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The 500 °C isothermal section of the Nd–Al–Ti ternary system

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Abstract

The phase relations in the Nd–Al–Ti ternary system at 500 °C were investigated by powder X-ray diffraction (XRD), differential thermal analysis (DTA), optical microscopy, and scanning electron microscopy (SEM) techniques. The existence of two ternary compounds $NdTi_2Al_{20}$ and $Nd_6Ti_4Al_{43}$ were confirmed. The isothermal section of this ternary system consists of 15 single-phase regions, 29 two-phase regions, and 15 three-phase regions. At 500 °C, the maximum solid solubilities of Ti in Nd_3Al, Nd_2Al, and $NdAl_2$ is about 2.4, 3.5, and 16.1 at.%, respectively, and that of Nd in Ti, Ti_3Al, TiAl is less than 1 at.%.

Keywords: Rare earth compounds; Transition metal compounds; Crystal structure; X-ray diffraction; Phase diagram

1. Introduction

Due to their good high-temperature properties and low density, the ordered intermetallic titanium aluminides, especially those based on Ti_xAl ($x = 3$ or 1), are currently under active development as attractive candidates for applications in advanced aerospace engine and air-frame components [1–3]. However, their application is hindered by low ductility and toughness at ambient temperature. Studies have revealed that certain alloying additions such as Cr, V, Nb, Ta, and rare earth elements to the binary Ti–Al system can improve ductility, oxidation resistance, and high temperature strength of titanium aluminides [4,5]. As a contribution of our systematic study of the RE–Al–Ti system [6–9], this present paper concerns the 500 °C isothermal section of the phase diagram of the Nd–Al–Ti ternary system.

The binary Al–Ti, Nd–Ti, and Nd–Al systems are accepted from Refs. [10,11]. At 500 °C there are four intermetallic compounds in the Al–Ti system, namely Ti_3Al, TiAl, $TiAl_2$, and $TiAl_3$, There are six intermetallic compounds in the Nd–Al system, namely Nd_3Al_{11}, $NdAl_3$, $NdAl_2$, NdAl, Nd_2Al, and Nd_3Al. No intermetallic phase was found in the Nd–Ti binary system.

No Nd–Ti–Al ternary phase diagram has been reported in the literature yet. However, two ternary compounds $NdTi_2Al_{20}$ and $Nd_6Ti_4Al_{43}$ have been identified by Niemann and Jeitschko [12]. The compound $NdTi_2Al_{20}$ crystallizes with the cubic $CeCr_2Al_{20}$ type structure (space group $Fd3m$) and the compound $Nd_6Ti_4Al_{43}$ crystallizes with the hexagonal $Ho_6Mo_4Al_{43}$ type structure (space group $P6_3/mcm$).

2. Experimental

One hundred and fifty samples, each weighing 2 g, were prepared starting from high purity metal blocks (purity > 99.9 mass%) of Nd, Al, and Ti. All samples were prepared by arc melting them three times under high purity argon. Then they were sealed in evacuated quartz tubes for homogenization annealing. The heat treatment temperature was determined by differential thermal analysis (DTA) results of some alloys or based on the previous work of binary systems. The Al-rich alloys and Ti-rich alloys were kept at 900 °C for 500 h, the other samples were homogenized at 700 °C for 500 h. Then the samples were cooled at a rate of 10 K/h to 500 °C and kept at 500 °C for 150 h. At last, the samples were quenched into liquid nitrogen.

The samples for X-ray diffraction (XRD) analysis were powdered and investigated by X-ray diffraction on a Rigaku D/Max 2500PC X-ray diffractometer (Cu Kα,

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monochromator), using JADE5 software [13] to analyze the angles, ranging from $2\theta = 20^\circ$ to 60° at 40 kV, 25 Ma. Some representative alloys were analyzed in an S-570 scanning electron microscope (SEM) or by differential thermal analysis. From all these result, the phase relations in the Nd–Al–Ti system were determined.

3. Results and discussion

3.1. Phase analysis

In the Nd–Al–Ti ternary system, ten binary compounds, namely Ti_3Al, TiAl, $TiAl_2$, $TiAl_3$, Nd_3Al_{11}, $NdAl_3$, $NdAl_2$, NdAl, Nd_2Al, and Nd_3Al, and two ternary compounds $NdTi_2Al_{20}$ and $Nd_6Ti_4Al_{43}$ have been reported. For all of them, excepting Nd_3Al_{11} and Nd_2Al crystallographic data are available on JCPDS PDF cards. With the crystallographic data of Nd_3Al_{11} and Nd_2Al taken from Ref. [14], using the LAZY program [15], we were able to obtain the calculated XRD pattern of the compound Nd_3Al_{11} and Nd_2Al. The results of XRD analysis of our alloy samples are in good agreement with the data on the respective JCPDS PDF cards or the calculated XRD patterns of Nd_3Al_{11} and Nd_2Al. Thus the existence of these 12 phases was confirmed.

Niemann and Jeitschko [12] reported the existence of two ternary compounds, namely $Nd_6Ti_4Al_{43}$ and $NdTi_2Al_{20}$. We prepared two alloy samples with composition of 11.3 at.% Nd, 7.6 at.% Ti, 81.1 at.% Al, and 4.3 at.% Nd, 8.7 at.% Ti, 87 at.% Al, respectively. The X-ray diffraction patterns of these samples are in agreement with the data on the respective JCPDS PDF cards, which confirms that the compounds $Nd_6Ti_4Al_{43}$ and $NdTi_2Al_{20}$ are stable phases at 500 °C. No other ternary compound was found in this system.

