the thermal defects which are activated in balanced combinations in order to maintain the overall composition of the alloy [8]. The site preference of ternary elements at finite temperature is also investigated in the present work. For each X element, Tc, Ru, V and Y, the corresponding equilibrium point defect concentrations, are obtained and shown in the Figure 2 (a-d) respectively. At T = 0K, rabahi et al [10] found that Y, and Tc elements prefer to substitute for Zr atoms while the Ru and V prefer to replace Fe ones. At finite temperatures, entropy will play an important role in determining the site preference of ternary elements. As shown in Figure 1, all the Ru atoms have substituted to the Fe ones at elevated temperature, in the entire range of Zr composition; this fact is related to the negative heat of formation obtained in the case of the $Ru^{Fe}$ defect. The Tc and Y elements exhibit a strong preference to the Fe and Zr sites respectively, while moderate preference to the Fe site is noticed for the V element. Finally, the defect concentration curves underwent a noticeable shift towards lower values of Zr concentration in the case of $Fe_2ZrY$ alloy. This fact is due to the sharp variation of the Zr concentration in the system, since a great part of this element is found to be replaced by Y atoms. This last one displays a great preference for the Zr sites, as is clearly visible from the high concentration of the $Y^{Zr}$ defect.

**Table 1:** Heats of formation, volume variations and total magnetization of Clean $Fe_2Zr$, defected $Fe_2Zr$ and $Fe_2ZrX$ with C15 Laves phase.

| | $\Delta H_f$ (eV/atome) | ΔV (%) | M ($\mu_B$/Atome Fe) |
|---|---|---|---|
| $Fe_2Zr$ | -0.280 | - | 1.68 |
| $Va^{Fe}$ | -0.165 | -1.304 | 1.54 |
| $Va^{Zr}$ | -0.157 | -3.055 | 1.58 |
| $Fe^{Zr}$ | -0.247 | -1.850 | 1.83 |
| $Zr^{Fe}$ | -0.228 | 3.125 | 1.60 |
| $Ru^{Fe}$ | -0.301 | 1.095 | 1.75 |
| $Ru^{Zr}$ | -0.263 | -1.450 | 1.90 |
| $V^{Fe}$ | -0.267 | 0.453 | 1.58 |
| $V^{Zr}$ | -0.243 | -1.705 | 1.61 |
| $Tc^{Fe}$ | -0.278 | 0.719 | 1.72 |
| $Tc^{Zr}$ | -0.198 | -2.648 | 1.74 |
| $Y^{Fe}$ | -0.167 | 4.314 | 1.61 |
| $Y^{Zr}$ | -0.251 | 1.211 | 1.68 |

**Table 2:** Heats of formation of isolated punctual defects ($H_d$ ) predicted at 0 K in the C15-$Fe_2Zr$ compound.

| | Va | Fe | Zr | Ru | Y | Tc | V |
|---|---|---|---|---|---|---|---|
| **Fe** | 2.640 | - | 1.195 | -0.497 | 2.706 | 0.037 | 0.313 |
| **Zr** | 2.822 | 0.752 | - | 0.411 | 0.703 | 1.975 | 0.879 |

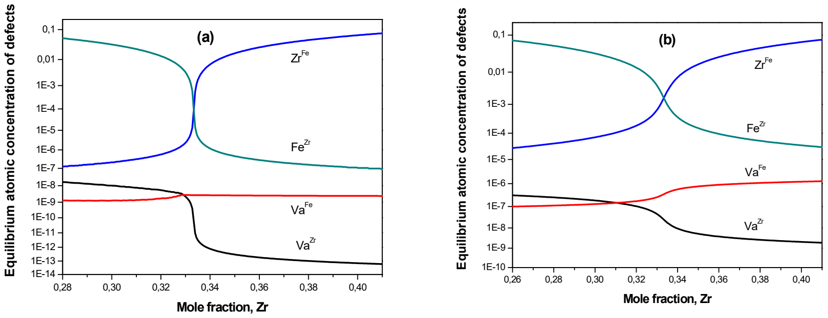

**Figure 1:** Equilibrium point defect concentrations in C15-$Fe_2Zr$ system at (a) T= 1373 and (b) T= 2073 K as function of Zr concentration.

