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Study of Dislocation in Crystallography of TiAl Intermetallic Compounds

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Abstract: *The crystallography of TiAl intermetallic compounds has been studied. It is found that dislocation and twins will occur in room temperature tensile test which explains the dislocation to be resolved into the Shockley $a/2[1\bar{1}1]$ and Frank partial dislocation $a/6[11\bar{2}]$ in TiAl intermetallic compounds. This is complete dislocation $a/2[10\bar{1}]$ and super dislocation <101] which causes the above two partial dislocations. This is both caused by α and γ phases according to this study. Furthermore, the many twins are formed in γ alloy that expresses the activated twins also play an important role as well in TiAl alloys. The Schmid factor will represent the size of dislocation that has different slide one. Meanwhile the CRSS means the precision size of dislocation and twins [1] slide and resolve. Through the critical resolved shear stress the force applied to will be attained which is the main method to proceed in deformation course of TiAl intermetallic compounds.*
Keywords: *dislocation; crystallography; twins; CRSS(critical resolved shear stress); TiAl alloys; intermetallic compounds; Schmid factor*

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I. Introduction

TiAl alloys as an important material have potential promise in turbine component of aircraft engine. So the research has been proceeded on it in many countries widely. In the deformation course the many dislocations and twins are found which cause the good strain to happen, so we must pay attention to them. The complete and super dislocations will resolve into the Shockley partial and Frank partial one which play an important role in crystallography change in Ti-48at.%Al alloy. Additionally the many twins are observed in this alloy to demonstrate its existence in deformation course. As for it the relative proof has been deficient currently. Therefore, the explanation on twins will be described in this paper.

The CRSS value will express the super dislocations $<01\bar{1}]$ and twins $<11\bar{2}]$ appearance according to the calculation value. If it is the lowest the defect will be easy to be formed which is a criteria to judge their big or small deformation. The Schmid factor is to be calculated according to X-ray diffraction one which is a terminological constants applying to the CRSS. The Schmid factor has the similar meaning for the same materials to CRSS. Only if the different materials are it will have the new mean. [1~3]

In short, the further research may be proceeded in above two aspects will enhance the plastic deformation degree in the end, which we judge in this paper. As a promise material applied to high temperature structure it may be searched further for its wide usefulness and application to be substituted for Ni based super alloys in future, for example adding the third elements and fourth & higher ones. The produce method has been changed in order to attain better crystalline structures, like Single crystals、seed crystal method for DS(Directional solidification)& poly crystals. [5~7]

II. Experimental Methodology

The specimen of TiAl alloys has been produced in plasma arc melting furnace whose vacuum is maintained about 10×10^{-5} Torr. Then after blowing Ar gas into the furnace the combination materials which is raw Ti sponge (99.7wt.%) and Al bulk(99.9wt.%) is to be melted two times and then puts it into cylinder cavity instantaneously in order to attain the rapidly solidified rod figuration with ϕ12×60mm specimens for the tensile experiment to be adopted.

The test is done at room temperature in order to search tensile curve. The strain rate is used to 1.25×10^{-4}/s. The specimens are used to 8×3×1mm in gauge. The gauge length 8mm is made according to $l_0=4.52F_0^{1/2}$ from reference as Table1. The ratio 3 of width and thickness is no more than 4.21 which is criteria specification.

Table1 The relation of gauge length l_0 and width in TiAl intermetallic compounds.

gauge length l_0	Gauge width
$l_0=4.52A_0^{1/2}$	<4.21

Here gauge length l_0 is 7mm in the tensile specimen; F_{max} is 139Kg, σ_{max} is 454MPa. A_0 is Plate cross with $3mm^2$, A is 3mm smaller than 4.21 in right condition which is the crossing area for gauge part. Here, l_0=7.68mm, so both aspects have the qualified value, means the reasonable decision for this tensile test in the TiAl specimens.

