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On the structure of the *B2* phase in Ti–Al–Mo alloys

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The structure of the *B2* phase has been investigated in Ti-26Al-20Mo and Ti-37.5Al-12.5Mo alloys using Rietveld refinement of x-ray diffraction data in homogenized conditions. Different initial structure models have been used for the refinement. The site occupancy of the *B2* phase has been calculated and compared to those of earlier experimental and theoretical investigations. © 2008 American Institute of Physics. [DOI: 10.1063/1.2931004]

I. INTRODUCTION

There has been substantial and sustained interest in the research and development of the titanium based *B2* intermetallic compounds since it is one of the constituents of Ti₃Al (α_2 +*B2*), *O*-phase (Ti₂AlNb+*B2*), and TiAl (γ +*B2*) based alloys being developed for high temperature applications.^{1–3} The *B2* is an ordered body-centered cubic (*Pm*-3*m*) phase designated as *L2*₀ in ternary alloys (Fig. 1). It is formed by three groups of metallic elements, namely, *X* (Ti, Zr, and Hf), Al, and *M* (V, Nb, Ta, Cr, Mo, and W). Both *X* and *M* may correspond either to an individual element or to a combination of elements of each group.⁴ All the elements in *X* and *M* groups are α (cph) and β (bcc) phase stabilizers, respectively. The stoichiometry of the *B2* phase has been reported as either *X*₂Al*M* or *X*₄Al₃*M*, although it has been observed to have several nonstoichiometric compositions with wide range of *X*, Al, and *M* concentrations.^{4–10} The degree of order and corresponding sublattice occupation of the *B2* phase strongly depend on the alloy composition, which in turn affects the mechanical properties.

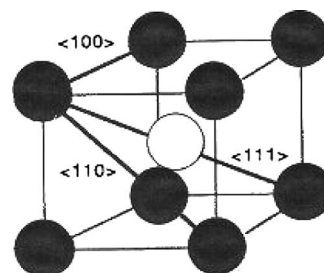
The *B2* phase has been observed in Ti–Al–Mo system in a series of alloys.^{4,5,7–11} These alloys possess both the stoichiometric as well as nonstoichiometric compositions either having the single *B2* phase or mixture of two or three phases (α_2 +*B2*, α_2 + γ +*B2*). The site occupancy of *B2* phase in Ti–Al–Nb alloys has been studied using channeling enhanced microanalysis,^{12,13} and Rietveld refinement of neutron diffraction data.¹⁴ Recently, the site occupancy of the *B2* phase in the Ti-25Al-25Mo alloy has been reported using Rietveld refinement of x-ray and neutron diffraction data.⁵ However, such a study has received limited attention in the *B2* phase of nonstoichiometric Ti–Al–Mo alloys.⁹ Azad *et al.* have predicted the site occupancy of *B2* phase in the Ti-42Al-6Mo alloy by comparing the intensity of calculated and observed *B2* reflections in x-ray diffraction (XRD) pattern.⁹ The present work is thus concerned to study the structure of the *B2* phase in two non-stoichiometric Ti-26Al-20Mo and Ti-37.5Al-12.5Mo alloys using Rietveld refinement of XRD data. The attempt has been made to study the site occupancy of alloying elements of the *B2* phase in these alloys. It is to

be noted that the composition of these experimental alloys are similar to those of the *B2* phase observed in *O*+*B2* and γ +*B2* based alloys, which are currently being developed for high temperature structural applications.^{1–4}

II. EXPERIMENTAL PROCEDURE

The alloys with nominal compositions Ti-26Al-20Mo and Ti-37.5Al-12.5Mo were prepared by using nonconsumable arc melting. 600 g pancakes of these alloys were melted six to seven times to ensure chemical homogeneity. The Ti-26Al-20Mo alloy was homogenized at 1200 °C for 30 min and air cooled while the Ti-37.5Al-12.5Mo alloy was solution treated at 1400 °C for 60 min and air cooled. The idea of selecting these temperatures for homogenization was to get the single phase *B2* structure after homogenization/solution treatment. The microstructures of the cast and homogenized alloys were initially examined using an optical microscope and a scanning electron microscope (SEM). The specimens for optical and SEM observations were prepared following standard metallographic techniques for titanium and its alloys and etched with Kroll's reagent (5 ml HF, 10 ml HNO₃, and 85 ml H₂O). After confirming that the homogenized alloys contain a single *B2* phase, the analyzed chemistry was obtained by electron probe microanalysis. The analyzed chemistry was found to be Ti 56.2, Al 25.3, and Mo 18.5 (at. %) and Ti 50.1, Al 37.8, and Mo 12.1 (at. %) for the Ti-26Al-20Mo and Ti-37.5Al-12.5Mo alloys, respectively.

