SITE OCCUPANCY OF TRANSITION ELEMENTS IN C15 NbCr$_2$ LAVES PHASE: A FIRST-PRINCIPLES STUDY

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Abstract

Using first-principles calculations, site occupancy behaviors of transition elements in C15 NbCr$_2$ Laves phase are systematically investigated. Elements Y, Sc, Zr, Hf, Cd, Ta, Ti and Ag prefer to occupy the Nb site, and elements Zn, Pt, Re, Tc, Ir, V, Os, Rh, Ru, Ni, Co, Mn, Fe and Cu favor to occupy the Cr site; whereas elements Mo, W, Pd and Au have weak site preference for Cr or Nb site. The present calculations agree well with the available experimental and previously calculated results. It was found that the site occupancy behavior of transition elements in NbCr$_2$ is mainly affected by the radii of transition elements. The present calculations also propose the correlation between the site preference energy and radii of transition elements.

Keywords: Laves phase, first-principles, site occupancy, NbCr$_2$

1. Introduction

Laves phases with an AB$_2$ stoichiometry are among the important intermetallic compounds [1]. NbCr$_2$ is a typical Laves phase with the TCP crystal structure of cubic C15, and it has a great potential for high temperature structural applications due to its high melting temperature, high strength and good high temperature oxidation resistance [2-7]. However, NbCr$_2$ is very brittle at low temperatures, as reported by Takasugi et al. [8, 9]. Consequently, many studies have been conducted on NbCr$_2$ to improve the physical and mechanical properties, especially the low ductility and fracture toughness at low temperatures [9, 10]. Adding an alloying element into NbCr$_2$ is an effective method to improve its mechanical properties.

To find which elements should be added into NbCr$_2$, it is necessary to understand the site occupancy behavior. So far, the site occupancy behavior for many elements in C15 NbCr$_2$ Laves phase has been studied extensively via both experiment and calculation. For example, the site occupancy of V was studied by using transmission electron microscope (TEM) and atom location with electron channeling-enhanced microanalysis (ALCHEMI) method, high-resolution synchrotron X-ray powder diffraction and Rietveld structure refinement [11, 12]. According to the isothermal section of the Cr–Zr–Nb system, the site occupancy of Zr was predicted [13]. The measured phase diagram and lattice parameters were used to reveal the site occupancy of Ti [14, 15]. Energy Dispersive Spectroscopy (EDS) analysis was used to unveil the site occupancy of Ni in C15 NbCr$_2$ Laves phase [16]. In the theoretic aspect, the first-principles calculation and thermodynamic modeling were used to study the site occupancy of several elements, such as Hf, Mn, Mo, Ta, Ti, V, W and Zr [17, 18]. Though many studies have been conducted on the site occupancy of many elements in C15 NbCr$_2$, the main focus is about those elements, which are close to Nb or Cr in the periodic table. So far, there is no systematical investigation for site occupancy of transition elements in C15 NbCr$_2$, and the rule for site occupancy is not established.

The present work systematically investigated the site occupancy behavior of transition elements in C15 NbCr$_2$ Laves phase by means of first-principles calculations. Based on the extensive calculations, the relation between the site occupancy and the radii of the transition elements is established.

2. Details of first-principles calculations

C15 NbCr$_2$ Laves phase is a complex face-centered cubic with 24-atom in the unit cell. The space group is $Fd\bar{3}m$, and Pearson symbol is *cF24*

[19]. In this work, calculations were performed using a 24-atom in the unit cell for the $NbCr_2$ Laves phase with ternary additions. When a transition element X occupies the Nb site in $NbCr_2$, the chemical formula is $Cr_{16}Nb_7X$ with a 4.17 at.% X concentration in $NbCr_2$. When X occupies the Cr site, the chemical formula is $XCr_{15}Nb_8$ with the same X concentration in $NbCr_2$.

