



Interactions of the components in the Al–V–Nd system at 773 K

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ABSTRACT

The phase equilibria of the Al–V–Nd ternary system at 773 K were investigated for the first time, mainly by means of X-ray powder diffraction (XRD), scanning electron microscope (SEM) and energy dispersive analysis (EDX). The existence of 11 binary compounds, i.e. $Al_{21}V_2$, $Al_{45}V_7$, $Al_{23}V_4$, Al_3V , Al_8V_5 , $Al_{11}Nd_3$, Al_3Nd , Al_2Nd , $AlNd$, $AlNd_2$ and $AlNd_3$ were confirmed. At 773 K, one ternary-phase $Nd_6V_4Al_{43}$ was confirmed and it was indicated that this compound has a hexagonal structure with space group $P6_3/mcm$ (no. 193) and the lattice parameters of $a = 1.1028$ nm, $c = 1.7931$ nm, $c/a = 1.626$ and $V = 1.893$ nm³. The isothermal section of the Al–V–Nd ternary system consists of 15 single-phase regions, 28 binary-phase regions and 14 ternary-phase regions. The solid solubility of Al in V is up to 39 at.% Al at 773 K.

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1. Introduction

Aluminum alloys are important structural materials for many fields due to their prominent properties like light weight, corrosion resistance, reasonably good strength and ductility, easy fabrication and favorable economics [1]. The alloys of aluminum with the rare earth metals have shown some interesting phenomena. For example, Lanthanide additions to Al-based alloys are very effective in enhancing mechanical properties [2–5] and corrosion resistance [6]. It is of academic interest to investigate into the phase equilibria related to the Al–RE (RE = rare earth)–M (M = metallic alloying elements for Al alloys) systems [7–9], so as to provide useful information for the study of the mechanism of rare earths on Al alloys. Up to now, the phase diagram of the Al–V–Nd ternary system has not been reported yet. The purpose of the present work is to experimentally determine the isothermal section of the phase diagram of the ternary system Al–V–Nd using equilibrated method.

In the binary Al–V system five phases have been reported, namely $Al_{21}V_2$ (also designated $Al_{11}V$ or $Al_{10}V$, cF184, $Fd\bar{3}m$, $Al_{21}V_2$ -type), $Al_{45}V_7$ (also designated Al_7V , mC104, C2/m, $Al_{45}V_7$ -type), $Al_{23}V_4$ (also designated Al_6V , hP54, $P6_3/mmc$, $Al_{23}V_4$ -type), Al_3V (tI8, I4/mmm, Al_3Ti -type) and Al_8V_5 (cI52, $I\bar{4}3m$, Cu_5Zn_8 -type). It also shows that Al with some solid solubility in V. The phase equilibria in the Al-rich part of the Al–V system are quite complex and were later reinvestigated by Richter and Ipser [10]. On the V-rich side, high melting temperatures make the liquidus and solidus temperatures difficult to measure and also make equilibrium diffi-

cult to achieve in the solid state. Interest in the possibility that AlV₃ would have good superconducting properties has led to numerous investigations around 75 at.% V, with conflicting results [11].

According to previous papers [7,8], there are six intermetallic compounds, i.e. $Al_{11}Nd_3$ (oI28, Immm, $Al_{11}La_3$ -type), Al_3Nd (hP8, $P6_3/mmc$, Ni_3Sn -type), Al_2Nd (cF24, $Fd\bar{3}m$, Cu_2Mg -type), $AlNd$ (oP16, Pbcm, AlDy-type), $AlNd_2$ (oP12, Pnma, Co_2Si -type) and $AlNd_3$ (hP8, $P6_3/mmc$, Ni_3Sn -type) in the Al–Nd system. Crystal structures and lattice constants of all the Nd–Al phases can be found in Ref. [12].

The Nd–V binary-phase diagram was reported in Ref. [13], the existence of any compounds was not observed.

For the Al–V–Nd ternary system, one ternary compound named $Nd_6V_4Al_{43}$ has been reported by Wolff et al. [14] and Niemann et al. [15].

2. Experimental details

In the present work, each sample was prepared with a total weight of 1.5 g by weighing appropriate amounts of the pure components (Nd: 99.9 wt.%, Al: 99.99 wt.%, V: 99.99 wt.%). 89 alloy buttons have been produced by arc melting on a water-cooled copper crucible with a non-consumable tungsten electrode under pure argon atmosphere. Titanium was used as an oxygen getter during the melting process. Each as-arc-cast button was melted three times and turned around after melting for better homogeneity. For most alloys, the weight loss is less than 1% after melting.