The XRD studies of cast alloys were carried out with the bulk samples using Cu *K* α radiation (operated at 40 kV and 25 mA). A scanning speed of 1/4deg/min in continuous mode was used and x-ray diffractograms were recorded with a range of 38°–120°. The powders of homogenized alloys

FIG. 1. Crystal structure of the *B2* phase.

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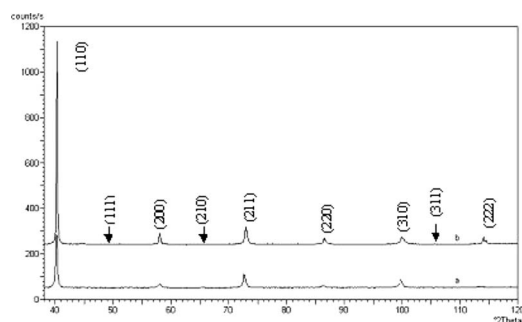


FIG. 2. XRD patterns of the as cast alloys: (a) Ti-26Al-20Mo and (b) Ti-37.5Al-12.5Mo.

were made by filing and then subjected to stress relieving treatment at 400 °C for 100 h. The XRD patterns of stress relieved powder samples were recorded in a Philips PW3020 diffractometer equipped with a graphite monochromator operated at 40 kV and 25 mA in a step size of 0.01° (2θ) and counting time of 3 s step. The XRD data were subjected to the Rietveld refinement program using Philips Xpert plus.

III. RESULTS AND DISCUSSION

The XRD patterns of the as cast alloys exhibit the presence of the *B2* phase only (Fig. 2). Both the alloys exhibit very high intensity of (110) reflection in comparison with other planes, which indicates the presence of strong (110) texture in the as cast materials. The XRD patterns of the powders of homogenized alloys (Figs. 3 and 4) also reveal the presence of a single *B2* phase. The intensity ratios of I_{hkl}/I_{110} of the XRD patterns (Figs. 3 and 4) of both the alloys do not indicate the true nature of the powder patterns of the *B2* phase and this can be attributed to graininess referred as an inadequate powder average.¹⁵ The backscattered electron micrographs confirm the presence of a single phase microstructure. A typical representative of this microstructure for the homogenized Ti-37.5Al-12.5Mo alloy is shown in Fig. 5.

The *B2* phase contains two distinct sublattices *A* and *B*, which are located at the cell corners (0, 0, 0) and at body-centered positions ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$), respectively (Fig. 1). The struc-

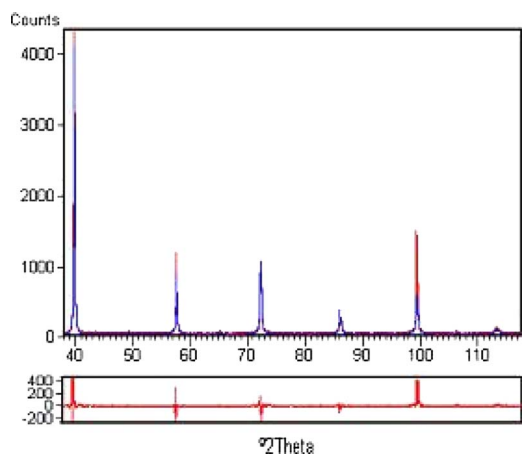


FIG. 3. (Color online) Observed and difference XRD patterns of the Ti-26Al-20Mo alloy.

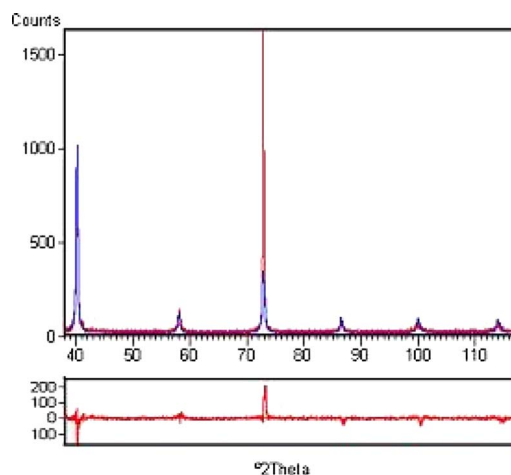


FIG. 4. (Color online) Observed and difference XRD patterns of the Ti-37.5Al-12.5Mo alloy.

ture may be considered to be chemically layered in the [001] direction with alternate planes consisting of *A* and *B* sublattices. The {110} planes, on the other hand, contain equal proportion of both the sublattices and are representative of the unit cell chemistry.