All first-principles calculations were performed by means of Vienna Ab initio Simulation Package (VASP) code [20, 21] with the ion-electron interaction depicted by the projector augmented wave (PAW) method [22, 23] and the exchange - correlation functional described by the generalized gradient approximation (GGA) of Perdew-Burke-Eruzerhof (PBE) [24]. During the VASP calculations, the cutoff energy was set as 300 eV. Sampling of the irreducible Brillouin zone was done by a 11*11*11 *k*-point mesh during relaxation and 15*15*15 in static calculations. The self-consistent convergence of total energy was set to be 10^{-4} eV/atom, and the relaxation of atoms was finished when the maximum force on each atom was less than 0.01 eV/Å.

3. Results and discussion
3.1 Formation energies of binary and ternary $NbCr_2$ Lave phase.

In order to understand whether the substitutional elements have tendency to alloy with the $NbCr_2$ phase or not, we calculated formation energies of binary and ternary $NbCr_2$ Lave phase. Calculated lattice parameter and formation energy of $NbCr_2$ in the present work along with the experimental data [1] and calculations by others [7, 26] are listed in Table 1. The lattice parameter of C15 $NbCr_2$ Laves phase in the present calculation is 6.948 Å, which agrees well with the experimental value of 6.991 Å [25]. As a consequence, the formation energy calculated to be -1.027 eV in the present work for the formula unit of $Cr_{16}Nb_8$ is considered to be more reasonable than that in refs. [7, 26]. The higher formation energy obtained in the present work than the work in refs. [7, 26] due to the bigger lattice parameters calculated in the present work means more weaker bond strength. Among the ternary Laves phase with the chemical formula $XCr_{15}Nb_8$, $CoCr_{15}Nb_8$, $FeCr_{15}Nb_8$, $IrCr_{15}Nb_8$, $MnCr_{15}Nb_8$, $OsCr_{15}Nb_8$, $PtCr_{15}Nb_8$, $ReCr_{15}Nb_8$, $RhCr_{15}Nb_8$, $RuCr_{15}Nb_8$, $TcCr_{15}Nb_8$, $TiCr_{15}Nb_8$ and $VCr_{15}Nb_8$ show lower formation energies than that of binary $Cr_{16}Nb_8$. This means that the occupancy of Co, Fe, Ir, Mn, Os, Pt, Re, Rh, Ru, Tc, Ti and V on the Cr sites stabilizes the $NbCr_2$ Laves phase. Other elements Ag, Au, Cd, Cu, Hf, Mo, Ni, Pd, Sc, Ta, W, Y, Zn and Zr on the Cr site reduces the phase stability of $NbCr_2$. In particular, the occupancy of Ag, Cd, Sc, Y and Zr on the Cr sites highly destabilizes the $NbCr_2$ Laves phase because $AgCr_{15}Nb_8$, $CdCr_{15}Nb_8$, $ScCr_{15}Nb_8$,

$YCr_{15}Nb_8$ and $ZrCr_{15}Nb_8$ have positive formation energies. $Cr_{16}Nb_7Hf$, $Cr_{16}Nb_7Ir$, $Cr_{16}Nb_7Pt$, $Cr_{16}Nb_7Ta$, $Cr_{16}Nb_7Ti$ and $Cr_{16}Nb_7Zr$ exhibit lower formation energies than the binary $Cr_{16}Nb_8$ among the ternary Laves phases with the chemical formula $Cr_{16}Nb_7X$. Thus, the occupancy of Hf, Ir, Pt, Ta, Ti and Zr on the Nb sites stabilizes the $NbCr_2$ Laves phase, while Ag, Cd, Co, Cu, Fe, Mn, Mo, Ni, Os, Pd, Re, Rh, Ru, Sc, Tc, V, W, Y and Sn on the Nb sites reduces the phase stability of $NbCr_2$. All of the formation energies of for $NbCr_2$-based ternary are listed in Table 2.

