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Structure Transformations in the Polycrystalline $(Ti,Nb)_3Al$ Alloy under Shock-Wave Loading

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Abstract

Structure transformations in the two-phase $(Ti, Nb)_3Al$ alloy, induced by shock-wave loading, were studied. The samples were subjected to an impact of a steel plate. The maximum pressure on the samples' surfaces was 100 GPa, while the maximum temperature was 573 K. The $\beta_0 \rightarrow \alpha_2$ phase transformation occurred during strong deformations. High temperature rectilinear dislocations (such types of dislocations usually could arise at 1073 K) with the ***c***-component, which occasionally formed slip bands, were located at the α_2-phase grains after the shock. The deformation α_2-phase twins were not observed.

Keywords: Ti_3Al, Phase Transformation, Shock Waves

1. Introduction

Shock waves in materials produce unusually great numbers of the dislocations that substantially change mechanical properties of metals, such as the strength, plasticity, resistance to damage, or cracking [1-3]. Stresses arising in materials may be relaxed because of the rearrangements of the dislocations to configurations with more favorable energy, twinning, or phase transformations. Plate impact is considered as the standard diagnostic means to characterize the dynamic response of the materials. These experiments are very important for the structural materials. In particular, the developments of jet turbine engines require knowledge of the materials' responses to impact events, such as the bird strikes, damages by foreign objects, and blade containments. Ti_3Al-base alloys are an interesting subject for studying. Excellent elevated-temperature properties and low density make the titanium aluminides attractive candidates for both engine and airframe applications, particularly in the aerospace industry. However, poor ductility and low fracture toughness have been the key limiting factors in utilizing the alloys.

Absence of the deformation twinning has frequently been referred to as one of the reasons for the brittleness of Ti_3Al, especially in its polycrystalline form [4]. This is also the case when Ti_3Al is deformed at high-strain rates, such as those achieved by shock loading [5]. The shock-wave loading in [5] was done by the technique of the plate impact; the maximum pressure on the samples' surfaces was 12 GPa. Brief information on the phase transformations in Ti_3Al-base alloy under shock-wave loading was given in [6].

It is assumed that the twinning process is independent of temperature and is governed by only the applied stress. This process is considerably facilitated in crystals with defects that serve as stress concentrators, as well as by alloying that leads to changes in the stacking-fault formation energy. In [7] it is found that the deformation twinning occurs only in the Ti-36.5 at.%Al single crystals under specific conditions (*i.e.*, off-stoichiometric compositions, high temperatures, and if the compression axis is close to the ***c***-axis). In [8] the authors have suggested the occurrence of the deformation twinning in Ti_3Al grains coexisting with grains having the B2 superstructure in Ti-24 at.%-11 at.%Nb alloys.

The purpose of this work is a detailed study of the deformation behavior of the two-phase polycrystalline $(Ti, Nb)_3Al$ alloy under the shock-wave loading with a maximum pressure of 100 GPa on the samples' surfaces.

2. Materials and Methods

The subjects of this study, the $(Ti, Nb)_3Al$ polycrystals,

were smelted from titanium iodide (99.95%), extra-pure aluminum (99.9%), and niobium (99.9%) in an argon atmosphere in an arc furnace (**Table 1**). The ingots were homogenized at 1400˚C for 5 h in a helium atmosphere. For our study, the samples were cut to sizes of 10 × 10 × 10 mm from the ingots and placed on a steel plate; the loading was done with another steel plate. Shock-wave loading of the samples was done at the Academician E. I. Zababakhin Russian Research Institute of Technical Physics, Russian Federal Nuclear Center, Snezhinsk, Russia. The samples were exposed to an impact of the steel plate, and the maximum presure on the samples' surfaces was 100 GPa, while the pulse duration was 1 μs. We used a chamber for saving samples after the shock-wave loading. The X-ray diffraction analysis was performed using a DRON-3 diffractometer with the Co k_α and Cu k_α radiation. The TEM analysis was performed with a JEM-200CX transmission electron microscope.

