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Comments

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Abnormal deformation behavior in Polysynthetically-twinned TiAl crystals with A and N orientations─── **an AFM study**

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Abstract

Polysynthetically-twinned TiAl crystals were deformed by compression with loading axis parallel and perpendicular to the lamellar interfaces. The deformation structures on the free surfaces were scanned using a dimension AFM with scan directions parallel and perpendicular to the lamellar interfaces. Abnormal deformation behaviors were observed to occur in both orientations. When the compression axis is parallel to the lamellar interfaces, the gamma and alpha lamellae deform primarily by shear in planes inclined with the lamellar interface, while the shear vectors lie in the interface. However, in-plane shear, shear in slip planes parallel to the lamellar interfaces, also occurs along the lamellar interfaces. When the loading axis is perpendicular to the lamellar interface, in-plane shear was found to be dominant at the beginning stage of plastic deformation and contributes more to the macroscopic strain. These behaviors are controversial to the Schmid's Law since the applied resolved shear stress for these deformation systems is zero. The abnormal phenomenon was explained by the large coherency stresses along the lamellar interfaces.

Introduction

 It has long been accepted that the lamellar interfaces play an important role in the deformation process of γ-based TiAl materials with lamellar structures. [1-3] However, it is a difficult job to investigate the interaction between the lamellar boundaries and the deformation systems, due to the complexity of boundaries in the polycrystals. In early 90s, Dr. Yamaguchi's group [4] produced the so-called polysynthetically-twinned (PST) TiAl crystals, which are big lamellar grains, and used them to study the deformation process with the existence of lamellar interfaces. Since then, a lot of achievements have been made in discovering the deformation behavior of PST crystals. It was found that the yield of PST samples changes with their orientations, [2-6] and the plastic deformation is anisotropic at some orientations. [3,6] TEM results show that the special deformation behavior comes from the selective activation of deformation systems in the gamma phase and alpha 2 phase, which results from the confinement of the lamellar interfaces [3].

 In our research, Atomic Force Microscopy (AFM) was chosen to study the deformation behavior of PST crystals. By scanning the free surfaces of the deformed samples with different orientations, deformation structure at different size scale can be investigated so that a more comprehensive view can be obtained. The AFM results showed [7] that there are three deformation modes with the change of sample orientation. When the angle between the loading axis and the lamellar interfaces is below 20 degree, the lamellae deform by shear on slip planes inclined with the lamellar interfaces, but the shear vectors are parallel to the lamellar boundaries. In-plane shear (shear in planes parallel to the lamellar interfaces) dominates when the angle is between 20 and 80 degrees. When the loading axis is close to perpendicular to the lamellar

interfaces, cross-lamellar shear dominates at high strain levels. The results suggest that in-plane shear is the easiest deformation mode in PST crystals, because it brings lest disturb to the lamellar interfacial structure. Consequently, in-plane shear was even observed in A orientation (loading axis parallel to the lamellar interface) and N orientation (loading axis perpendicular to the lamellar interface) even though the applied shear stress on these slip planes is zero. In this paper, the abnormal deformation behavior occurred in these two orientations will be discussed.

Experimental details

 PST crystals with a nominal composition of Ti-48at%Al were grown using optical floating zone furnace. Crystals were oriented by Laue back diffraction technique and samples were cut using electrical discharge machining (EDM). The free surfaces of the samples were mechanically polished and electro-polished. Compression tests were carried out under room temperature at a speed of 1×10^{-6} /s using an Instron machine. The geometries for the compression tests at A and N orientations are schematically shown in figure 1.

 The deformation structures emerged on the free surfaces were studied using a DI 3000 Dimension AFM. In AFM observation, the feature parallel to the scan direction is weakened due to the signal process. In order to obtain the true topography, scan directions parallel and perpendicular to the lamellar interfaces were both chosen.

Results and discussions

1. In-plane shear in A-oriented sample

 In-plane shear typically occur as interfacial sliding at the lamellar interfaces. As we discussed elsewhere, [8] in A orientation samples, the neighboring lamellae tend to deform in such a way that the deformation bands have the same offset height and offset angle, so that no strain incompatibility will be produced at the lamellar interface. However, this cannot be always satisfied since some of the gamma domains deform by combination of twinning and ordinary dislocation slip with vectors inclined with lamellar interfaces. Strain incompatibility and complex stress state will be inevitably induced at the lamellar interfaces, although the offset across the lamellar interfaces is only tens of nanometers. The built-up stress along with the coherency stress might be high enough to stimulate the in-plane shear at these places, since the C.R.S.S for the in-plane shear is much lower. [3,6,9]

Figure 1. Geometry of the PST samples during compression test

Figure 2. Interfacial sliding at the γ**/**γ **lamellar interface (Deflection image)**

As shown in figure 2, there is an intense band at the γ/γ interface pointed by the black arrows. The lamella at the left side has deformation bands going across the lamellar interface, as a result, stresses were built up and in-plane shear occurs to dissipate the energy. The interfacial sliding also occurs at the α_2/γ interfaces when there is a strain incompatibility.