Table 1. *The lattice parameter and formation energy of $NbCr_2$.*

Method	Lattice parameter (Å)	Formation energy (eV / formation)	Ref.
PAW –GGA(PBE)	6.948	-1,027	This work
Experiment	6.991	-	[25]
LMTO-LDA	6.83	-1,750	[26]
FLAPW- LDA	6.82	-1,848	[7]

3.2 The strong site occupancy of elements in Nb or Cr site of the Laves phase

The extent for site occupancy of transition elements X in C15 $NbCr_2$ is judged by comparing formation energy of X in Cr and Nb sites, according to refs. [18, 27]. The formation energies of X in Cr and Nb sites can be expressed as Eqs. (1) and (2), respectively.

$$E_{X \rightarrow Cr}^{f} = E_{XCr15Nb8} + E_{Cr} - E_{Cr16Nb8} - E_{X} \qquad (1)$$

$$E_{X \rightarrow Nb}^{f} = E_{Cr16Nb7X} + E_{Nb} - E_{Cr16Nb8} - E_{X} \qquad (2)$$

Where $E_{X \rightarrow Cr}^{f}$ and $E_{X \rightarrow Nb}^{f}$ are the formation energies of X in Cr and Nb sites, respectively. $E_{XCr15Nb8}$, $E_{Cr16Nb7X}$ and $E_{Cr16Nb8}$ are the total energies of $XCr_{15}Nb_8$, $Cr_{16}Nb_7X$ and $Cr_{16}Nb_8$ compounds, respectively. E_{Nb}, E_{Cr} and E_X are the energies of per Nb , Cr and transition element X in their standard state.

The site occupancy behavior of ternary additions in C15 $NbCr_2$ Laves phase can be reflected by the energy difference between formation energy of X in Cr and Nb sites. The energy difference between formation energies of X in Cr and Nb sites is defined as site preference energy [27].

$$\Delta E = E_{X \rightarrow Cr}^{f} - E_{X \rightarrow Nb}^{f} = E_{XCr15Nb8} - E_{Cr16Nb7X} + E_{Cr} - E_{Nb} \quad (3)$$

When $\Delta E < 0$, the ternary atom X preferentially occupies the Cr site; otherwise X is energetically favorable on the Nb site in $NbCr_2$ Laves phase.

Based on formula (3) and our calculated results, the site occupancy of transition elements additions in $NbCr_2$ Laves phase can thus be determined, as can be seen in Table 3. Elements Y, Sc, Zr, Hf, Cd, Ta, Ti and

Table 2. *Formation energies for NbCr$_2$-based ternary*

Elements	XCr$_{15}$Nb$_8$: formation energy (eV/formula)	Cr$_{16}$Nb$_7$X: formation energy(eV/formula)	Elements	XCr$_{15}$Nb$_8$: formation energy (eV/formula)	Cr$_{16}$Nb$_7$X: formation energy(eV/formula)
Ag	0.857	0.526	Pt	-1,619	-1,339
Au	-0.203	-0.304	Re	-1,250	-0.570
Cd	0.859	0.230	Rh	-1,260	-0.773
Co	-1,189	0.036	Ru	-1,171	-0.413
Cu	-0.303	0.116	Sc	0.210	-1,002
Fe	-1,457	0.033	Ta	-0.677	-1,299
Hf	-0.118	-1,392	Tc	-1,124	-0.480
Ir	-1,543	-1,108	Ti	-1,105	-1,437
Mn	-1,145	0.405	V	-1,287	-0.702
Mo	-0.712	-0.538	W	-0.737	-0.640
Ni	-0.963	-0.138	Y	2,073	0.409
Os	-1,391	-0.539	Zn	-0.772	-0.486
Pd	-0.643	-0.577	Zr	0.270	-1,073

Table 3. *The site occupancy of transition elements additions to C15 NbCr$_2$ Laves phase. The relative difference (η) of atom's radius between X and Cr (or Nb) are listed to correlate it to the site preference energy (ΔE). The values in parentheses are the calculated results of Yao et al. [18] using first-principles method.*