The melted alloys were sealed in an evacuated quartz tube. The tube was placed in a resistance furnace for homogenization treatment and then annealed at different temperatures in order to attain good homogenization. The heat treatment temperature of the alloys was determined by differential thermal analysis (DTA) results of some typical ternary alloys or based on previous works of the three binary-phase diagrams. The Al-rich alloys containing more than 40 at.% Al were homogenized at 873 K for 600 h. The other alloy samples were homogenized at 1173 K for 480 h. Subsequently, the furnace was cooled down to 773 K and kept at this temperature for 240 h. Then, the samples were removed and quenched in liquid nitrogen.

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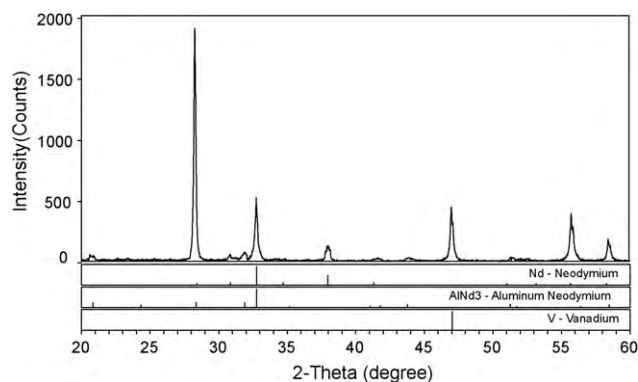


Fig. 1. XRD pattern of the equilibrated alloy (14 at.% Al, 12 at.% V and 74 at.% Nd) indicating the existence of Nd, V and AlNd₃.

All the equilibrated samples were powdered and then analyzed on a Rigaku D/Max-2500 V diffractometer with Cu K α radiation and graphite monochromator operated at 40 kV, 200 mA. The Materials Data Inc. software Jade 5.0 and Powder Diffraction File (PDF release 2003) were used for phase identification. Scanning electron microscopy (SEM) with energy dispersive analysis (EDX) was employed for microstructure and phase analysis. By all these means, the phase relationships of the Al–V–Nd ternary system at 773 K were determined.

3. Results and discussion

3.1. Binary system

3.1.1. V–Nd system

The present work has indicated that no binary compound exists in the V–Nd system. The XRD pattern of the equilibrated alloy with atomic proportion of 14 at.% Al, 12 at.% V and 74 at.% Nd shows that there is no intermediate compound at 773 K (Fig. 1), which agrees well with the results of Ref. [13].

3.1.2. Al–V system

The Al–V phase diagram [11] shows five intermediate phases, which are Al₂₁V₂, Al₄₅V₇, Al₂₃V₄, Al₃V and Al₈V₅. In this work, all the above intermediate phases have been confirmed in the Al–V system at 773 K. The XRD pattern of the equilibrated alloy with atomic proportion of 81 at.% Al, 15 at.% V and 4 at.% Nd shows that there are Al₂₃V₄, Al₃V and Nd₆V₄Al₄₃ phases exist, as illustrated in Fig. 2a. As an example, the microstructure of this sample was examined by SEM and it clearly indicated the existence of three-phases (Fig. 2b). EDX result indicated that the pale phase was Nd₆V₄Al₄₃, the gray one was Al₂₃V₄, and the black phase was Al₃V. In addition, the XRD pattern of the equilibrated sample with composition of 72 at.% Al, 25 at.% V and 3 at.% Nd clearly indicates the existence of three-phases, i.e. Al₃V, Al₈V₅ and Al₂Nd in Fig. 3a. From Fig. 3b, the microstructure of #48 sample (72 at.% Al, 25 at.% V and 3 at.% Nd) examined by SEM clearly reveals the above three-phases. EDX result indicated that the black phase was Al₃V, the gray one was Al₈V₅, and the white phase was Al₂Nd. Two other binary compounds i.e. AlV₃ and Al₅₀V₅₀ (also designated AlV) have been reported in Ref. [16]. It was also reported that the new compound AlV was discovered in the course of a re-investigation of the system at 773 K. In this work, the two compounds AlV₃ and Al₅₀V₅₀ (AlV) were not observed, which agrees well with Ref. [10]. In other words, they are considered to be high temperature phases in both experimental and thermodynamical ways.

