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A Study of Dislocation and Twins in Deformation of Ti_3Al-Nb Intermetallic Compounds

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Abstract: *The crystallography of Ti_3Al-Nb intermetallic compounds has been studied. It is found that dislocation and twins will occur in tensile test, which explains the pyramidal dislocation $<11\bar{2}6]$ and twins $<10\bar{1}\bar{1}]$ exists in Ti_3Al-Nb alloys and wields their ductility promotion certainly. That means many dislocations and twins are formed in α_2 alloy deformation that expresses the resolved dislocation and twins plays a certain role in this intermetallic compounds. The Schmid factor will represent the size of dislocation that has different slide, meantime the Critical resolved shear stress means the precision size of dislocation and twins slide. Through the Critical resolved shear stress the force applied to will be attained which is the main method to proceed in deformation course of Ti_3Al-Nb alloys. Meantime the twins have also certain roles in plastic deformation here. They conclude the whole deformation mechanism in this paper while the basal or prismatic dislocation exhibits the lowest stress with Schmid factor 0.*

Keywords: *pyramidal dislocation; twins; CRSS(critical resolved shear stress); Ti_3Al-Nb intermetallic compounds; deformation; Schmid factor*

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I. Introduction

Ti_3Al 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 dislocations will resolve into the Shockley partial dislocation which play an important role in crystallography change in Ti-25at.%Al-11at.%Nb alloys. 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 of dislocation and twins [1] will be described detail in this paper.

The CRSS value will express the pyramidal dislocations $<11\bar{2}6]$ and twins $<10\bar{1}\bar{1}]$ 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 deformation size. 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 substituted for Ni based and Ti based alloys in future, for example adding the third ones into Ti_3Al intermetallic compounds. The producing method has been changed a certain in order to attain better crystalline structures, like Making inclined solidification, Single Crystals & Poly crystals. [4~7]

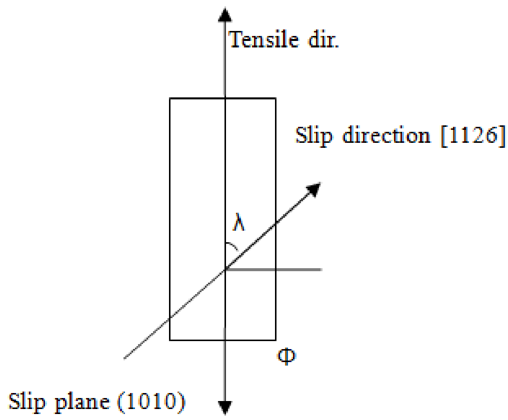

Figure 1 Schematic of the CRSS of [1126] in (1010) in Ti-Al Intermetallic Compounds.

II. Experimental Methodology

The specimen of Ti_3Al-Nb 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.%), Al bulk(99.9wt.%) & Plate Nb(99wt.%) 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 proceeded at room temperature in order to search tensile curve. The strain rate is used to 1.25×10^{-4}/s. Test times are processing two times whose average value is adopted with each composition specimens. The specimen after tensile test is adopted to proceed the TEM(Transmission electron microscopy) observation with both Ti-25at.%Al and Ti-25Al-13at.%Nb alloys. The specimen gauge specification uses 8×3×1mm for tensile experiment. The specimen has fitted to specification well.

In addition, 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 Ti_3Al 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 angle 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 very much. 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.

III. Result and Discussions

The results was proceeded with the equations of a certain equation, and according to Figure 1 the logic arrangement was done through the Schmid factor in the crystal. The dislocations and twins like (1010)[1126] has angle λ with tensile direction, meanwhile ϕ is perpendicular to tensile one. Hence here $\phi=90°-\lambda$. So we can obtain the some values as below discussed. The Schmid factor and CRSS(Critical resolved shear stress) presents the complete stress status in dislocations and twins in Ti_3Al-Nb. So we can judge their size value in terms of both them.

3.1 Schmid Factor

The 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 {1011} and basal slips in poly crystals. Furthermore, the dislocations having linear mode is observed to occur. The Schmid factor in basal or prismatic dislocation has become 0 whose stress will be the lowest one. But its strain can become the highest one which we speculate now.

Due to the complicate dislocations is there in deformation course in Ti_3Al 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 the direction{1010}<1126> pyramid and {1012}<1011> twins. 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. According to these two directions the directional dislocation and twins is searched for with the Schmid factor and CRSS respectively in this study. [8~11]

3.2 Default Status

The poly crystalline Ti-at.%25Al and no deforming twins are observed. However, {1011},{1012} and {1022} three types twinning planes is confirmed while the main twinning' is {1011}. [12] The volume fractions of formed twins with about 0.1 strains have increased with increasing temperature, meanwhile it will decrease slightly. At 1273K and 1173K the increasing volume fraction with total strain has increased in Al-rich ones.

The occurred twins has been relation to the dislocation with c composition and LRO(Long range order) which has been considered. The decreasing LRO is the reason of the twins to happen smaller than the size of APB(Antiphase boundary). The burgers vector B and (1210) to determine of APB [0001] and [1010] is the same as [1210]. Those super lattice with partial dislocations are <1010> which has been confirmed. The 1/3<1120> has been 15nm, meantime, 1/6<1120> in partial dislocation is 4nm. The 1/3<1121> in super dislocation has very low temperature so the role of partial dislocation is existed.