The stoichiometric compositions of both the experimental alloys Ti-26Al-20Mo and Ti-37.5Al-12.5Mo are Ti_2AlMo and $\text{Ti}_4\text{Al}_3\text{Mo}$, respectively. The possibilities of site occupancies in the stoichiometric Ti_2AlMo alloy having the *B2* phase can be classified as follows.

- (1) The Ti atoms may occupy *A* sublattice sites and Al and Mo atoms together occupy the *B* sites (model 1: $A\text{-Ti}_{100}$; $B\text{-Al}_{50}\text{Mo}_{50}$).
- (2) Mo and Al atoms may occupy *A* and *B* sites, respectively while Ti atoms are distributed on both the sites (model 2: $A\text{-Ti}_{50}\text{Mo}_{50}$; $B\text{-Al}_{50}\text{Ti}_{50}$).
- (3) Mo atoms are equally distributed on both *A* and *B* sites. The remaining vacancy of *A* sites are occupied by Ti atoms, while the excess Ti atoms, and Al atoms are occupied on *B* sites (model 3: $A\text{-Mo}_{25}\text{Ti}_{75}$; $B\text{-Mo}_{25}\text{Al}_{50}\text{Ti}_{25}$).
- (4) Al atoms are equally distributed on both *A* and *B* sites. The remaining vacancy of *A* sites are occupied by Ti atoms, while the excess Ti atoms and Mo atoms are occupied on *B* sites (model 4: $A\text{-Al}_{25}\text{Ti}_{75}$; $B\text{-Al}_{25}\text{Mo}_{50}\text{Ti}_{25}$).

The nature of interactions among Ti-Al, Al-Mo, and Ti-Mo bonds and corresponding bond energy finally decide the possibility of site occupancy in the alloy.

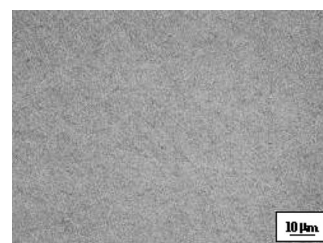


FIG. 5. BSE microstructure of the homogenized Ti-37.5Al-12.5Mo alloy.

TABLE I. The initial models of site occupancy and corresponding Rietveld refinement parameters of x-ray powder diffraction data of the Ti-26Al-20Mo alloy.

Serial No.	Site occupancy model		Rp	Rwp	Rexp	GOF	Lattice parameter (nm)
	A site	B site					
1	Ti (100)	Al (50.6) Mo (37.0) Ti (12.4)	19.31	24.26	12.96	3.504	0.3194
2	Mo (37.0) Ti (63.0)	Al (50.6) Ti (49.4)	22.67	29.60	12.96	5.216	0.3195
3	Mo (18.5) Ti (81.5)	Mo (18.5) Al (50.6) Ti (30.9)	21.47	27.13	12.96	4.382	0.3194
4	Al (25.3) Ti (74.7)	Al (25.3) Mo (37.0) Ti (37.7)	19.66	24.89	12.96	3.690	0.3194

The experimental alloy in the present study is not stoichiometric. As a result, the possibilities of site occupancies in this alloy are different than that of stoichiometric composition. These are given in Table I. Model 1 of stoichiometric alloy now exhibits a slightly different possibility. The Ti atoms are occupied on A sites, while the Al and Mo atoms tend to occupy on B sites. Since Ti atoms form occupation probability more than 1, the excess Ti atoms are occupied on B sites.

The site occupancy in model 2 (Table I) corresponds to the site occupancy of case (2) of the stoichiometric composition. The only difference in this case is that Ti atoms are not equally distributed on both the sites. Ti atoms are distributed according to the vacancy available on a particular site to make the same completely filled these sites. Structure models 3 and 4 (Table I) are equivalent of models 3 and 4 of the stoichiometric alloy, respectively, wherein Mo and Al atoms are equally distributed on both the sites. The remaining vacancy of A sites are filled with Ti atoms, while B sites are occupied by Al (model 3) and Mo (model 4) atoms, respectively. In both the models (3 and 4), the remaining vacancies of B sites are filled by excess Ti atoms.