3.1.3. Al–Nd system

In the Al–Nd system, the phase diagram [17,18] shows six intermediate phases, namely, Al₁₁Nd₃, Al₃Nd, Al₂Nd, AlNd, AlNd₂ and AlNd₃. It is confirmed in this work that these binary compounds

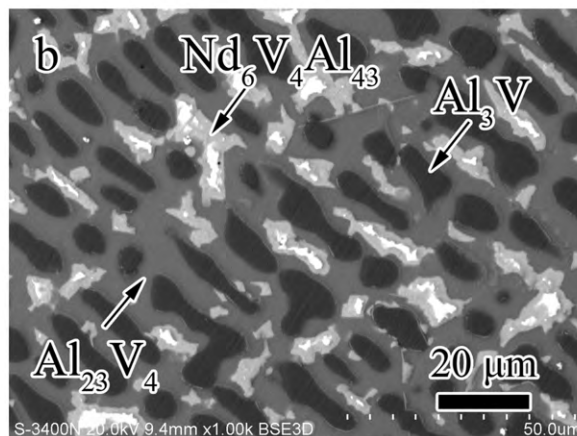
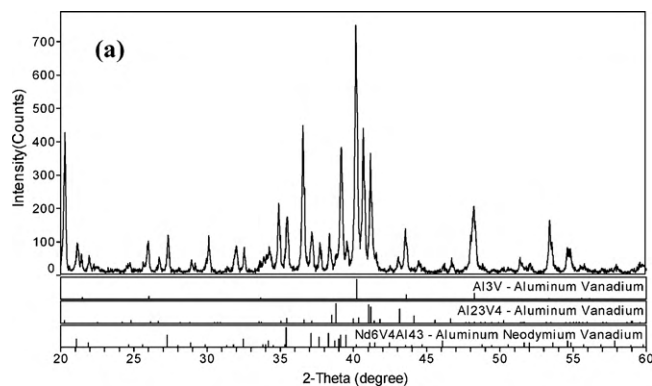


Fig. 2. XRD pattern (a) and SEM micrograph (b) of the equilibrated sample prepared with atomic proportion of Al 81 at.%, V 15 at.% and Nd 4 at.%, showing the existence of Al₂₃V₄, Al₃V and Nd₆V₄Al₄₃.

all exist at 773 K. As illustrated in Fig. 4a, the XRD pattern of the equilibrated sample containing 79 at.% Al, 2 at.% V and 19 at.% Nd clearly indicates the existence of Al₁₁Nd₃, Al₃Nd and Nd₆V₄Al₄₃. From Fig. 4b, SEM image of this sample shows three-phases of Al₁₁Nd₃, Al₃Nd and Nd₆V₄Al₄₃. EDX result indicated that the black phase was Al₁₁Nd₃, the gray one was Nd₆V₄Al₄₃ while the white phase was Al₃Nd. Fig. 5 illustrates the XRD pattern of the equilibrated alloy with atomic proportion of 67 at.% Al, 17 at.% V and 16 at.% Nd. It reveals the existence of Al₃Nd and Al₂Nd. Besides, in Fig. 6, AlNd and AlNd₂ can be clearly observed. Therefore, there are six binary compounds in the Al–Nd binary system at 773 K, which agrees well with Refs. [7,8].

3.2. Ternary-phases

The existence of ternary compound Nd₆V₄Al₄₃ at 773 K was confirmed in this work and its reported structural data is given in Table 1. In this work, the XRD patterns of #24 sample (81 at.% Al, 15 at.% V and 4 at.% Nd) and #25 sample (79 at.% Al, 2 at.% V and 19 at.% Nd) clearly indicates the existence of Nd₆V₄Al₄₃, as illustrated in Figs. 2a and 4a. The existence of this ternary-phase has been clearly indicated in Figs. 2b and 4b. Combined with the above results, the existence of the ternary compound Nd₆V₄Al₄₃ reported in Refs. [14,15] can be confirmed in this work.