3. Results and Discussion

The X-ray pattern of the initial sample is shown in **Figure 1(a)**. The phase composition of the initial sample had two components: α_2 (Ti_3Al, $P6_3/mmc$, DO_{19}) and β_0 (TiAl, Pm3m, B2). The lattice parameters of the phases in the initial state are given in **Table 2**.

The results of the X-ray analysis of the sample after the shock-wave loading showed that the intensity of the β_0-phase lines was severely reduced; the lines at intermediate angles disappeared (**Figure 1(b)**). The lattice parameters of the β_0-phase could not be accurately determined; however, those of the α_2-phase changed to a = 0.5774 nm; c = 0.4663 nm.

According to our optical study, in its initial state, the alloy included two species of grains, on average 20 μm in size (**Figure 2(a)**), whereas after the shock loading, the grains were fragmented (**Figure 2(b)**). Results of the micro- hardness measurements are presented in **Figure 3**.

The hardness of the sample increased after the shock-wave loading, the maximum hardness was observed at the edge of the sample.

Table 1. Chemical composition of the initial samples (weight %).

Al	Ti	Nb
14.6	64.8	20.3

Table 2. Phase composition of the samples in the initial state.

Phase composition	Volume fraction, %	Lattice parameters
$\alpha_2 + \beta_0$	80% α_2	α_2: a = 0.5766 nm c = 0.4661 nm β_0: a = 0.32628 nm

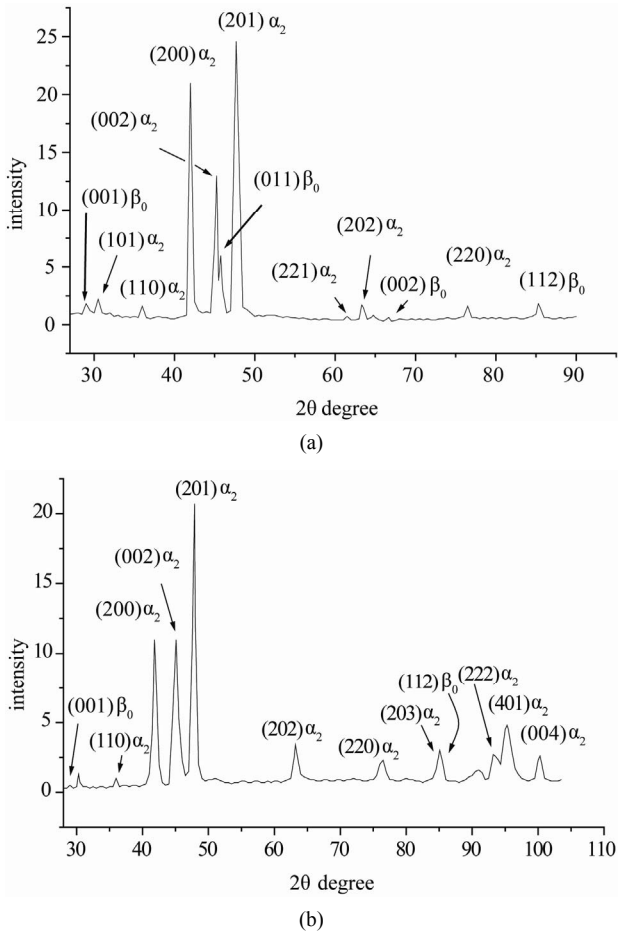

Figure 1. Results of the X-ray analysis of the (Ti, Nb)$_3$Al alloy: (a) the initial state; (b) the state after the shock loading.

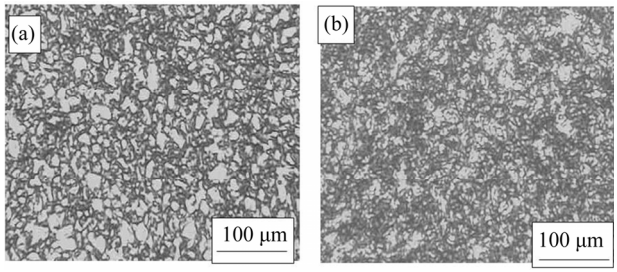

Figure 2. The microstructure of the (Ti, Nb)$_3$Al alloy, optical microscopy, polarized light: (a) the initial state; (b) the state after the shock loading.

