Site Occupancy of the B2 Phase in Ti-25Al-zMo Alloys

A. K. Singh, Materials Science Division, Defence Metallurgical Research Laboratory, Hyderabad, AP, India

M. Premkumar, Materials Science Division, Defence Metallurgical Research Laboratory, Hyderabad, AP, India

ABSTRACT

The structure of the B2 phase has been investigated in Ti-25Al-30Mo, Ti-25Al-35Mo and Ti-25Al-40Mo alloys using Rietveld refinement of X-ray diffraction data in homogenized condition. Different initial structure models have been used for the refinement based on the analyzed alloy chemistry. Site occupancy models for the general alloy compositions (xTi-yAl-zMo) wherein the Ti (x) is less than 50 atom % have been proposed. The site occupancy of the B2 phase has been calculated and compared with those of earlier experimental and theoretical investigations. The lattice parameter of the B2 phase decreases with increase in Mo content at constant Al.

Keywords: Alloys, Homogenized Conditions, Phase Transformation, Site Occupancy, Titanium Aluminides, X-Ray Diffraction

1. INTRODUCTION

The intermetallic compounds with B2 (ordered bcc, CsCl type) structure have been observed in several binary, ternary and multi-component alloys (Banerjee, 1993; Banerjee, 1997; Kim, 1989; Bradley & Taylor, 1937). The stoichiometric composition of this phase in binary alloy is AB while in ternary alloys is $A_2BC$ or $A_4B_3C$. However, these alloys often exist over a wide range of compositions on either side of the stoichiometric composition. The deviations from the stoichiometric composition are accommodated by constitutional defects namely vacancies on the different sublattice sites and/or antisites (Bradley & Taylor, 1937). The properties of the B2 phase change drastically with deviation from stoichiometric composition (Westbrook, 1967). This behavior is quite different from that of solid solution for which properties normally vary smoothly with compositions (Westbrook, 1967).

The existence of B2 phase has been identified in several Ti$_3$Al, Ti$_2$AlNb and TiAl based alloys as well as in Nb and Ta based alloys (Naka et al., 1992; Naka et al., 1993; Singh et al., 2007; Bendersky et al., 1990; Bohm & Lohberg, 1958; Hamajima et al., 1972; Azad et al., 2006; Das & Das, 2003; Chaumat et al., 1999; Banerjee et al., 1987; Nandy et al., 1988; Singh et al., 2008; Haddad et al., 1994). Naka et al. (1993) have proposed a classification of
alloying elements of titanium based B2 phase into three groups which are X (Ti, Zr, Hf), Al and M (V, Ta, Nb, Cr, Mo, W etc.). Both the X and M may correspond either to an individual element or to a combination of elements of each group. The elements in group X and M exhibit close packed hexagonal (cph) and body centred cubic (bcc) structures at room temperature, respectively.

Site occupancy of the B2 phase can be experimentally determined by several competing or supplementary techniques and also can be predicted theoretically. This has been summarized by Jones in his review article on the determination of locations of chemical species in ordered compounds using atom location by channeling enhanced microanalysis (ALCHEMI) (Jones, 2003). Rietveld refinement of X-ray and neutron diffraction data is one of the techniques which has been used to determine site occupancy of the B2 phase for stoichiometric and non-stoichiometric alloys (Chaumat et al., 1999; Singh et al., 2007; Singh et al., 2008).

The B2 phase has been observed in Ti-Al-Mo system in a series of alloys which possess both the stoichiometric as well non-stoichiometric compositions either having single B2 phase or mixture of two or three phases (α₂ + B₂, α₂ + γ + B₂) (Bohm & Lohberg, 1958; Naka et al., 1993; Das & Das, 2003; Azad et al., 2006; Singh et al. 2007, 2008). Singh et al. (2007, 2008) have determined the site occupancy of the B2 phase in Ti-Al-Mo alloys using X-ray and neutron diffraction data. These results are classified into two groups: (1) the alloys containing Ti<50 atom % and (2) the alloys containing Ti>50 atom %. In former case, A sites are occupied by Ti atoms while the B sites are occupied by Al and Mo atoms. The small amount of Mo atoms can also occupy A sites either due to excess of B sites or anti site effect in non-stoichiometric alloys. In later case, the A sites are occupied by Ti atoms while the B sites are populated by Al and Mo atoms. The excess Ti atoms are occupied B sites.

The site occupancy of the B2 phase in Ti-Al-Nb system has been studied by several investigators (Banerjee et al., 1987; Nandy et al., 1988; Hou et al., 1996; Chaumat et al., 1999). A detailed Rietveld analysis of the neutron diffraction data of the Ti-25Al-25Nb and Ti-27Al-20Nb alloys having a single B2 phase has been carried out by Chaumat et al. (1999). They have calculated the site occupancy and compared the experimental results to those obtained by cluster variation method. These 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 atoms on the sites. The Ti and Al atoms 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.

The site occupancy of the B2 phase in an alloy Ti-25Al-10Nb has been studied using ALCHEMI technique (Banerjee et al., 1987). It has been observed that Ti atoms have a tendency to occupy A sites, while Al and Nb atoms tend to occupy the B sites. This has been attributed to antisite effect that occurs in non stoichiometric compositions. The site occupancy in B2 phase has also been studied by an ordering Tie line (OTL) based on the atom configurations of two sublattices (Hou et al., 1996; Banerjee et al., 2001). The tendency for site occupancies can easily be deduced with the sublattice compositions determined using OTL analysis. The extent of ordering of the B2 phase is highest when all the Al atoms tend to occupy on one type of sublattice (say B sites).

Nandy et al. (1988) have studied the site occupancy of the B2 phase for a series of alloying elements to a base composition of Ti-24Al-11Nb using a simple Bragg-Williams approach by considering first neighbor interactions, in which total bond energy on alloying is computed for different sublattice occupations. The results obtained by thermodynamic analysis have been compared to experimentally determined site occupancy using ALCHEMI. It has been observed that Ti atoms tend to occupy A sites, while Mo atoms occupy on B sites along with Al and Nb atoms.
11 more pages are available in the full version of this document, which may be purchased using the "Add to Cart" button on the product's webpage:
www.igi-global.com/article/site-occupancy-phase-25al-zmo/77888?camid=4v1

www.igi-global.com/e-resources/library_recommendation/?id=2

Related Content

Wear Performance Optimization for Electroless Ni-P Coating
www.igi-global.com/article/wear-performance-optimization-for-electroless-ni-p-coating/138560?camid=4v1a

Cold End Forming Of Welded Steel Tubes
www.igi-global.com/article/cold-end-forming-welded-steel/51372?camid=4v1a

Capillary Tube as an Expansion Device in a CO2 (R744) Transcritical Heat Pump System
www.igi-global.com/chapter/capillary-tube-as-an-expansion-device-in-a-co2-r744-transcritical-heat-pump-system/136753?camid=4v1a
Slurry Erosion Behavior of Thermal Spray Coatings
www.igi-global.com/chapter/slurry-erosion-behavior-of-thermal-spray-coatings/128077?camid=4v1a