The XRD data of homogenized powder of the Ti-26Al-20Mo alloy was subjected to Rietveld refinement. The refinement was carried out for the B2 structure only by fixing the space group and corresponding Wyckoff positions. The occupancies of Ti, Mo, and Al atoms on A and B sites were systematically varied (models 1–4), as described in Table I to refine the B2 structure. The important refinement parameters such as residual profile (Rp), residual expected (Rexp), residual weighted profile (Rwp), and goodness of fit (GOF) and corresponding lattice parameters are given in Table I. It is to be mentioned here that a small value of GOF along with the correct chemistry of the alloy results in the best solution of the refinement. The lattice parameter of the experimental alloys calculated by the Rietveld refinement of XRD data in the present study along with those reported in literature in Ti_2AlM systems are given in Table II.

The GOF values of structure models 2–4 are higher than that of model 1. This in turn shows that site occupancies of

structure models 2–4 for the B2 phase do not result in the best solution for refinement. Therefore, these models do not have the right choice of site occupancy. Structure model 1, however, exhibits the lowest value of GOF indicating the best solution for refinement. Hence, structure model 1 represents the right choice of site occupancy in the Ti-26Al-20Mo alloy.

The possibilities of site occupancies in the stoichiometric Ti_4Al_3Mo alloy having the B2 phase can be classified as follows.

- (1) The Ti atoms may occupy A sublattice sites and Al and Mo atoms together occupy the B sites (model 1: A-Ti₁₀₀; B-Al₇₅, Mo₂₅).
- (2) Mo and Al atoms may occupy A and B sites, respectively, while Ti atoms are distributed on both the sites (model 2: A-Ti₇₅, Mo₂₅; B-Al₇₅Ti₂₅).
- (3) Mo atoms are equally distributed on A and B sites. The remaining vacancies of A sites are occupied by Ti atoms, while the excess Ti atoms and Al atoms are occupied on B sites (model 3: A-Mo_{12.5}, Ti_{87.5}; B-Mo_{12.5}, Al₇₅Ti_{12.5}).
- (4) Al atoms are equally distributed on A and B sites. The remaining vacancy of A sites are occupied by Ti atoms while the excess Ti atoms and Mo atoms are occupied on B sites (model 4: A-Al_{37.5}, Ti_{62.5}; B-Al_{37.5}, Mo₂₅, Ti_{37.5}).

TABLE II. Lattice parameter of the B2 phase in Ti–Al–M systems obtained by x-ray and neutron diffractions.

Alloy	Lattice parameter (nm)	Technique	References
Ti-25Al-10Nb-3V-1Mo	0.323(1)	XRD	16
Ti-25Al-25Nb	0.324(5)	Neutron diffraction	14
Ti-27Al-20Nb	0.326(5)	Neutron diffraction	14
Ti-25Al-25Mo	0.317	XRD	7
Ti-25Al-25Mo	0.318(3)	XRD	5
Ti-25Al-25Mo	0.318(5)	Neutron diffraction	5
Ti-26Al-20Mo	0.319(4)	XRD	Present work
Ti-37.5Al-12.5Mo	0.319(5)	XRD	Present work

TABLE III. The initial models of site occupancy and corresponding Rietveld refinement parameters of x-ray powder diffraction data of the Ti-37.5Al-12.5Mo alloy.

Serial No.	Site occupancy model		Rp	Rwp	Rexp	GOF	Lattice parameter (nm)
	A site	B site					
1	Ti (100)	Al (75.6) Mo (24.2) Ti (0.2)	24.11	31.04	12.92	3.067	0.3194
2	Mo (24.2) Ti (75.8)	Al (75.6) Ti (24.4)	25.58	33.12	12.92	4.453	0.3194
3	Mo (12.1) Ti (87.9)	Mo (12.1) Al (75.6) Ti (12.3)	24.12	31.05	12.92	3.211	0.3194
4	Al (37.8) Ti (62.2)	Al (37.8) Mo (24.2) Ti (38.0)	24.35	31.25	12.92	3.243	0.3194

The experimental alloy in the present study is not stoichiometric. As a result, the possibilities of site occupancies in this alloy are different than those of stoichiometric composition. These are given in Table III. In model 1, the Ti atoms are occupied on A sites, while the Al and Mo atoms tend to occupy on B sites. The excess Ti atoms are also occupied on B sites. The site occupancy in model 2 (Table III) corresponds to the site occupancy of case (2) of the stoichiometric composition. The only difference in this case is that Ti atoms are distributed on both the sites according to the vacancy available on a particular site to make the same completely filled. Structure models 3 and 4 (Table III) are equivalent to models 3 and 4 of the stoichiometric alloy, respectively, wherein Mo (model 3) and Al (model 4) atoms are equally distributed on both the sites. The remaining vacancies of A sites are filled with Ti atoms, while B sites are occupied by Al (model 3) and Mo (model 4) atoms, respectively. In both the models (3 and 4), the remaining vacancies of B sites are filled by excess Ti atoms.

