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Original Research Article

Effects of Composition on Structure & Mechanical Property of TiAl Based Intermetallic Compounds

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Abstract

The effects of Al content and ternary additions such as Mo, V and Si in as cast γ based alloys made by plasma arc melting on solidification structures and mechanical properties were studied. The Columnar γ /α_2 lamellar structures in Al-lean alloys due to primary α solidification had higher room temperature fracture strength and strain than γ phase structures through the reaction of L+α=γ in Al-rich alloys. The fraction of α_2 phase was found to decrease with increasing Al content in binary alloys. Fractography revealed that fine translamellar fracture is a man fracture mode in Ti-48at.%Al alloy which led to a high fracture with more than 5%. The RT fracture strain was improved by the addition of 1.5at.% Mo and 1at.%Si. The mechanical propertied have been discussed in term of changes in unit cell volume and axial ration. In the case of Si, tensile properties coincided well with the change of axial ratio c/a. The strength and strain could be raised slightly to compare with binary system. The standard deviation has been low in lattice constant so deviation of c/a is 0.43% which is good one to help to analyze the strain in TiAl-X alloys. The first factor is c/a which means atomic anisotropy then is $c*a^2$ which is unit atomic volume of γ phase. The decreasing c/a is to decrease the atomic anisotropy and increase the materials atomic ductility in TiAl-X alloys.

Keywords: Solidification, Composition, Structure, Mechanical property, TiAl.

1. INTRODUCTION

γ-TiAl with high ratio strength had been promised in the high temperature structures in the future. The TiAl alloys developed by now had excellent casting property so that they could be used to the engine of craft and automobile with good evaluation [1]. However they were still limited actually due to their weak ductility and fracture toughness. So the alloys were still in the original stage in industry.

Al content which was one of the important factor to affect process and mechanical property was chosen by controlling microstructure in TiAl base alloys [1, 2]. According to Al content the casting structure was obtained with different primary phase. In general, equiaxed grains had been trend to form when primary phase was β, columnar's had been trend to form when primary phase was α. The lamellar structure was still brittle in spite of good toughness. Moreover the coarse lamellar with no crystallizing was produced with continuous and slow growth so that structure was not easy by heat treatment. However the full lamellar would fit to promote high temperature strength because the lamellar was possible to use in high temperature.

The element such as V [1, 3, 4] will improve the ductility. In addition, Mo [3-5] and Si [3, 5] could have the effect of raising the ductility at room temperature. The B2 was escaped in order to enhance the ductility so that the additional element was limited in the range of 1~3at.%. There were the factors affected the ductility as below. The reducing c/a [6, 7], the change of lattice volume [6, 7], the activation of strained twins and 1/2[110] full dislocation [8] would be divided into.

In this research the cases would be considered to melt cast specimens to enhance the mechanical properties so that the third elements for example Mo, V and Si was added in the condition of TiAl. The effect of

the type and quantity on the solidification structure and physical properties were investigated [9, 10].

2. METHODOLOGY

2.1 Materials & Specimens Preparation

The binary and ternary alloys in TiAl were produced to analyze. The 99.7wt.% sponge Ti, 99.9wt.% bulk Al and 99.9wt.%Mo,V and Si were used to produce specimen. They were melted under 99.9% Ar gas in plasma arc furnace. For homogeneous specimen they were melted more than 3 times.

2.2 Tests

The compositions were investigated used EDS (energy dispersive X-ray spectroscopy). Micro- and macrostrucuture were observed with OM (optical microscopy) and SEM (scanning electron microscopy). The etching solution was 10mlHF+ 5mlHNO_3+ 35mlH_2O_2+ 100mlH_2O. Transition temperature and composition of solid and liquid phase in Ti-48at.%Al were observed to use DTA(differential thermal analysis). The scanning rate was 10°C/min and the highest temperature was defined to 1560°C. The lattices constant were investigated on X-ray diffraction and lattice program. The microstructure and strained microstructure were investigated with JEM-2010 TEM (transmission electron microscopy). The jet solution was 60%methanol+ 35%n-butanol+ 5%perchloric acid. The content was measured with the energy dispersive X-ray. The test was done at room temperature in order to search tensile curve. The strain rate was used to 1.25×10^{-4}/s. The specimens were used to 8×3×1mm in gauge.