Our TEM study of the sample in its initial state showed the structure with the α_2-phase and β_0-phase grains, as well as the grains with plates of the α_2 phase piercing throughout the β_0-phase grains. Single α_2-phase grains were much coarser than the two-phase grains (**Figure 4**).

The TEM study of the sample after the shock-wave loading revealed the rectilinear dislocations inside the α_2

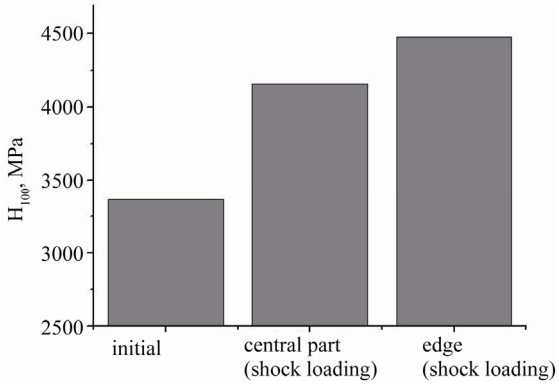

Figure 3. Results of the micro-hardness measurements.

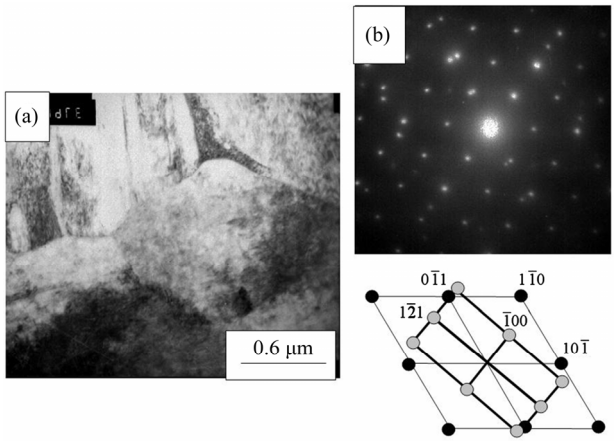

Figure 4. The microstructure of the (Ti, Nb)$_3$Al alloy in the initial state, TEM: (a) bright field image; (b) diffraction pattern to a); zone axis [111] β_0 II [012] α_2.

grains. **Figure 5** shows the dislocation systems; we found that they are ***c***-component dislocations, because they are clearly seen in reflection $\boldsymbol{g}$ = 0002 (**Figure 5(a)**, **(b)**). For the dislocations in **Figures 5(c)**, **(d)**, the condition $\boldsymbol{gb}$ = 0 is fulfilled in reflection $\boldsymbol{g}$ = $1\bar{1}00$.

It is known that the slip on $\{1\bar{1}00\}\prec 11\bar{2}0\succ$ (prism ***a***-slip), $(0001)\prec 11\bar{2}0\succ$ (basal ***a***-slip), $\{0\bar{2}21\}\prec 11\bar{2}6\succ$ (type-I pyramidal 2***c*** + ***a***-slip) and $\{11\bar{2}1\}\prec 11\bar{2}6\succ$ (type-II pyramidal 2***c*** + ***a***-slip) are the operative slip systems in Ti_3Al, among which the prism slip is the most-readily operative one because of a considerably lower critical resolved shear stress [9].

In the Ti_3Al alloy, during the deformation by compression at the room temperature, along with the main slip system $\{1\bar{1}00\}\prec 11\bar{2}0\succ$, the slip system $\{11\bar{2}1\}\prec 11\bar{2}6\succ$ contributes to the deformation. In the latter slip system, the edge dislocations are less mobile.