There are some fine γ lamellae separated by fine α_2 lamellae in the PST crystals. These lamellae have the width of several tens of nanometers and look like a pure α_2 lamella in the SEM. [10] Because of the high density of lamellar interfaces inside this kind of lamellar bundle, the deformation process is strongly restricted. Figure 3 (a) shows the deformation structure of a sample deformed by about 3%. Fewer deformation bands exist inside the lamella between the two dashed lines. The deformation bands look like vertical traces which might be formed by prismatic slips in the α_2 phase. [8] However, a closer look in figure (b) reveals that these bands are actually not vertical, but composed of many zigzagged bands in different lamellae. The width of the bundle is about 2µm, and it contains about 20 lamellae. There are not only fewer inclined bands inside the bundle, but also fewer and smaller in-plane bands. Only at the two boundaries of the bundle are there large in-plane shear steps, which have the height of tens of nanometers and are comparable to that of the inclined bands. The possible reason for this deformation behavior is that it is difficult for the fine lamellae to deform while maintaining compatible strain with each other in such a small scale. In other words, the energy increase associated with the deformation might be huge, so the PST crystal tends not to deform inside these lamellae bundles. Rather, it dissipates the energy by interfacial sliding at the boundaries of the bundles.

 It is not clear whether the lamellar sliding is a superficial effect or it occurs throughout the whole sample. No direct TEM observations and discussions are available on this issue, although it can be seen from the TEM images that fringes of tens of nanometers in width usually present at the lamellar interfaces. [11,12] The details of the structure inside these fringes need further investigation. In fact, based on the AFM observations, interfacial sliding does not occur everywhere. Resultantly, additional strain incompatibility will be produced at the domain boundaries, especially at the intersections of the domain boundaries and the lamellar interfaces. However, since the domain boundaries are weak barriers to the shear transmission, and the lamellar shear is just on the nanometer scale, the strain incompatibility will not cause large stress concentration at the domain boundaries.

Figure 3. The deformation structure inside a 'lamellar bundle'. Picture (b) is a magnified view of the dashed square in picture (a).

Figure 4. The deformation structure in the lightly deformed area on the two free surfaces. (a) Deflection image; (b) Amplitude image.

2. In-plane shear in N orientation

 AFM results show that in-plane bands are the dominant species at low strain level as shown in figure 4. Detail analyses [13] indicate that only in-plane shear can produce bands parallel to the lamellar interfaces on both free surfaces. But how can this happen since the Schmid factors for the in-plane shear systems are all zero when the loading axis is perpendicular to the lamellar interface?

 One possible reason for the appearance of these unexpected slip traces might be that the crystal is incorrectly oriented so that the loading axis is not perfectly perpendicular to the lamellar interfaces. This would induce deformation mode similar to those seen in the B-oriented samples. [14] Since the possible error in sample orientation using the Laue back diffraction technique is about 2 degrees, the maximum Schmid factor for the deformation systems on the (111) plane is about 0.001. The CRSS of deformation systems on (111) plane parallel to the

lamellar interfaces in the γ phases is around 100MPa, [2,3,6,9] so if the in-plane shear is caused by this misorientation, the axial yield stress should be around $10⁵ MPa$, which is 100 times higher than the experimental results, about 1000MPa.

 Clearly, misorientation is not the primary reason for the occurring of in-plane shear. A reasonable explanation might be to include the coherency stress and complex stress state at the lamellar interfaces. Previous calculations and measurements have shown that coherency stresses with amplitude of 100MPa exist in the PST crystals. Hazzledine's calculation and CBED results [15] suggest that the residual stress is biaxial in the lamellae, but pure shear in the interfaces. Results from Appel et al. [1] also suggest that the direction of the coherency stress is randomly oriented and the amplitude of the stress ranges from several MPa to over 400MPa. This shear stress, along with the induced shear stress by the pileups might be high enough to activate the dislocations in the lamellar interfaces and produce parallel traces on the free surface. The interfacial shear will then lead to shear stress inside the lamellae and cause the broadening of the parallel bands.

 Similar to the A orientation, it is unclear whether the formation of these parallel bands are just a superficial effect or not, since no twinning or dislocation slip on planes parallel to the lamellar interfaces in N-oriented samples was ever observed in TEM. And since many misfit dislocations are present in the lamellar interfaces, it might be very difficult for the dislocations to move throughout the entanglements. However, this question still needs further investigation since the TEM samples are typically cut parallel to the lamellar interfaces [1-3] it is difficult to observe in-plane shear using this kind of thin films.

 With the increase of strain level, cross-lamellar shear becomes to take over since only these bands can produce strain in the compression direction. However, in-plane shear still contributes a lot to the overall strain as shown in figure 5.

yz **surface** *xz* **surface**

Figure 5. The deformation structure in the heavily deformed area. Black arrows indicate the in-plane shear bands. (Deflection images)

Conclusions

 In-plane shear is the easiest deformation mode for the PST crystals due to the confinement of the lamellar interfaces. As a result, in-plane shear occurs whenever possible even when the applied shear stress for this deformation system is zero. In A-oriented samples, in-plane shear occurs along lamellar interfaces when there is a strain incompatibility and stress concentration. In N-oriented samples, in-plane shear is the dominant deformation mode at low strain level and contribute a lot to the overall strain. This abnormal deformation behavior might result from the complex coherency stress state at the lamellar interfaces.

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