The crystal structure of the Nd₆V₄Al₄₃ was investigated using X-ray power diffraction, and the XRD pattern was indexed using Jade 5.0. The results indicated that the single-phase has a hexagonal structure with space group P6₃/mcm (no. 193) and the lattice parameters of $a = 1.1028$ nm, $c = 1.7931$ nm, $c/a = 1.626$ and $V = 1.893$ nm³. The composition of the sample, the intensity of the reflection and the obtained lattice parameters all proved that this

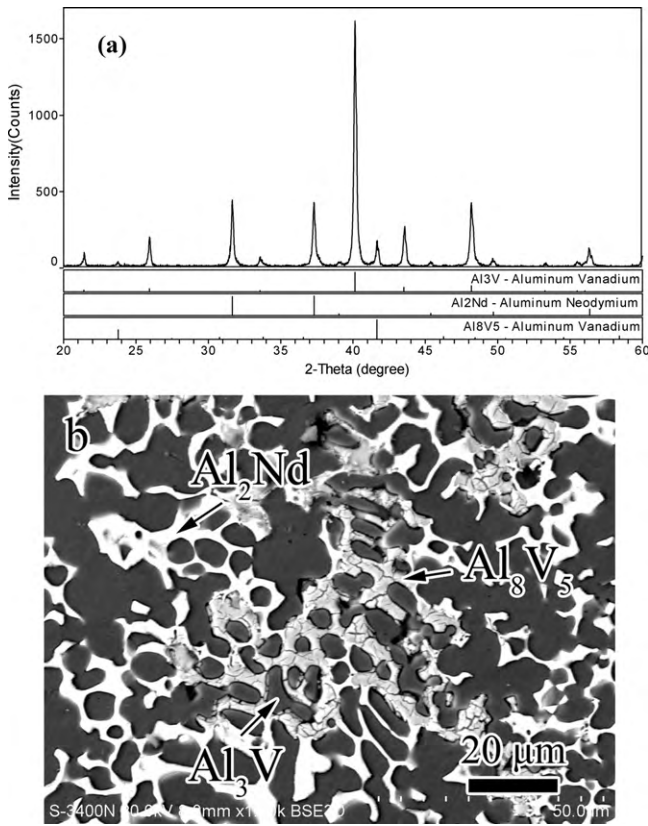


Fig. 3. XRD pattern (a) and SEM micrograph (b) of the equilibrated sample with chemical proportion of 72 at.% Al, 25 at.% V and 3 at.% Nd reveal three-phases i.e. Al_3V , Al_8V_5 and Al_2Nd .

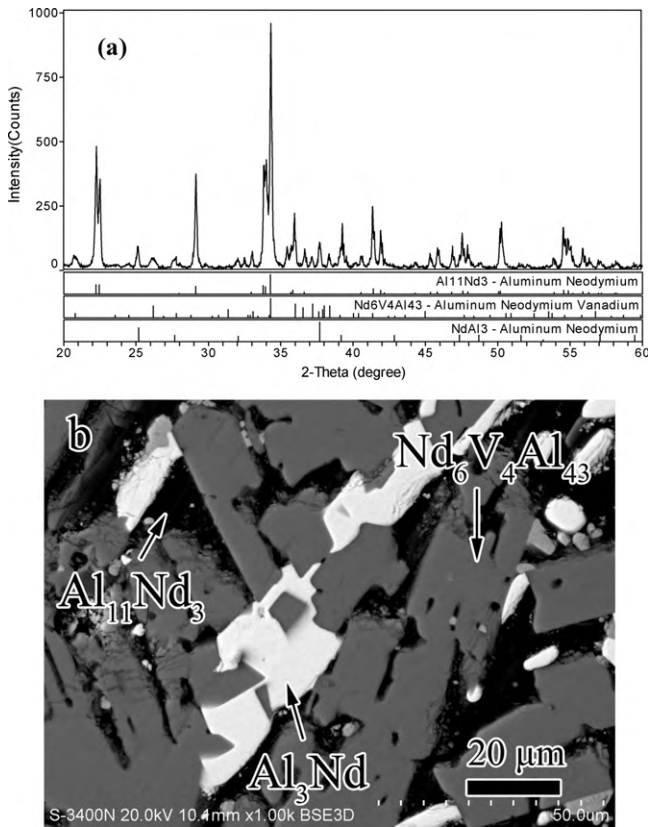


Fig. 4. XRD pattern (a) and SEM micrograph (b) of the equilibrated sample with chemical proportion of 79 at.% Al, 2 at.% V and 19 at.% Nd reveal three-phases i.e. Al_3Nd , $Al_{11}Nd_3$ and $Nd_6V_4Al_{43}$.