The XRD data of homogenized powder of the Ti-37.5Al-12.5Mo alloy was subjected to Rietveld refinement for the B2 structure only by fixing the space group and corresponding Wyckoff positions. The occupancies of Ti, Mo, and Al atoms on A and B sites were systematically varied (models 1–4), as described in Table III to refine the B2 structure. The important refinement parameters such as Rp, Rexp, Rwp, and GOF and corresponding lattice parameters are given in Table III. Structure model 1 (Table III) results in the smallest value of GOF in comparison with those of models 2–4. This indicates that structure model 1 exhibits the best solution for refinement amongst all the four models and hence represents the correct choice of site occupancy in the Ti-37.5Al-12.5Mo alloy.

Another scheme of site occupancy has also been considered for both the alloys, wherein A sites are occupied by Ti atoms, while B sites are occupied by Al and Mo atoms. It is to be noted that the total numbers of Ti atoms in both the alloys give occupation probabilities greater than 1. This implies the presence of constitutional vacancies on B sites.

Therefore, vacant sites have also been allowed for on B sites during Rietveld refinement of XRD data. This has resulted in high GOF values in comparison with structure model 1 of Tables I and III. This suggests that the consideration of vacant sites in both the experimental alloys gives poorer refinement. Singh *et al.* have recently studied the site occupancy of the Ti-25Al-25Mo alloy based on the Rietveld refinement of x-ray and neutron diffraction data and observed poorer refinement after consideration of constitutional vacant sites.⁵ Therefore, based on the Rietveld refinement of XRD data of the present study, it appears that the B2 phase of the Ti-26Al-20Mo and Ti-37.5Al-12.5Mo alloys does not indicate the presence of constitutional vacant sites.

The site occupancy of B2 phase in the Ti-25Al-10Nb alloy has been studied by Banerjee *et al.*¹² based on channeling enhanced microanalysis technique. It has been shown that the Ti atoms tend to occupy A sites, while Al and Nb atoms tend to occupy the B sites. A small amount of Nb is also observed on the A sites. This has been attributed to the antisite effect, which occurs in nonstoichiometric compositions. On the other hand, Konitzer *et al.*¹⁷ have observed that the Nb atoms go to Ti sites in the Ti-20Al-5Nb and Ti-25Al-5Nb alloys. It is to be noted that the alloys used by Banerjee *et al.*¹² and Konitzer *et al.*¹⁷ exhibit ($\alpha_2 + B2$) and α_2 phases, respectively.

The sublattice occupation of the B2 phase has been studied by Nandy *et al.*¹³ through a simple Bragg–Williams approach by considering first neighbor interactions, in which total bond energy on alloying is computed for different sublattice occupations and this has been used as a parameter for determining site occupancy. They have selected a series of alloying elements such as Mo, V, Hf, Ag, and Co in the range of 2–4 at. % to a base composition of the Ti-24Al-11Nb alloy. The results obtained by thermodynamic analysis have been compared to experimentally determined site occupancy using channeling enhanced microanalysis by transmission electron microscopy. It has been shown that the Ti atoms occupy A sites, while Mo atoms occupy on B sites along with Al and Nb atoms.

Chaumat *et al.*¹⁴ have performed a detailed Rietveld

analysis of the neutron diffraction data of the Ti-25Al-25Nb and Ti-27Al-20Nb alloys having a single $B2$ phase and calculated site occupancy. They have compared the experimental results to those obtained by the cluster variation method calculation. Neutron diffraction results have shown that the sublattice occupation of the $B2$ phase is sensitive to the alloy composition. They have also observed that there is a constraint on the Ti and Al atom distribution on the sites. The Ti and Al atom preferably occupy on A and B sites, respectively. The occupancy of Nb atoms depends on the vacant occupation according to the concentration of the alloy. However, a slight ordering of Nb atoms on the B sites has been observed.