X[a]	R(Å)	η_{X-Cr}	η_{X-Nb}	ΔE (eV)	TSO[b]	Reference	
						Experiment	Calculation
Y	1.8	40.63%	22.45%	1,664	Nb site	Nb site [28]	
Sc	1.64	28.13%	11.56%	1,211	Nb site		
Zr	1.6	25%	8.84%	1.328(1.386)	Nb site	Nb site [13]	Nb site [17, 18, 29, 30]
Hf	1.58	23.44%	7.48%	1,256	Nb site	Nb site [31]	Nb site [17, 29, 30]
Cd	1.57	22.66%	6.80%	0.629	Nb site		
Nb	1.47	14.84%	0		Nb site		
Ta	1.47	14.84%	0	0.622	Nb site	Nb site [31]	Nb site [17, 29, 30]
Ti	1.46	14.06%	0.68%	0.320(0.347)	Nb site	Nb site [14, 15, 32]	Nb site [17, 18, 33], WPS [29]
Ag	1.45	13.28%	1.36%	0.331	Nb site		
Au	1.44	12.50%	2.04%	0.101	WSP[c]		
W	1.41	10.16%	4.08%	-0.098(-0.085)	WSP[c]	Nb site [34]	WSP[c] [17, 18, 29, 30]
Mo	1.4	9.38%	4.76%	-0.173(-0.201)	WSP[c]	Nb site [9, 35]	WSP[c] [17, 29, 30], Cr site [18]
Zn	1.39	8.59%	5.44%	-0.287	Cr site		
Pt	1.39	8.59%	5.44%	-0.280	Cr site		
Re	1.38	7.81%	6.12%	-0.680	Cr site		
Pd	1.38	7.81%	6.12%	-0.066	WSP[c]		
Tc	1.36	6.25%	7.48%	-0.644	Cr site		
Ir	1.36	6.25%	7.48%	-0.690	Cr site		
V	1.35	5.47%	8.16%	-0.585(-0.600)	Cr site	Cr site [9, 11, 12, 35, 36]	Cr site [18], WPS [17, 29]
Os	1.35	5.47%	8.16%	-0.861	Cr site		
Rh	1.35	5.47%	8.16%	-0.487	Cr site		
Ru	1.34	4.69%	8.84%	-0.758	Cr site		
Ni	1.25	2.34%	14.97%	-0.880	Cr site	Cr site [16]	Cr site [33]
Co	1.25	2.34%	14.97%	-1,224	Cr site		Cr site [33]
Mn	1.26	1.56%	14.29%	-1,544	Cr site		Cr site [17]
Fe	1.27	0.78%	13.61%	-1,500	Cr site	Cr site [37, 38]	
Cu	1.28	0	12.93%	-0.526	Cr site		
Cr	1.28	0	12.93%		Cr site		

[a]Transition elements. [b]Theoretical site occupancy. [c]Weak site preference.

Ag, which have positive ΔE, prefer to occupy the Nb site. Elements Zn, Pt, Re, Tc, Ir, V, Os, Rh, Ru, Ni, Co, Mn, Fe and Cu prefer to occupy the Cr site, and these elements have ΔE lower than 0 eV.

Experimental methods have been extensively adopted to discover the site occupancy of ternary additions. Site occupancy of elements Y, Zr and Hf in NbCr$_2$ Laves phase was studied by Lu et al. [28], Kim et al. [13] and Fujita et al. [31], respectively. They confirmed that all of them take the site of Nb. Fujita et al. [31] confirmed that Ta prefers for the site of Nb. Several groups [14, 15, 32] had investigated site occupancy of Ti, and their investigations show that Ti takes the site of Nb. V takes the site of Cr according to a few groups of authors [9, 11, 12, 35, 36]. Site occupancy of Ni was reported by Nie et al. [16], who showed that Ni takes the site of Cr. According to the isothermal section of the system Fe-Cr-Nb [37, 38], Fe takes the site of Cr. From Table 3, we can see that our calculations agree well with the experimental results.

Calculations have also been extensively adopted to reveal the occupancy of transition elements in NbCr$_2$. It was reported that Zr, Hf, Ta and Ti take the site of Nb [17, 18, 29, 30]. Through first-principles calculation, Yao et al. [18] showed that V prefers to take the site of Cr. The occupancy of elements Ni and Co was investigated by Li et al. [33], and Wu et al. [17] studied the site occupancy of Mn in NbCr$_2$ by combining thermodynamic modeling with first-principles calculation. Their results [17, 33] show that these elements take the site of Cr. Tien et al. [39] had studied the occupancy behavior of Ru additions to Cr-TaCr$_2$. Ru was found to mainly occupy the Cr site in TaCr$_2$ Laves phase. We can predict that Ru would also take the site of Cr in C15 NbCr$_2$, because Ta and Nb have similar mechanical and physical properties. As shown in Table 3, we can see that our calculations agree well with the other calculations in the literature.