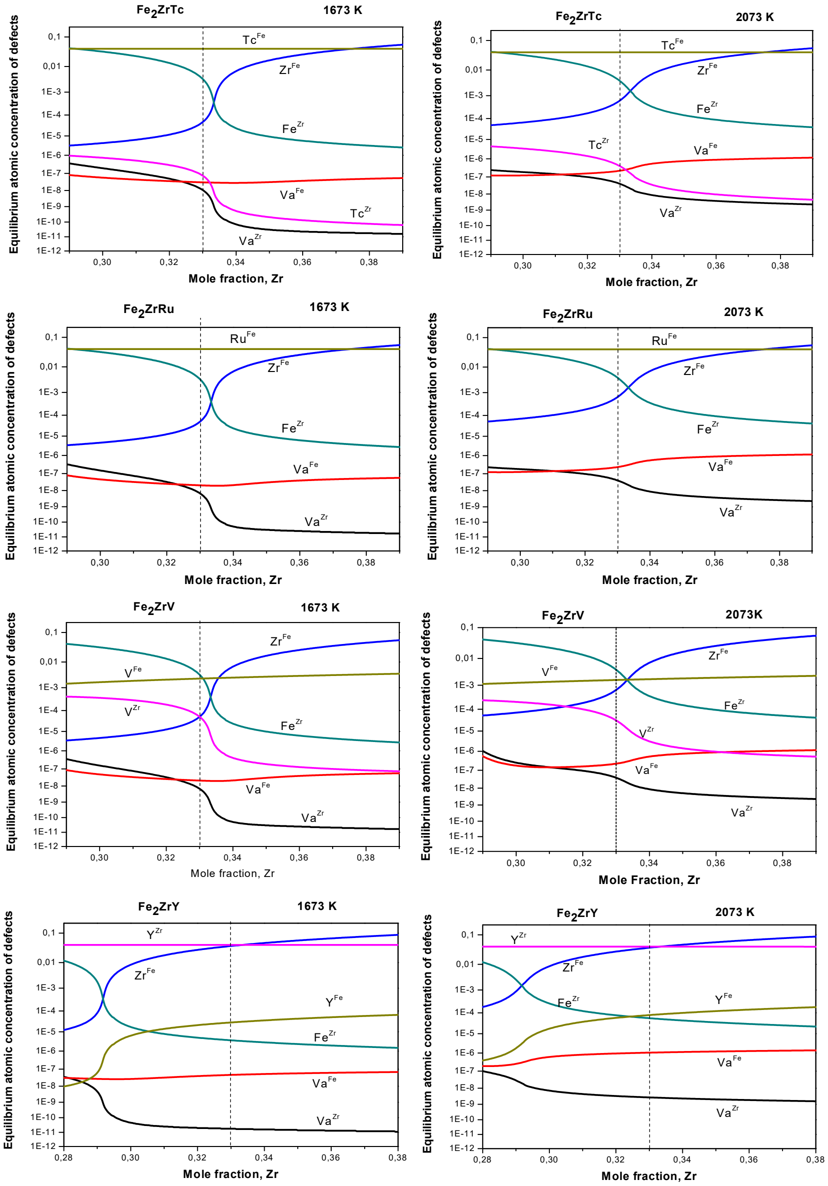

**Figure 2:** Equilibrium point defect concentrations in C15-$Fe_2ZrX$, (X =Tc, Ru, V and Y) system at T= 1673 K (left) and T= 2073 K (right) as function of Zr concentration.

## 4. Concluding remarks

In this work, the evolution with temperature of the point defect concentrations in the C15-ZrFe2 Laves phase in the presence of several ternary additions X (X=V, Y, Tc, Ru) is investigated. To this purpose, the DFT-based pseudo-potential method combined with the statistical Wagner-Schottky model is applied. The obtained results indicate a strong dependency of the stability of the C15-Fe2Zr compound on the point defect kind; the RuFe antisite increases the stability of the system, while the opposite effect is found when vacancies VaFe, VaZr and YFe antisite are created. At finite temperature, the antisites are found to be the dominant constitutional point defects, and the entropy plays an important role in determining the site preference of ternary elements. The Ru atoms have substituted for the Fe ones at elevated temperatures and in the entire range of Zr composition, whereas the Tc and Y elements exhibit a strong preference for the Fe and Zr sites, respectively.

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