Recently, Singh *et al.*⁵ have studied the site occupancy of the Ti-25Al-25Mo alloy using Rietveld refinement of x-ray and neutron diffraction data. It has been shown that the Al atoms are occupied on B sites and most of the Mo atoms are also occupied on the same site. The excess Mo atoms tend to occupy A sites wherein the Ti atoms are occupied. It is to be noted here that either the presence of excess Mo or due to antisite effect (as shown by Banerjee *et al.*¹²), the A sites in $B2$ phase will be occupied by Ti and Mo atoms, while the B sites will be occupied by Al and Mo atoms. In this case, the concentration of Ti in the alloy should be less than 50 at. %.

The site occupancy in the $B2$ phase has also been studied based on concept that the atom configuration in an ordered alloy with two sublattices can be described by an ordering tie line (OTL).^{18,19} The OTL is similar to a tie line in a ternary phase diagram. This is defined as the tie line connecting the compositions of the individual sublattices when these are plotted on a compositional diagram. It has been shown that the trend for site occupancies can easily be deduced as soon as the sublattice compositions are determined using OTL analysis. The $B2$ phase is in most ordered state only when all the Al atoms tend to occupy on one type of site (say, B site). Banerjee *et al.*¹² have made the same assumption for determining the site occupancy of $B2$ phase in the Ti-25Al-10Nb alloy. In addition, most of the Nb atoms occupy the same sites that are occupied by Al atoms.

The present result thus shows that the Ti atoms are occupied on A sites, while the Al and Mo atoms are occupied on B sites. The excess Ti atoms tend to occupy B sites since the concentration of Ti in both the alloys are greater than 50 at. %. It is to be noted here that either the presence of excess Ti atoms or due to antisite effects (as discussed by Banerjee *et al.*¹²), the B sites in $B2$ phase of the present experimental alloys will be occupied by Al, Mo, and excess Ti atoms, while the A sites will be occupied by only Ti.

The $B2$ phase stabilized within a wide range of compositions of both the Ti and Al along with the β -stabilizing element M (M =Nb, Mo, Ta, V etc.). The site occupancies of $B2$ phase can therefore be classified into two groups: (1) the alloys containing Ti \leq 50 at. % and (2) the alloys containing Ti \geq 50 at. %. In the case of the alloys containing \leq 50 at. % Ti, the A sites are occupied by Ti atoms, while the B sites are occupied by Al and M atoms. The small amount of M atoms can also occupy A sites either due to the excess from B site or antisite effect in nonstoichiometric alloys. The results ob-

tained by Singh *et al.*⁵ and Banerjee *et al.*¹² are such examples. In the case of alloys containing Ti \geq 50 at. %, the A sites are occupied by Ti atoms, while the B sites are occupied by Al and M atoms. The excess Ti atoms are occupied on B sites. The $B2$ phase of the present experimental Ti-26Al-20Mo and Ti-37.5Al-12.5Mo alloys and that of the Ti-42Al-6Mo alloy reported by Azad *et al.*⁹ belongs to this class.

This has been shown by the calculation of Saunders²⁰ that the strongest pair of interaction in Ti-Al- M (M =Nb, Mo, Ta, V, etc.) systems is between Al and Ti and, M respectively. As a result, the $B2$ phase is stabilized by obtaining the maximum number of first neighbor Ti-Al and/or Al-Mo bonds. It appears that the site occupancy in alloys having a $B2$ phase follows the same criteria and variation of the occupation on A and B sites strongly depends on the alloy composition.

It has been clearly demonstrated in the present experimental alloys having Ti concentration greater than 50 at. % that the excess Ti atoms tend to occupy B sites. As discussed above that when the Ti concentration is $<$ 50 at. %, the excess of Mo atoms occupies the A sites.⁵ The Al atoms are not permitted to occupy A sites consisting of mostly Ti atoms. The $B2$ phase has also been observed in several other technologically important systems such as FeAl and NiAl based alloys. In all these alloys, finer details of the structure of the $B2$ phase play significant role in controlling the mechanical properties. Therefore, it is important to understand the nitty-gritty of this class of alloys having both the stoichiometric and nonstoichiometric compositions. This will provide an exact basis to classify the $B2$ phase based on the composition, site occupancy, and presence of constitutional vacant sites and their correlation to mechanical properties.

IV. CONCLUSION

The site occupation of the $B2$ phase in Ti-26Al-20Mo and Ti-37.5Al-12.5Mo alloys has been calculated using the Rietveld refinement of XRD. It has been shown that the Ti atoms tend to occupy A sites, while Al and Mo atoms occupy B sites. The excess Ti atoms occupy B sites.

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