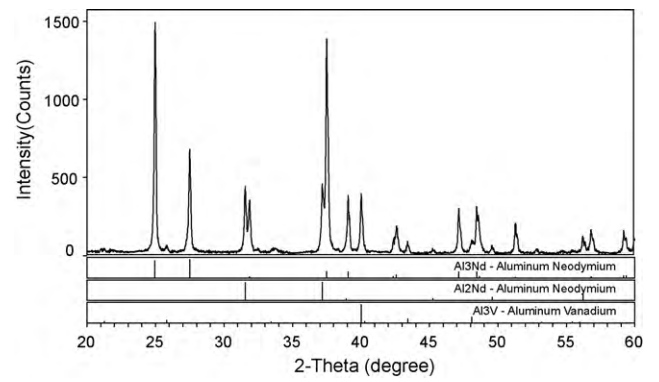


Fig. 5. The sample containing 67 at.% Al, 17 at.% V and 16 at.% Nd consists of Al_3V , Al_3Nd and Al_2Nd .

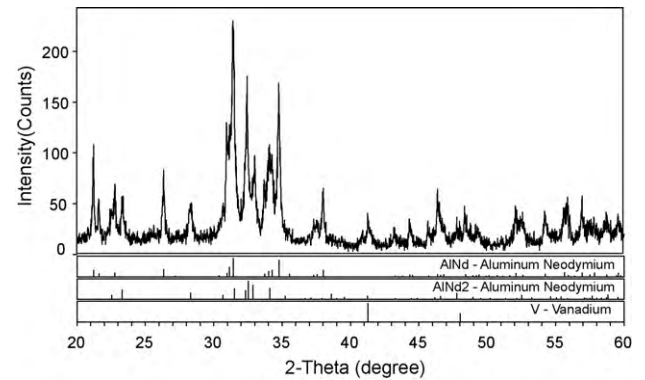


Fig. 6. XRD pattern of the equilibrated sample prepared with atomic proportion of Al 27 at.%, V 28 at.% and Nd 45 at.%, containing Al_3V , Al_3Nd and Al_2Nd .

Table 1

Crystal structure data of the intermetallic compounds in the Al–V–Nd system at 773 K.

Phase	Space group	Lattice parameters (nm)			References
		a	b	c	
$Al_{21}V_2$	$Fd\bar{3}m$	1.4492 (4)	–	–	[19]
$Al_{45}V_7$	$C2/m$	2.5604 (14)	0.76213	1.1081	[19]
$Al_{23}V_4$	$P6_3/mmc$	0.76928	–	1.704	[19]
Al_3V	$I4/mmm$	0.3772	–	0.8305	[19]
Al_8V_5	$I43m$	0.9234 (5)	–	–	[19]
$Al_{11}Nd_3$	$Immm$	0.4359	1.2924	1.0017	[19]
Al_3Nd	$P6_3/mmc$	0.647	–	0.4603	[19]
Al_2Nd	$Fd\bar{3}m$	0.8	–	–	[19]
$AlNd$	$Pbcm$	0.594	1.1728	0.5729	[19]
$AlNd_2$	$Pnma$	0.6716	0.5235	0.965	[19]
$AlNd_3$	$P6_3/mmc$	0.8000 (2)	–	–	[19]
$Nd_6V_4Al_{43}$	$P6_3/mcm$	1.1036 (3)	–	1.7939 (4)	[15]

Table 2

Crystal structure data of the ternary compound $Nd_6V_4Al_{43}$.

Compound	$Nd_6V_4Al_{43}$
Structure type	$Ho_6Mo_4Al_{43}$
Space group	$P6_3/mcm$ (no. 193)
Cell parameters	$a = b = 1.1028$ nm, $c = 1.7931$ nm, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$
Volume of unit cells (nm^3)	1.8885
Calculated density (g/cm^3)	3.9206
Formula units per cell	$Z = 2$