3.3 The weak site preference of a few elements in Nb or Cr site of Laves phase

According to the refs. [18, 27] and our calculation results, Au should take the site of Nb, and W, Mo and Pd should take the site of Cr. However, experimental result [34] and extensive calculations [17, 29, 30] show that the site preference of W depends on composition and temperature of NbCr$_2$ Laves phase. According to the experimental results [9, 35], Mo takes the site of Nb. On the contrary, Yao et al. [18] show that Mo prefers to take the Cr site. The site preference of Mo depends on composition and temperature of NbCr$_2$ Laves phase according to the ref. [17, 29, 30].

In fact, according to Eq. (3), the more negative of ΔE, the more favorable X occupies the Cr site; the

more positive of ΔE, the more probability of X takes Nb site. When ΔE is close to zero, X has weak site preference. When a element has weak site preference [18], it either occupies Cr site or Nb site depending on composition and temperature of NbCr$_2$ Laves phase. ΔE of W is equal to -0.098 eV, which is very close to zero. Therefore, W has weak site preference. Which is consist with the experimental [34] and calculated results [17, 18, 29, 30]. ΔE of Mo is equal to -0.173eV, which is close to zero. Therefore, Mo also has weak site preference [17, 18, 29, 30]. In addition, we can predict tha elements Pd ($\Delta E = -0.066 eV$) and Au ($\Delta E = 0.101 eV$) also have weak site preference.

3.4 The relation between site occupancy and atomic radii of transition elements

Based on the extensive calculations about the site occupancy behaviors of transition elements in C15 NbCr$_2$, as shown in Table 3, the relation between site occupancy and atomic radii of transition elements can be established. All of the atomic radii were obtained from ref. [40]. We drew a figure to compare atomic radii of Cr, Nb and X and the site occupancy behavior of X. As can be seen in Fig.1, the relation between the site occupancy and atomic radii can be classified into the following three parts. R_{Cr}, R_{Nb} and R_X represent atomic radius of Cr, Nb and transition element X, respectively.

(i) $R_X \geq R_{Nb}$: X always prefers to take the site of Nb. The elements include Y, Sc, Zr, Hf, Cd and Ta.

(ii) $R_X \leq R_{Cr}$: X always prefers to take the site of Cr. The elements include Ni, Co, Mn, Fe and Cu.

(iii) $R_{Cr} < R_X < R_{Nb}$: the region can be divided into three situations according to the relative difference (η) between atomic radii of X and Cr (or Nb). The relative difference of atomic radii between X and Cr (or Nb) is expressed as follows:

$$\eta_{X-Cr} = \frac{|R_X - R_{Cr}|}{R_{Cr}} \tag{4a}$$

$$\text{or } \eta_{X-Nb} = \frac{|R_X - R_{Nb}|}{R_{Nb}} \tag{4b}$$

η_{X-Cr} represents the relative difference of atomic radii between X and Cr, and η_{X-Nb} represents the relative difference of atomic radii between X and Nb. As shown in Fig. 1, when $0 < \eta_{X-Cr} < 9.38\%$, X prefers to occupy the site of Cr. The elements include Ru, Rh, Os, V, Ir, Tc, Re, Pt and Zn. An exception is element Pd. Pd has a weak site preference though the relative difference of atomic radii between Pd and Cr is 7.81%. When $9.38\% < \eta_{X-Cr} < 12.50\%$, X has weak site preference for Cr or Nb. The elements include Mo, W and Au. In this region, whether X occupies Cr or Nb depends on composition and temperature of

NbCr$_2$ [17, 29]. When $0 < \eta_{X-Nb} < 2.04\%$, X prefers to occupy the site of Nb. The elements include Ag and Ti.