Table 1: EDS analysis of γ base alloys. (at.%)

Nominal composition	Ti	Al	3rd element
Ti-44Al	57.23	42.77	-
Ti-46Al	56.80	43.20	-
Ti-48Al	52.34	47.66	-
Ti-50Al	50.82	49.18	-
Ti-52Al	46.84	53.16	-
Ti-54Al	46.12	53.88	-
Ti-50Al-1Mo	50.14	48.70	1.16
Ti-50Al-1.5Mo	47.49	50.84	1.67
Ti-50Al-1V	50.44	48.86	0.70
Ti-50Al-3V	48.51	48.49	3.00
Ti-50Al-1Si	50.03	49.01	0.96
Ti-50Al-2Si	48.89	48.48	2.63

3. RESULT AND DISCUSSIONS

3.1 Phase analysis and crystallography

The results measured with EDS had been shown as Table 1. The deviation with 2at.% was found. In equilibrium the solid was complexed and sensitive to concentration Al. According to the phase diagram beyond 55at.% the primary γ was been solidified. That means that they were transformed with L→β in the case of Ti-(44~48)at.%Al, there were the solidified course as follow,

44~46at.%Al: L→ L+β→ L+β+α→ β+α→ α→ α+γ

48at.%Al: L→ L+β→ L+β+α→ α→ α+γ

In the case of Ti-(50~54)at.%Al they were transition through L→α

50at.%Al: L→ L+α→ α→ α+γ→ γ

52~54at.%Al: L→ L+α→ L+α+γ→ α+γ→ γ

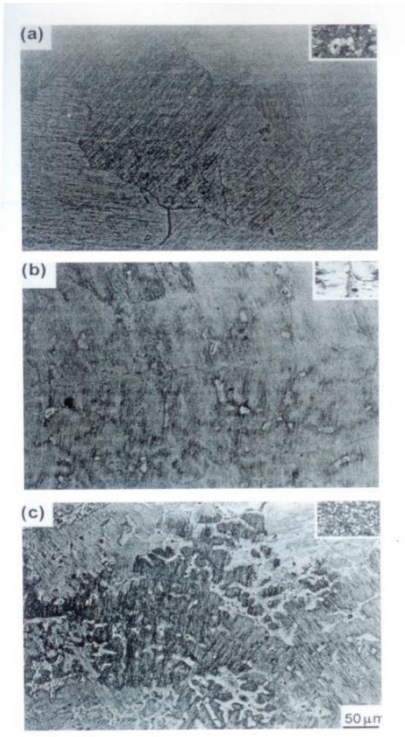

Fig 1: Optical micrographs of as cast binary γ base alloys

The lamellar structures were thought to be upon α → (α+γ)L →(α_2+γ)L to obtain the plate nucleation [1]. The microstructures of binary alloys were shown in Fig. 1. It was found that in the Ti-44at.%Al the equiaxed in center and slight columnar in edge with the binary structure was formed. The grain growth was formed from edge to center in the Ti-48at.%Al. On the contrary the fine grain was formed and those growths did not occur in the Ti-52at.%Al. In Ti-44at.%Al the full lamellar structure was shown, and they were thought to be through primary β. In Ti-48at.%Al the fine γ/α_2 lamellae were formed mostly with the 80~90 ˚ direction with grain growth. Other boundaries among grain growth were found. Upon Y. Shimada et al. those distribution was formed by the primary α from liquid. So it was thought that growth rates would be fast which was formed from primary α in those alloys. In the Ti-48at.%Al it was supposed that they were nucleated from primary α because those columnar grains were nucleated from α solidification [1]. The Ti-52at.%Al evident dendrite was formed so that the coarse lamellae γ/α were grown with different directions in varied grains. It was found that they were due to the random growth directions to view in general. That was through the reaction of L+α→ γ to form the γ grains which had surround the lamellae. On the other hand in those fine structures the segregation and heterogeneous were observed. The deep Al seperation