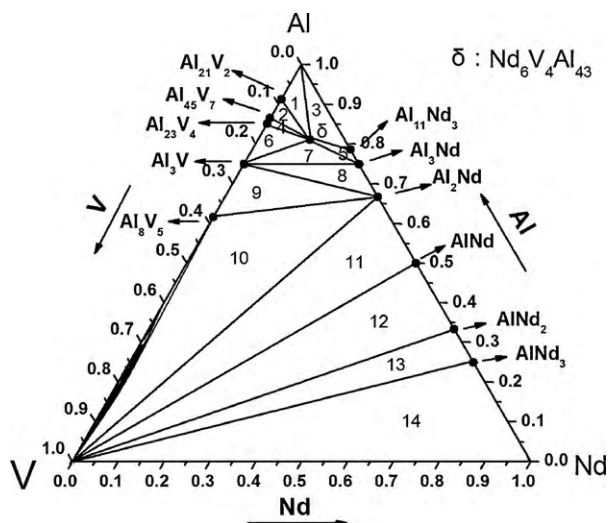


Fig. 7. The 773 K isothermal section of the Al-V-Nd ternary system.

Table 3

Details of the ternary-phase regions in the Al-V-Nd system at 773 K.

Phase regions	Alloy composition (at.%)			Phase composition
	Al	V	Nd	
1	90	6	4	Al + Al ₂₁ V ₂ + Nd ₆ V ₄ Al ₄₃
2	87	11	2	Al ₂₁ V ₂ + Al ₄₅ V ₇ + Nd ₆ V ₄ Al ₄₃
3	85	3	12	Al + Al ₁₁ Nd ₃ + Nd ₆ V ₄ Al ₄₃
4	84	12	4	Al ₂₃ V ₄ + Al ₄₅ V ₇ + Nd ₆ V ₄ Al ₄₃
5	78	2	20	Al ₃ Nd + Al ₁₁ Nd ₃ + Nd ₆ V ₄ Al ₄₃
6	81	15	4	Al ₂₃ V ₄ + Al ₃ V + Nd ₆ V ₄ Al ₄₃
7	78	9	13	Al ₃ V + Al ₃ Nd + Nd ₆ V ₄ Al ₄₃
8	72	6	22	Al ₃ V + Al ₃ Nd + Al ₂ Nd
9	68	27	5	Al ₃ V + Al ₈ V ₅ + Al ₂ Nd
10	52	39	9	Al ₂ Nd + Al ₈ V ₅ + V
11	48	18	34	AlNd + Al ₂ Nd + V
12	34	18	48	AlNd + AlNd ₂ + V
13	24	19	57	AlNd ₂ + AlNd ₃ + V
14	14	12	74	AlNd ₃ + Nd + V

compound is isostructural with Ho₆Mo₄Al₄₃. The crystal structure of the Nd₆V₄Al₄₃ compound is shown in Table 2.

3.3. Solid solubility and isothermal section

The solid solubility ranges of all single-phases at 773 K were determined by XRD using phase-disappearing method and comparing the shift of the XRD pattern of the samples near the compositions of the binary-phases [20]. The solid solubility of Al in V is determined to be up to 39 at.% Al at 773 K (Fig. 7). For the other compounds, the results showed that the diffraction patterns did not show shift and the diffraction patterns of the second phase could easily be detected when the composition of the alloys deviated from its single-phase region by 1.0 at.%. Therefore, none of the

other phases in this system revealed a remarkable homogeneity range at 773 K.

Based on the phases analysis of XRD patterns of 89 samples and assisted with the results of SEM and EDX analysis of selected samples, the 773 K isothermal section of the Al-V-Nd ternary system was determined, as shown in Fig. 7. This isothermal section consists of 15 single-phase regions, 28 binary-phase regions and 14 ternary-phase regions. The details of the three-phase regions and compositions of the typical alloys of each region in the Al-V-Nd system are shown in Table 3.

4. Conclusions

By comparing and analyzing the XRD patterns of 89 equilibrated samples, the phase equilibria of the Al-V-Nd ternary system at 773 K has been determined for the first time. The 773 K isothermal section consists of 15 single-phase regions, 28 two-phase regions and 14 three-phase regions. The existence of 11 binary compounds, namely, Al₂₁V₂, Al₄₅V₇, Al₂₃V₄, Al₃V, Al₈V₅, Al₁₁Nd₃, Al₃Nd, Al₂Nd, AlNd, AlNd₂ and AlNd₃ were confirmed at 773 K. The AlV₃ and Al₅₀V₅₀ compounds are not confirmed at 773 K. The existence of the ternary-phase Nd₆V₄Al₄₃ has been confirmed and the crystal structure is refined. The solid solubility of Al in V is determined to be up to 39 at.% Al at 773 K.

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