As the temperature increases (to 923 K), the slip morphology changes, such that the dislocations are localized in the slip bands and split according to the reaction [10]:

$$1/3<\bar{1}\,\bar{1}26>\rightarrow 1/6<\bar{1}\,\bar{1}26>+\text{APB}+1/6<\bar{1}\,\bar{1}26>.$$

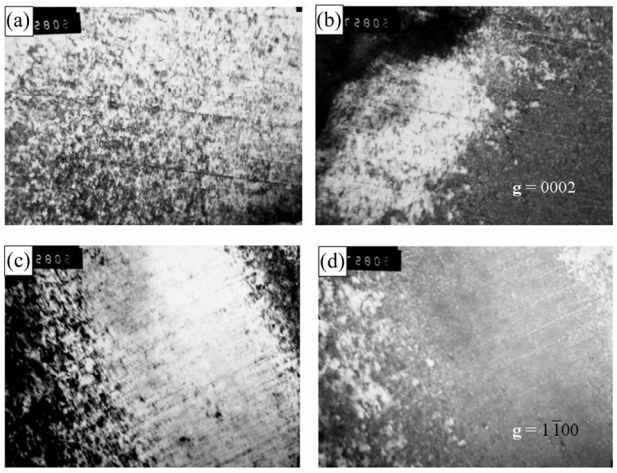

Figure 5. Dislocations in the (Ti, Nb)$_3$Al alloy after the shock loading: (a) bright-field image to (b), (b) dark-field image in g = 0002; (c) bright-field image to (d), (d) dark-field image in g = $1\bar{1}00$.

According to [9], a similar dislocation picture with the ***c***-component dislocations, as in our case, is observed in the range of the thermal strengthening for Ti_3Al crystal (~1073 K) and during the deformation at the room temperature. In our experiment, the maximum temperature on the samples' surfaces was 573 K.

We also found the band structure resembling the twin inside the α_2-grains (**Figure 6**); however, in reality it is not a twin. The diffraction pattern taken from the region with the band structure did not have the reflections of the β_0 phase. The β_0 reflections must appear according to the orientation relationship between the crystal lattice of the α_2- and β_0- phases: $(0001)\alpha_2 \parallel (110)\beta_0$; $<11\bar{2}0>\alpha_2 \parallel <\bar{1}11>\beta_0$.

The presence of certain orientation relationships between the lattices of the different phases allows one to precisely identify (within a single grain) the selected-area electron-diffraction (SAED) patterns obtained from different sites of the same grain. For indexing the diffraction patterns, we calculated the matrices of the correspondence between the planes and zone axes of the crystal lattices of the α_2- and β_0-phases in our alloy. The calculation is based on the solution of the following ma-

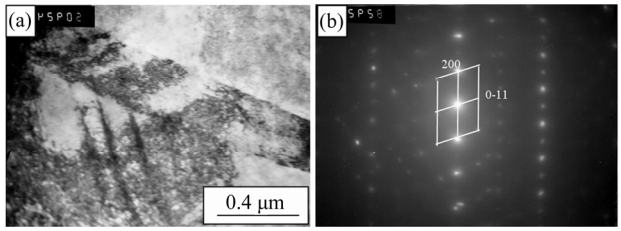

Figure 6. Band structure in α_2-phase: (a) bright-field image, (b) diffraction pattern to a), zone axis [011] α_2.

trix equations that allow one to find the indices of the corresponding phases: $H_{\beta 0} = A^* H_{\alpha 2}$; $U_{\alpha 2} = A^T * U_{\beta 0}$, where H and U are the column vectors containing the indices of the planes and directions in the crystal lattices of the phases, respectively; A and A^T are the transformation matrices for the determination of the planes and directions in these two lattices. With the lattice parameters of the phases presented in **Table 2**, the A and A^T matrices in our alloy are calculated as:

$$A = \begin{pmatrix} 0.46 & \overline{0.196} & 0.495 \\ \overline{0.46} & 0.196 & 0.495 \\ 0 & 0.59 & 0 \end{pmatrix},$$

$$A^T = \begin{pmatrix} 0.46 & \overline{0.46} & 0 \\ \overline{0.196} & 0.196 & 0.59 \\ 0.495 & 0.495 & 0 \end{pmatrix}$$

We find that the band structure resembling twins is observed only in the α_2 grains. We carefully checked the diffraction pattern taken from the place with the band structure and reflections of twins were not observed.

Our TEM study also showed that greater changes occurred in the β_0-phase grains. In the initial state, the β_0-phase was observed in the form of the grains or layers between the α_2 plates. After the shock loading, the dark-field images showed this phase as fine particles (**Figure 7**).