and non stable phases were formed and the primary α forms the second phase to form the non equilibrium structures due to Al seperation within the boundaries through the peritectic reaction. Moreover it was thought that peritectic transformation α+γ→ γ was not proceeded upon confining the solid diffusion with kinematics. The separated γ- interdendrites was shown obviously in the Ti-(52~54)at.%Al so that the following reaction was obtained. Etc. L→ L+α→ L+α+γ segregation→ α+γ segregation.

The results would be confirmed with DTA. In the phase diagram the solidified course would be L→ L+β→ L+β+α →α → α+γ as they were discussed above. That would be results with DTA in 48at.%Al. The high exothermic reaction between 1160 and 1412˚C was (α_2+γ)lamellar→ (α+γ) lamellar transformation, and the other was between 1478 and 1492˚C with α→ L+α. The low exothermic reaction was up to 1518˚C with L+β→ L. So the heat to be necessary for (α_2+γ)lamellar→ (α+γ) lamellar would be high. It means that the fine lamellae were highly resistant to heat so that it had been known that they would be steady even above 1160˚C. It was known that the dissolved of lamellae would start and end at 1412˚C and 1478˚C respectively. Moreover it had been shown that the peak of L+β→ γ will be not formed fully so that the course would be neglected to form the primary α directly in the case of rapid solidification.

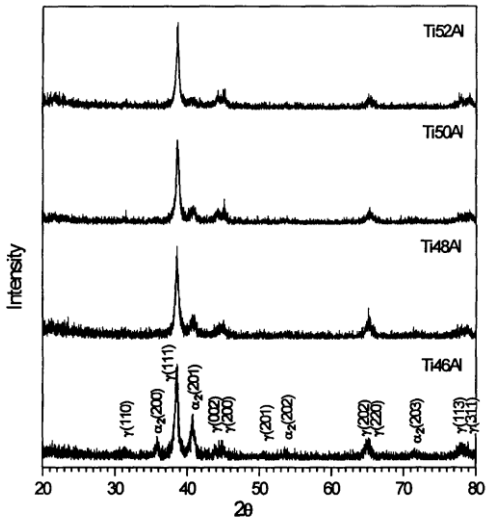

Fig 2: The variation of X-ray diffraction spectra in binary γ base alloys

In the case of ternary alloys it will be observed that the grain could be fine and coarse grains to grow in the Ti-50at.%Al-1at.%Si and Ti-50at.%Al-2at.%Si respectively. It was thought that the flow could be increased so that the grain growth can be good to growing with increasing Si additions. The grain growth was known to form in Ti-50at.%Al-1at.%Mo, and fine grains would be formed Ti-50at.%Al- 1.5at.%Mo respectively. In contrast the grain growth would not take place in Ti-50at.%Al-1at.%V. The grain growth will be shown obviously in Ti-50at.%Al- 3at.%V.

The precipitation existing in lamellar boundary would be observed in fine structure with SEM. Those precipitations were known as the Si content which should be high obviously with EDS. That was thought to be silicides particle with Ti_5Si_3. We could find that even the Si was reduced the silicides would be big, and

the fraction of silicides will be reduced. And in the Mo and V addition alloys nothing were found obviously in microstructure. So It was thought that the research with that direction will be proceeded.