Thus we can come to a conclusion that the site occupancy of X in NbCr$_2$ is mainly affected by radii of transition elements. Elements with smaller atomic radii prefer to take the site of Cr. Conversely, elements with larger atomic radii prefer to take the site of Nb. This is consist with the relation between the site preference energy (ΔE) and radii of transition elements (see in Fig.2). The tendency of site preference energy (ΔE) against radii of transition elements is as follows: the smaller radius of X, the more negative of (ΔE); the larger radius of X, the more positive of ΔE.

It is worth to mention that in a larger range of relative difference of atomic radii ($0 < \eta_{X-Cr} < 9.38\%$), X prefers to occupy the site of Cr. But in a small range of relative difference of atomic radii ($0\% < \eta_{X-Nb} < 2.04\%$), X prefers to occupy the site of Nb. This may be due to the fact that both atomic radius and the proportion of Nb and Cr in C15 NbCr$_2$ Laves phase should be considered.
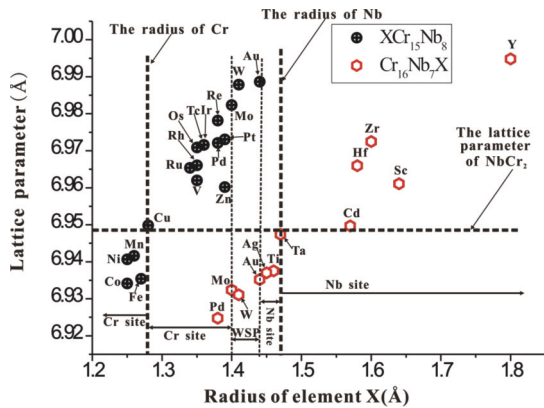

Figure 1. *The relation between site occupancy and radii of transition elements. WSP represents weak site preference.*
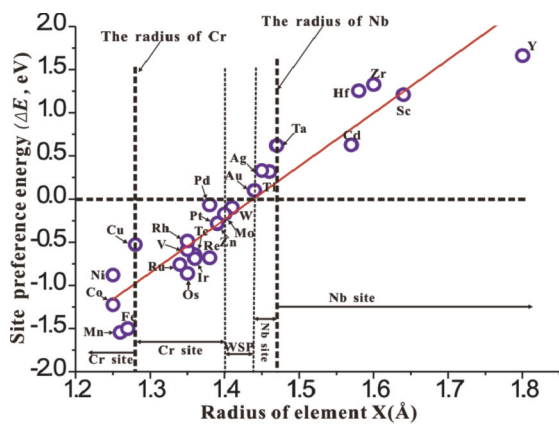

Figure 2. *The relation between site preference energy (ΔE) and radius of transition element X. WSP represents weak site preference. The elements with ΔE close to zero have weak site preference for Cr or Nb site.*

Conclusions

The site occupancy of transition element additions to the NbCr$_2$ Laves phase was systematically studied by first-principles calculations. The major conclusions are as follows:

(1) Elements Y, Sc, Zr, Hf, Cd, Ta, Ti and Ag prefer to occupy the Nb site; elements Zn, Pt, Re, Tc, Ir, V, Os, Rh, Ru, Ni, Co, Mn, Fe and Cu prefer to occupy the Cr site; while elements Mo, W, Pd and Au have weak site preference for Cr and Nb.

(2) The relation between site occupancy behavior and atomic radii of transition elements is established: (i) When $R_x > R_{Nb}$, element X would take the Nb site. (ii) When $R_X < R_{Cr}$, element X would take the Cr site. (iii) In the case of $R_{Cr} < R_X < R_{Nb}$, according to the relative difference (η) of atomic radii between X and Cr (or Nb), the occupancy behavior of X can be divided into three situations. When $0 < \eta_{X-Cr} < 9.38\%$, X prefers to occupy the Cr site except for element Pd. When $9.38\% < \eta_{X-Cr} < 12.50\%$, X has weak site preference. When $0 < \eta_{X-Nb} < 2.04\%$, X would occupy the Nb site.

(3) The site occupancy behaviors of X in NbCr$_2$ is mainly affected by radii of transition elements. This is consist with the relation between site preference energy (ΔE) and radii of transition elements.

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