III. Result and Discussions

Due to the complicate dislocations is there in deformation course in TiAl intermetallic compounds. It shall express many resolved dislocations which needs to be explained in details. From the CRSS its information will be formed and known by us through the resolved ones including in Shockley partial dislocations and Frank partial dislocations by the super one <101] and another super one a/2[112]. Additionally the ordinary one a/2[110] will have the same transformation as well. We will discuss and narrate details as below. Here we suppose that the [0001] growth direction is the preferring direction in α_2 Intermetallic Compounds, meanwhile the [100] is the preferring one in TiAl Intermetallic Compounds respectively. According to the two directions the directional dislocation and twins is searched for with the Schmid factor and CRSS respectively in this study. [8]

3.1 Crystallography in α_2 Intermetallic Compounds

The $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin has 6 slips. The a/6$(10\bar{1}0)[11\bar{2}6]$ pyramid dislocation has the same slips. The a/6$[11\bar{2}0]$basal one has 3 slips. The total twin and dislocations are 15 slips. The $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin has high CRSS According to data.[8~9] the deformation dislocation in α phase is the $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin. The $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin is short and the quantity is not much. From the CRSS the this twin is the least. It stated that the $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin is hardest dislocation. It is the hardest happening dislocation. it can happen at last in those other dislocations and twins. The other one is twin in α matrix. From the data the one is dislocation which is a/6$[11\bar{2}6]$ pyramid dislocation. The one is the least in those two dislocation and twins. It will happen easily in two dislocation and twins.

According to the calculation the CRSS of $(10\bar{1}0)$ $[11\bar{2}6]$ dislocation is 264MPa. It is formed firstly. That of $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin is 294MPa. That is due to the growth direction of crystal which is probably not [0001] direction simplicity. That need more measurement to define the growth direction of crystal. But the ideal condition can also explain the trend of dislocation and twin deformation. So we will notice the easy twin will play an importance role on deformation.

In this experiment to align load axis being parallel to lamellar direction, we can gain good strength. We gain small twin and dislocations. That means that the strain will become good if we could increase dislocation and twin specially the a/6$[11\bar{2}6]$ pyramid dislocation. On the other hand, the $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin is also needed to increase.

A Schmid factor is calculated for twin systems. It depends on the easy slip plain and directions. A higher value at [0001] axis will be decreased if it is remote direction. So that several orientated specimens with deformed twins in SC(Single crystals）will be confirmed by compression as shown in literature [10]. It is orientated by [0001] above 45° . It has been observed that there is the existence of pyramidal slip with $\{10\bar{1}1\}$ and basal slips in poly crystals. Furthermore, the dislocations having linear mode is observed to occur.

3.2 Crystallography in TiAl Intermetallic Compounds

It is the easy dislocation to happen. If we find method to increase the full dislocation it is possible to affect the strain of specimen. For example changing to directional solidification and seed directional solidification. The former is columnar solidification direction and the later is lamellar direction. Or adding element to align the lamellar direction by β solidification. It is reported that adding element for example Nb can affect lamellar parallel to columnar solidification direction as to new solidification in seed DS. The columnar solidification growth direction is perpendicular to loading direction, which leads to some poor mechanical properties. If we grow columnar direction parallel to load axis the more good properties will be gained. But the lamellar direction will be good when it is parallel to loading direction too. This can affect the strain properties more effectively.

But that its value is 150MPa similar to twin one means the role will as big as twins. The easy full dislocation has the lowest energy with easy slip plane. the angle with loading axis is near 0° which forms the lowest critical resolved shear stress. That means the dislocation will happen more, we can gain good strain. Other two kinds of resolved dislocations are the same to this kind. The highest super dislocations aren't found in this experiment, substituting for that, the same orientation twins are found to play a biggest role in three dislocations. The same orientation super dislocation and twins will be investigated further more. Probably there are some relations between them or they affect the gliding commonly. So the dislocation and twins in this direction is main reason to influence the total slip systems. Because the found slips are these two only. The three twins with parallel to load direction are main slip system in this research. The super dislocation is little relation to slips as it high density. As to strain the super dislocation happen partially. The dislocation density with full dislocation is low it is considered that the deep Peierls stress with big curve has been the reason due to its Anisotropic bond.