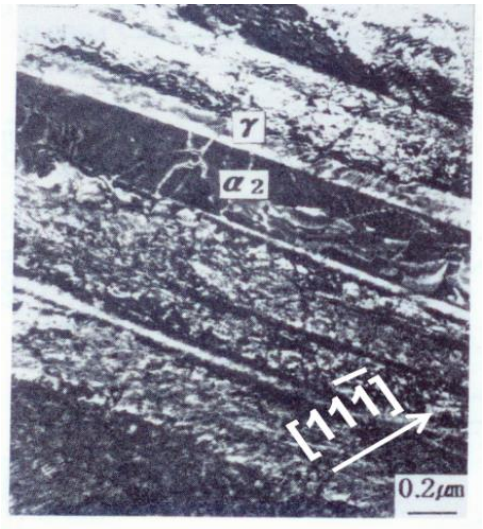

Fig 3: TEM micrographs of Ti-48at.%Al structure

The phase changes with the binary alloys composition could be observed by XRD as shown in Fig 2. In the binary alloys it was observed that the peak of α_2 would be high when the Al content was low. That meant the α_2 was distributed highly. In the binary and ternary alloys the lattice constant was measured shown in Fig 5 and 9. The following behaviors were found.

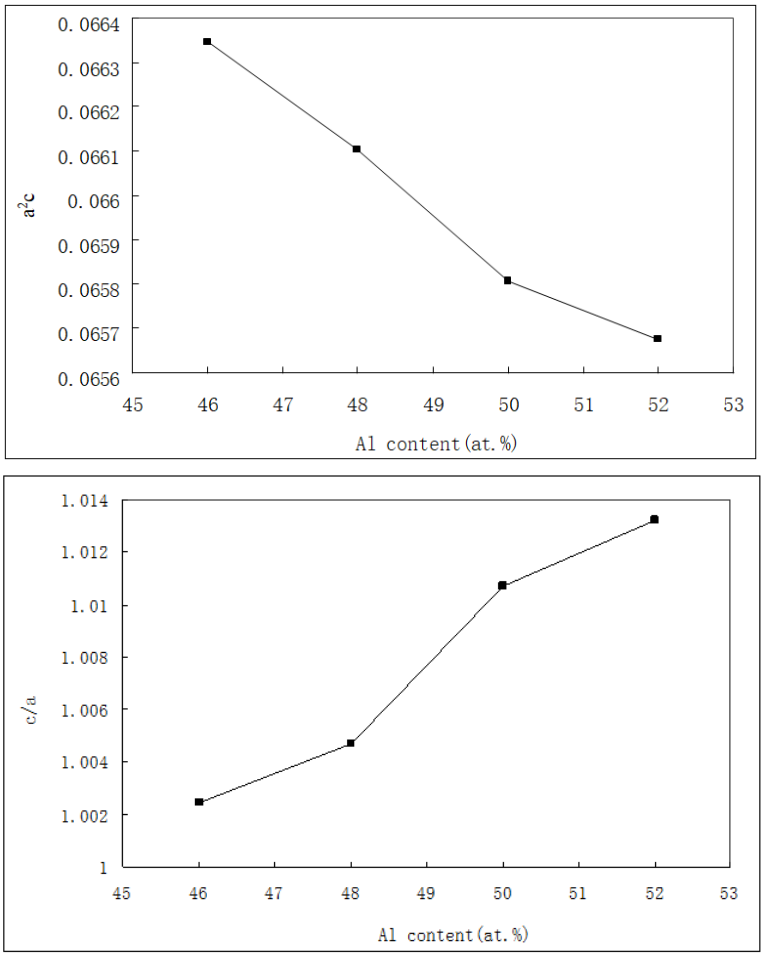

Fig 4: The variation of unit cell volume and axial ratio of γ phase in γ base alloys