The super lattice with partial dislocation has extensive defects. The APB energy may be increased with high temperature. The volume ratio has been reduced with increasing temperature which is main reason on the LRO. In results non stoichiometric and ternary element has reduced LBO so that is promoted ductility.

The prismatic slips having activated as SC(Single crystal) are compressed near c axis. The volume fraction of twins will increase with raising temperature up to 1373K. It will increase under the high temperature. The fraction of twins increase according to the total strain at the HT(High temperature) while the fraction of the twins reduces. Non a dislocation and APB in Ti-33at.%Al has been observed.

3.3 Strength style status

A large data on the types of planes has been formed on which the cleavage fracture has occurred in {1012}, {1123}, {1011} and {0001}. In order to calculate the Griffith surface energy, it specifies the crack-opening ability for the detected cleavage. It is found that the low decoherence energy is compared with pure metals for one of the reasons of the brittlement. [12]

It is important that we will analyze the types of dislocation and their transformations in the plastic zone of a growing crack nucleation and growth in a slip band in the basal plane have been analyzed in detail. Experimental studies have proved that The basal slip results in shear-type crack.

In some papers in theoretical analysis the structure of the screw a super dislocation in the basal slip. The model is found to be in agreement with experimental results. As for other orientations of deformed SC, the crack nucleation process studies. In this work, we perform some analysis of dislocations making up a plastic cracks in α_2 deformed at room temperature. The cracks show to grow on {0111} pyramidal planes and in the slip bands of 2c+a super dislocations on {2021} and {1121} pyramidals'. Because the formation of a slip band has lay in the basal plane at a micro crack tip, the propagating crack is liken rather than linear. Nucleation can be formed at the intersection line of {1121} pyramidal and prismatic planes. [13]

The α_2 with ordered structure is the promise for practical application in HT(Heat treatment) resistance. They have a low density and high mechanical properties at HT. It has low RT(Room temperature) plasticity. A strong orientation dependence of σ_y and the present of a complicated structure will occur by a variety of Bergurs vectors and slip planes with SC. That is a, c+a and 2c+a super dislocation in the basal, prismatic or pyramidal slip. The earliest deformation mode in it i a/3<1120>{1100} prismatic slip. In the basal plane the deformation also involves in a super dislocations. [14]As for $D0_{19}$ the peak in the $\sigma(T)$ curve is given by a minimum value in plasticity. A mechanical formation of the shear type micro cracks will happen due to the intersection for the screw a dislocation in a basal slip band.

The super α_2 having more stabilized elements has gradually improved strength as the solution temperature will approach the transus'. Under heat treatment temperature the Martensite transforms to the stabilized secondary α_2+O+B2 which will distribute finely. The amount of refining α_2 increases strength in super' so the transformation is supposed and the strength promotion in not available. [15~17]

The varied treatment has used to define the volume and morphology of α_2. It has higher influence on the crack evolving. So through the behavior of two phases of $\beta+\alpha_2$ it is investigated that the fine colony showed no variation as the function will change. In contrast to the equiaxed and basket weave it appears to increase crack growth resistance as the fraction is reduced. A quantitative measurement for test crack closure is done to explain.

The crack resistance attributes to a sessile of evolving path herein it results in a reducing in the driving force to acquire from deflection and roughness'.

There is the boundary of the ribbon of stacking default, herein it can resolve two Shockley partial dislocations. The space of partial dislocations are in proportion to stacking default energy reversely. There is the trend that slips will be confined in basal plane of Hcp. There are two reasons. Firstly, the fully dislocations are resolved in basal plane. Secondly, with non dense plane to be intersection in basal plane, and the interactive slips can not occur, which is not the same to Fcc. However the slips to be basal plane are observed often.

The dislocation has been mostly on basal plane in large crystalline alloys. It can make effect on the intersection slip. The no resolved screw dislocation will more generally in the basal plane for the barriers to be difficult to move, herein the movement will be possible through the pyramidal and prismatic plane. However, in order to form the resolved screw dislocation and shrink stacking default energy it will occur only in pyramidal slip$\{10\bar{1}1\}$ and prismatic slip $\{10\bar{1}0\}$.

3.4 Conclusive narrative

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 slip and twins to be difficult to happen in crystallography of Ti_3Al phase for high stress. 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 dislocation{1010}<1126> can wield more roles in plastic deformation than the twins $\{10\bar{1}2\}$<$10\bar{1}\bar{1}$> in the Ti_3Al-Nb alloys.

For the needs of higher temperature and light quality, new advanced materials would be searched: 1) high melting point; 2) low density; 3) elastic modulus; 4) good structure stability and excellent oxidized resistance [16] in the high temperature application, such as engines. [17] Through the changing their elements the above needs has been combined, therein the new material α_2 intermetallic compounds can be formed in the end. So the new properties can be evaluated for us to search for in the future.

IV. Conclusions

The more pyramidal dislocation <1126> and twins <1120> can wield more roles in plastic deformation of the Ti_3Al alloys because the pyramidal dislocation and twins has big effectiveness according to CRSS value in Ti_3Al-Nb alloys. The former has bigger strain than the later due to its low value of CRSS with 264MPa and 294MPa respectively in this paper.

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