The grain size is the smaller the higher strength will be gained in usual. To gain higher strength we add element such as B or N etc. To reduce it. In this paper increase the Al to 44~48at.% it will deformation column which has the fine lamella, we hope the high stress and strain to be obtained. The other hand adding Mo will reduce the grain size. Adding Si raise the flow property and V to raise RT ductility. As to 48at.%Al twin and the full dislocation will be found in TEM observation. That twin [11] consists of low CRSS with easy dislocation, which fit to calculation. If twin and dislocation is activated enough, the good strain will be attended. We shall notice the twin owned large size will promise occurring matter. But the full dislocation is the problem to be activated further in research. The dislocation resolves two partial dislocation is demonstrated by calculation.

The fracture mode is trans granular, which means the fracture crack will propagate through grain, i.e. column. As the lamellar aligns vertical to column growth, that will make barries to crack propagation. But the column length is too big which makes weak effect to fracture stress. In total the lamella is main factor that affect the fracture propagation. So the high stress is obtained while the little strain is gained. If we use DS specimen the lamella is main factor to inhibit the stress. But it promotes strain due to vertical direction. The column will be benefit to the stress secondarily. The little stress and high strain is predicted if we gain the lamellar direction vertical to load axis. If we control the specimen with near 45^0 lamella, the good stress value will be obtained as prediction. The best strength is for lamella parallel to loading axis.

The flow of easy dislocation slip is to be proposed by Peierls stress method. So at the low temperature the brittlement has been in relation to defining dislocation flow. As to the strain the super dislocation happens to partially. Defect loops with resolved a/6[112] Shockley partial is formed. In additional dislocation density with a/2[110] easy dislocation slip is low. [11] It is considered that the deep Peierls stress with the curve had caused the anisotropic force.

In addition to, the XRD(X-ray diffraction) value can be used to acquire plain distance and transform it into lattice constant for solving the directional dislocation movement in TiAl intermetallic compounds. The error between the measured lattice constant and criteria one has been analyzed with variance method as well. Then we find the little deviation happens here, so it is judged that the former is feasible within this differences. Because the angel above 120° in XRD has too little peak to occur that has not allowance to utilize for us as saying in book, the peak value adopted from 0~90° is available enough. We used the value of measurement to attain the lattice constant that has completely precision as well. For these phases the deviation will be neglected.

In short, the two aspects are searched here to analyze so as to observe the differences of them. It has been found that Schmid factor will instruct the directional dislocation slip to ensure that the easy slip and difficult one to happen in crystallography of TiAl phase. The CRSS has the more transformed value than Schmid factor in practice. Through it we can solve the force to identify the size precision of them. The 45° lamella is the better force to attain the good plastic deformation. The usual lamellar angel is 0~10° with weak strain in DS alloys, so the lamellar angel with 45~75° will be excellent one in general. The more Shockley partial dislocations $a/2[1\bar{1}1]$ and Frank partial dislocations $a/6[1\bar{1}2]$ can wield more roles in plastic deformation in the Ti-Al alloys.

IV. Conclusions

The 45° lamella is the synthesized optimum angle which owns strong strength and toughness after all upon the comparing with 0~90° ones. Thereby maintaining this angle is significant results for us to search further in future because it can be replaced for the complicate 90° one. The 90° lamella is difficult to be produced since producing the single crystalline and seed crystalline methods in order to form this angle so the producing cost will be very high.

The more Shockley partial $a/2[1\bar{1}1]$ and Frank partial dislocations $a/6[11\bar{2}]$ can wield more roles in plastic deformation of the Ti-Al alloys.

The complete dislocations with a/2<110] and super dislocations <101] can be used into resolved ones i.e. the Shockley $a/2[1\bar{1}1]$ and Frank partial dislocation $a/6\ [11\bar{2}]$ has big effectiveness according to CRSS value in TiAl alloys.

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