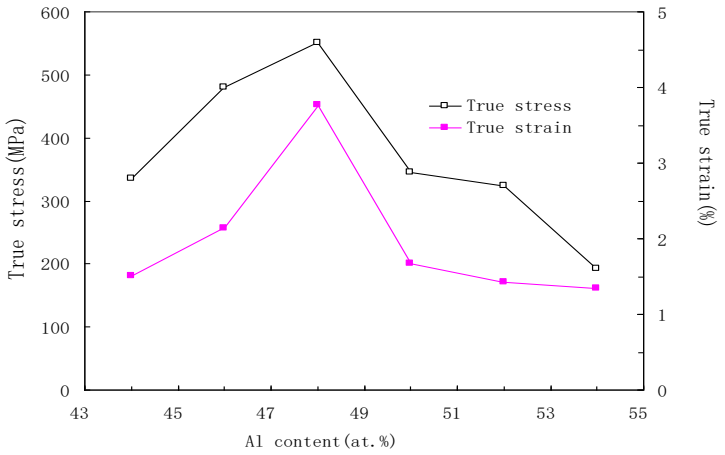

Fig 5: The variation of tensile properties for binary γ base alloys at room temperature in air. (strain rate: 1.25×10^{-4}/s)

The Ti-48at.%Al had been observed to find the plate distributed lamellar structure by TEM shown in Fig 3. The two phases had the following relation. They were γ plate with $L1_0$ at the zone axis [011] and α_2 with $D0_{19}$ at the zone axis $[2\bar{1}10]$. They became lamellar structure by alternation mode as shown in the bright field image. All the plate had the same boundary direction. It had the relation of $(0001)\alpha_2$// $(111)\gamma$ and $[2110]\alpha_2$// $[110]\gamma$ [1]. That was because the (111) dense plane had been several. However there was only one (0001) dense plane in α_2. So it was a certain direction. The lamellar would be arranged in a certain direction in grain boundaries.

A concept of distribution has given a set of measurements of n being lattice constant of TiAl. For measuring change quantitatively the analysis had been taken as reference. The high of standard deviation σ means the high of the deviation. By the analysis the value had good credit from the deviation. That means the constant had approached more to near 0.406nm and 0.403nm with c and a respectively as Table 2. It was included that measurement standard deviations was 0.064% and 0.11% in c and a lattice constant respectively as below with the range of scope were happened according to variance in TiAl alloys. The lattice c is preciser than a in terms of their deviation value, therein it is explained that the standard deviation is very small whose value is feasible to use in measuring lattice of TiAl specimen. In additional the c/a has been measured with variance. It is found that the calculated value c/a is 1.01 meantime volume of $c*a^2$ has been $0.07nm^3$ and their standard deviation is about 0.43% and 0.026% respectively. It expresses that the later $c*a^2$ is preciser than the former c/a. The effective turn of these four respects is lattice a> c/a>lattice c> $c*a^2$. It means that lattice a is the best one and then c/a& lattice c and finally $c*a^2$ in terms of deviation.

Table 2: Variance and standard deviation analysis results of γ base alloys

Item	Lattice c	Lattice a	c/a	$c*a^2$
Mean value	0.406nm	0.403nm	1.01	$0.07nm^3$
Deviation σ^2	4*E-6	1*E-5	2*E-4	1*E-6
Standard deviation σ %	6.4*E-2	1.1*E-1	4.3*E-1	2.6E-2

3.2 Mechanical properties in TiAl

The true stress and true strain at room temperature for solidified specimens with the tensile axis arranged parallel to the specimen direction is shown in Fig 5. The average value in the alloy is about 371MPa while addition of Al amount does not seem to cause a drop in true strain. The further the Al content was raised, the further the yield strength to 600MPa.would be formed [4] in the 44~48at.%Al. It was observed that the hardness was low when the Al content was increased in the binary alloys. That might be explained by reducing hard α_2. In the Ti-50at.%Al-X alloys in the case of V and Mo the hardness would be high, however in the case of Si that was similar to the binary alloys. It was found that would be depended on no effects by Silicide particles.