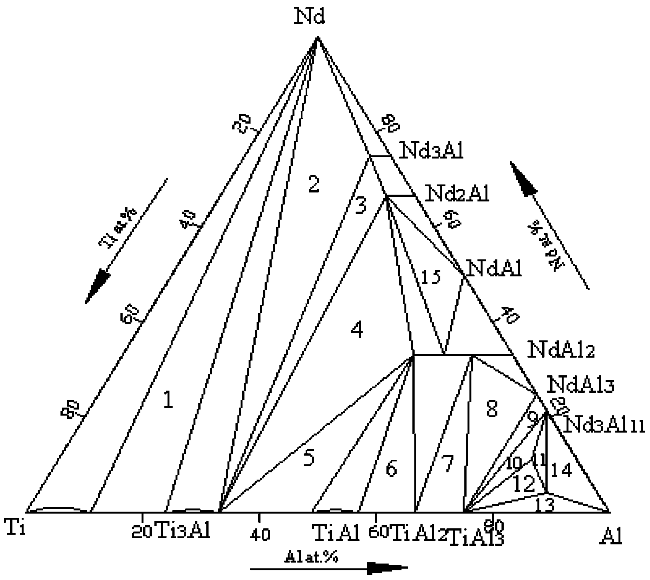

Fig. 1. The isothermal section of the phase diagram of the Nd–Al–Ti ternary system at 500 °C. A: $Nd_6Ti_4Al_{43}$; B: $NdTi_2Al_{20}$.

Table 1
Three-phase regions of the Nd–Al–Ti ternary system at 500 °C

Region number	Phase 1	Phase 2	Phase 3
1	Ti	Nd	Ti_3Al
2	Ti_3Al	Nd	Nd_3Al
3	Ti_3Al	Nd_3Al	Nd_2Al
4	Ti_3Al	Nd_2Al	$NdAl_2$
5	Ti_3Al	$NdAl_2$	TiAl
6	TiAl	$NdAl_2$	$TiAl_2$
7	TiAl	$NdAl_2$	$TiAl_3$
8	$TiAl_3$	$NdAl_2$	Nd_3Al
9	$TiAl_3$	Nd_3Al	Nd_3Al_{11}
10	$TiAl_3$	Nd_3Al_{11}	$Nd_6Ti_4Al_{43}$
11	$Nd_6Ti_4Al_{43}$	$NdTi_2Al_{20}$	Nd_3Al_{11}
12	$TiAl_3$	$Nd_6Ti_4Al_{43}$	$NdTi_2Al_{20}$
13	$NdTi_2Al_{20}$	Al	Nd_3Al_{11}
14	$NdTi_2Al_{20}$	$TiAl_3$	Al
15	Nd_2Al	NdAl	$NdAl_2$

3.2. Solid solubility

The single-phase regions in the 500 °C isothermal section were determined by X-ray diffraction. The results show that the maximum solubility of Ti in Nd_3Al, Nd_2Al, and $NdAl_2$ is about 2.4, 3.5, and 16.1 at.%, respectively, and that of Nd in Ti, Ti_3Al, TiAl is less than 1 at.%. The single phase ranges of Ti, Ti_3Al, and TiAl are from 0 to 10.5 at.% Al, from 23 to 34 at.% Al, and from 50 to 56.5 at.% Al, respectively.

3.3. Isothermal section at 500 °C

From the combination of XRD analysis, optical microscopy and SEM results of 145 alloy samples, we come

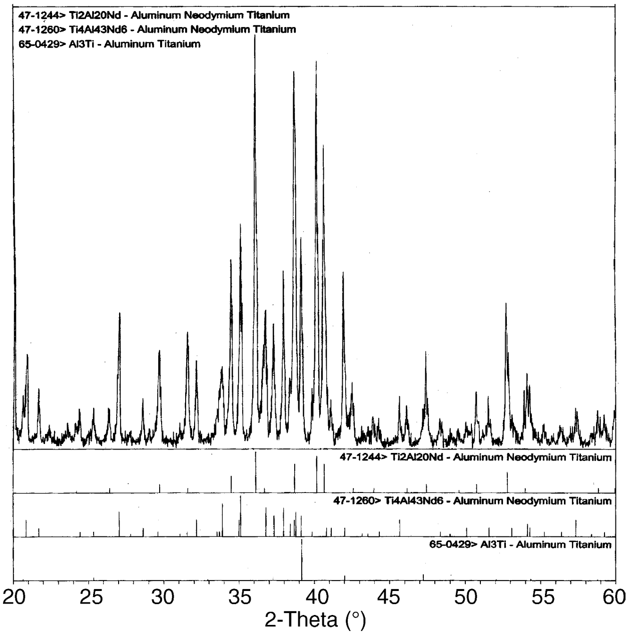

Fig. 2. X-ray diffraction (XRD) pattern of alloy the $Nd_6Ti_{12}Al_{82}$ situated in the three-phase region no. 12.

to the conclusion that no new ternary compound exists in this system at 500 °C. The phase relations in the Nd–Al–Ti ternary system are shown in Fig. 1. Details of the phase relations are shown in Table 1. The three-phase region $TiAl_3 + NdTi_2Al_{20} + Nd_6Ti_4Al_{43}$ is (no. 12) of particular interest. The XRD pattern of the alloy $Nd_6Ti_{12}Al_{82}$ which falls in this region and the corresponding three-phase equilibrium is illustrated by means of Fig. 2. The isothermal section of the Nd–Al–Ti ternary system at 500 °C consists of 15 single-phase regions, 29 two-phase regions, and 15 three-phase regions.

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