Since alloys with this composition usually are severely deformed only at high temperatures owing to the room-temperature brittleness, we compared the structures obtained here with those of a similar two-phase alloy after rolling at 1173 K [11].

The authors of [11] also observed the $\beta_0 \rightarrow \alpha_2$ phase transformation during strong deformations and re-crystallizations of both α_2- and β_0-phases during the cooling of the alloy. When the sample was deformed to 85 %, the β_0 phase transformed fully to the α_2 phase [11].

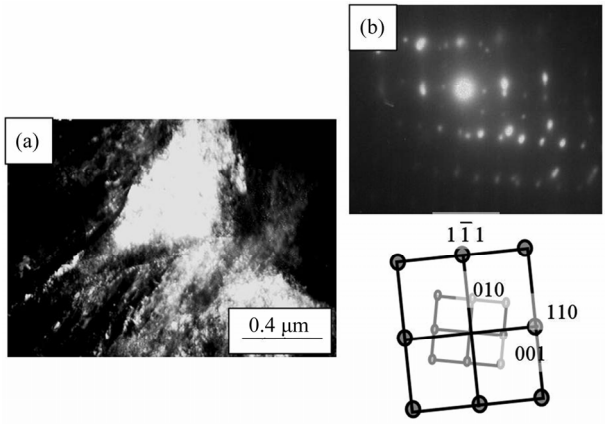

Figure 7. Microstructure of the (Ti, Nb)$_3$Al alloy after shock loading, TEM: (a) dark-field image in (110)$_{B2}$; (b) diffraction pattern to (a), zone axis $[\bar{1}1\bar{2}]\,\beta_0$ II $[100]\alpha_2$.

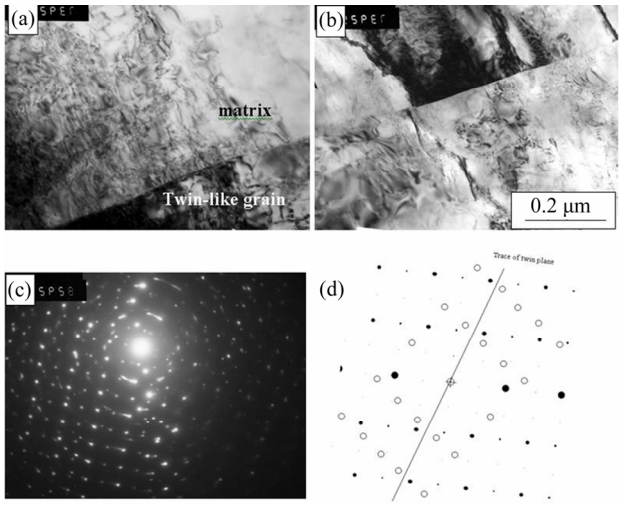

Figure 8. Twin-like α_2 grains: (a) dark field image in twin-like reflex, (b) dark-field image in matrix reflex; (c) diffraction pattern to (a)-(b) zone axis [010]; (d) bright-field image, d-diffraction pattern to (d), zone axis [011].

Figure 8 shows a structure that looks like a twin. The diffraction pattern shown in **Figure 8(b)** is quite similar to that reported for the $\{2\ 12\ \overline{10}\ 3\} \prec 5\overline{1}46 \succ$ twin by Kishida *et al.* [7]. But in reality it is not a twin. We could not obtain the dark-field or bright-field images from this place to prove the formation of the twin. Probably, in this case, we found the grain boundary, that looks like a twin.

4. Conclusions

The structure of the two-phase (Ti, Nb)$_3$Al polycrystal after the shock-wave loading has been studied in detail using the X-ray analysis, optical microscopy, and transmission electron microscopy. Our results can be summarized as follows.

1) Strong instantaneous (100 GPa, 1 μs) shock-wave loading of the two-phase (Ti, Nb)$_3$Al alloy caused the phase transformations $B2 \rightarrow DO_{19}$.

2) The rectilinear high temperature dislocations with the ***c***-component formed the slip bands that were observed inside the α_2 grains after the shock-wave loading.

3) No deformation twin was found in the α_2 grains after the shock-wave loading.

5. Acknowledgements

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