In the Fig 5 the strength and strain depended on the Al were shown in the binary alloys. It was observed that the Al difference based on 48at.%Al had been high the effects would be low. On the other hand in low Al the fracture strength and strain might be high compared with low Ti. From that it was found that the structure and properties were relative to Al concentration. That meant that the tensile strength and ductility would be the largest at (47~48)at.%Al [1]. That was formed by the α_2 with wave boundary of lamellae in large columnar grains. In the content beyond 48 at.%Al it was existent with the report that γ

phases would be formed by boundaries so that the toughness will be reduced highly [1].

From the binary photographs as shown in Fig 6. the fracture structures, and the different types with fracture plane was observed. In the Ti-46at.%Al the translamellar fracture was the main mode while in the Ti-48at.%Al the transgranular fracture was the most genneral mode. In the Ti-50at.%Al the translamellar and transgranular were main fracture mode simultaneously, which was observed in this research. Moreover coarser fracture would be observed in the Ti-46at.%Al rather than Ti-48at.%Al. It was supposed that the shear strain in those translamellar fracture would cross lamellar boundaries {111} in the case of parallel between tensile direction and lamellar boundaries so that the high toughness resistance to crack was maintained. The typical transgranular with brittlement fracture being no relation to lamellar direction was across γ phase particles so that it was thought that the low toughness was owned.

The strain structures after tensile test at room temperature with Ti-48at.%Al was shown to analyze with TEM as shown in Fig 7. The strained twins were observed in γ phase zone meanwhile dislocations were in γ/α_2 phase lamellar zone. Those twins strain in γ phases had satisfied the polycrystals plasticity to show high toughness with compensate no enough slip systems. The twin may be caused by shear stress meanwhile the dislocation has been done by tensile stress [11, 12].

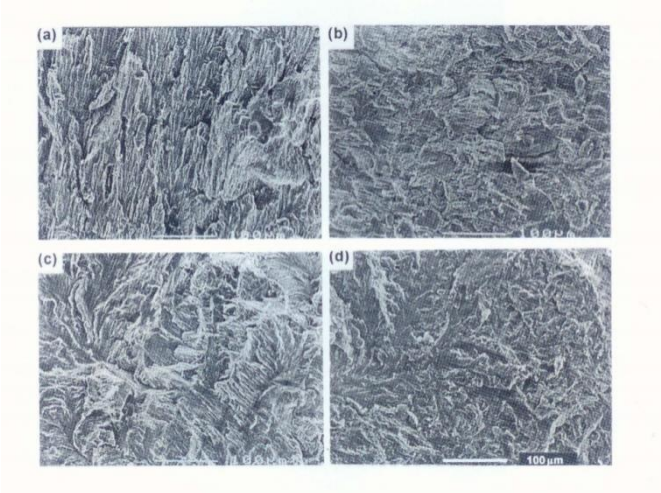

Fig 6: Top views of fracture surface for binary γ base alloys, (a) Ti-46at.%Al (b) Ti-48at.%Al (c) Ti-50at.%Al (d) Ti-52at.%Al

On the other hand the reducing unit cell volume will enhance the bond force between Ti and Al to affect Peierls stress. In the TiAl the Burgers vector [101] and 1/2[112] super dislocation and 1/2[110] and 1/6[112] Shockley partial full dislocation was in relation to strain. It was 1/2[101] >1/2[110] because c/a>1 in the γ alloys. It had been speculated that the super dislocation with high Burgers vector would be higher Peierls stress and lower movement than the full dislocation. So the super dislocations would have the high energy. Then the c/a reduction would decrease the movement difference of the [101] super dislocation and 1/2[110] full dislocations so that they would decrease the anisotropy and increase the ductility [6, 7, 12].

The fracture strength as shown in Fig. 9 had been consistent with hardness in the Ti-50at.%Al-X alloy. As for Mo in the 0~1.5at.%Mo the c/a ratio as shown in Fig. 8 would decrease the fracture strength will become high with the increasing the Mo. That would be due to reduction of c/a. It was thought that the dislocations with Burgers vector [101] were increased. The volume with increasing Mo would be decreased, and the strength will be increased as for the change of cell volume. Up to 3at.%V the fracture strength and strain would be increased. However the c/a might increase with the increasing addition amount. In the state of up to 2at.%Si the strength could be a certain. With the addition of up to 1at.%Si the strain could be raised then reduced beyond the content. That c/a was reduced highly so that it would cause to enhance the strain. However the cell volume may not fit to them. Additionally it was thought that the silicides particle would be low in 1at.%Si, which might have relation to low fraction of silicides particle [11]. It was supposed that the change of c/a would be main factor in binary to compare with the cell volume. The results of yield stress and true strain in terms of additional elements showed that some raising trend may explain the good effect by a certain elements. That may fit well to the change of lattice constant.

The dislocation moving directions were consistent with Burgers vector. The planes of their movement would be existent with Burgers vector and dislocation line. According to plane and directions for movement of atoms which were limited, it was defined that they would take place under the planes with the

highest atomic density. The yield of material took effect in atomic structure highly, and work hardening could be affected by dislocation density.

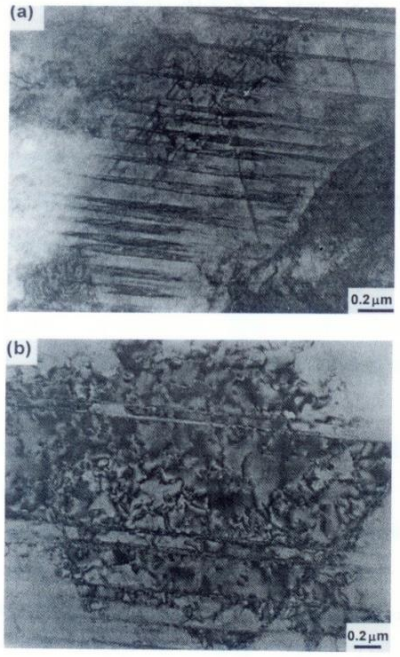

Fig 7: TEM micrographs of Ti-48at.%Al showing (a) twin and (b) dislocation formed by tensile deformation at room temperature

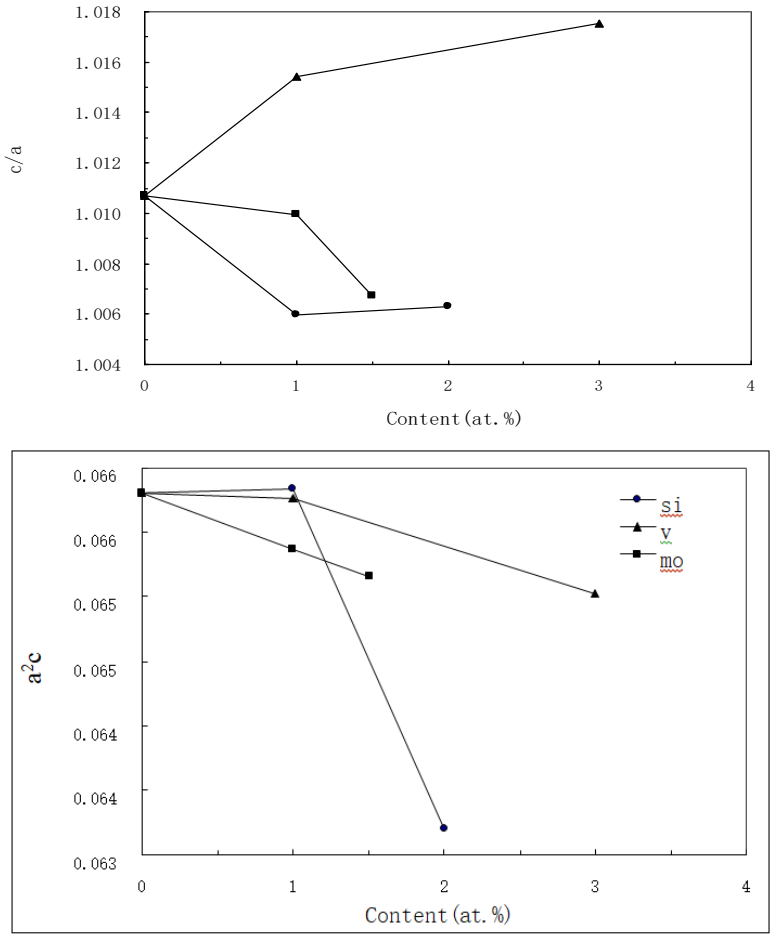

Fig 8: The variation of unit cell volume and axial ratio of γ phase in γ base alloys

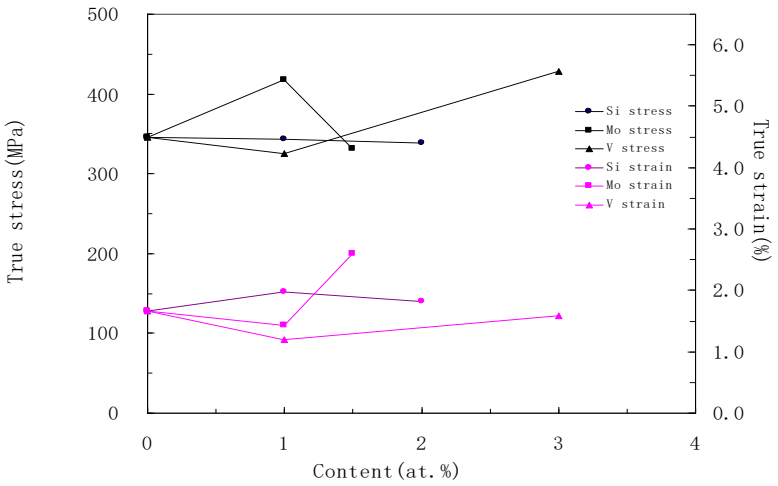

Fig 9: The variation of tensile properties for TiAl-X (X=Mo, V, Si) alloys at room temperature in air. (strain rate: 1.25×10^{-4}/s)

The strain in TiAl-X alloys is better in Si addition meantime the value is good in Mo and then in V addition, ie. Si>Mo>V is the turn according to experimental ternary TiAl alloys. in additional the stable Si is gained in this study and meantime the decreasing strain then increasing one has been attainable in Mo and V. As for the stress the stable Si and increasing Mo and then decreasing relationship may be attainable meanwhile the opposition relation with Mo in V element may be gained here. The interstitial element in position of Ti and Al happens to if the element is more than 2at.%, so the 3at.% V may increase the strength, ie. Solution strength which is important theory to promote the V strength. The substitution strength will happen in 1at.%Mo whose strength has been bigger.

4. CONCLUSIONS

1. The lower Al content would be, the higher fraction of α_2 will be, and the c/a was decreased so that the properties would be enhanced. With increasing Al the fracture mode was changed from translamellar to transgranular so that the fracture properties became bad.
2. In the Ti-48at.%Al with primary α the tensile direction and lamellar boundaries were parallel so that shear strain would cross the lamellar boundaries. The high strength and strain were obtained. In addition, twins and dislocations in straining structure were observed.
3. As for the Mo content up to 1.5at.% in TiAl the c/a would be reduced and the strain be raised. In the case up to 1at.%Si the strain would be raised. The strain will decrease beyond the content, which fit to the c/a. As for 3at.%V the fracture strength and strains were raised to compare with 1at.%V.
4. The mean true strain is 1.98% to be less than 4%. The mean value is slightly small. The addition of Al and elements to be the stabilization α_2 was high so that the strength and strain would be increased.

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