Influence of silicide on fracture behavior of a fully lamellar Ti-46Al-0.5W-0.5Si alloy

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Abstract: The fracture behavior of fully lamellar binary γ-TiAl alloys is extremely anisotropic with respect to the lamellar orientation. For the fully lamellar Ti-46Al-0.5W-0.5Si alloy, the existence of silicide clusters plays a critical role on the fracture behavior. In the present study, tensile test and three point bending test were performed at room temperature with the loading axis parallel and perpendicular to the lamellar orientation, respectively. To investigate the influence of silicide clusters on the initiation and propagation of cracks, the fracture surface and the cracks adjacent to the fracture zone of the specimens have been analyzed. Results show that the fracture process is related to the morphology and distribution of the silicide clusters. Crack preferentially initiates at and propagates along the interface of silicde and αγ lamellar with the loading axis perpendicular to the length direction of silicide. While the silicide can prevent the propagation of cracks from running across with the crack growth direction perpendicular to the length direction of silicide.

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Due to their low density and high temperature properties, intermetallic γ-TiAl based alloys have attracted significant applications in the aerospace and automotive industries [1-3]. The addition of a small amount of silicon into γ-TiAl based alloys not only increases the oxidation resistance, but also improves the tensile stress and creep resistance through introducing ξ-Ti5Si3 phase [4-6]. Research shows that the solubility of Si is limited at both room temperature and elevated temperatures in the γ-TiAl based alloys [7]. So far, silicides have been only found in Si-containing γ-TiAl alloys. There are usually two kinds of ξ-Ti5Si3 phase in these alloys, the primary relatively large particles formed during solidification and the small particles generated from solid eutectoid phase transformation [8].

There are four typical microstructures of γ-TiAl based alloys: fully lamellar (FL), near lamellar (NL), near γ phases (NG), and duplex (DP). Among them, aligned lamellar orientated microstructures usually manifest a good combination of strength and ductility over a wide range of temperatures [9]. So far, the mechanical properties and the fracture mechanism of γ-TiAl alloys have been widely studied. It is reported that the fully lamellar (FL) microstructure consisting of γ-phase (TiAl) and α2-phase (Ti3Al) can display a better fracture toughness, and the fracture toughness increases with an increasing grain size [10]. The weakest link is lamellar interface in the two-phase fully lamellar γ-TiAl alloys [11-13]. Therefore, usually valid mechanical properties can only be obtained when the loading axis is parallel to the lamellar orientation. Most research has focused on the relationship between the loading axis and the lamellar orientation. However, for Si-containing γ-TiAl alloys, the influence of the presence of silicide clusters on the mechanical properties has been rarely reported. In this work, a fully lamellar Ti-46Al-0.5W-0.5Si alloy, composed of α2/γ lamellar and silicides, was prepared and dedicated experiments were performed to study the fracture behavior. Specific objectives of this study include: (A) Investigating the initiation and propagation of cracks near the primary silicides, and (B) Analyzing the effect of silicides on the fracture behavior.

1 Experimental procedure

The nominal composition of the γ-TiAl based alloy used in the present study was Ti-46Al-0.5W-0.5Si (at.%). The master materials were titanium sponge, high purity aluminum (99.99wt.%), silicon (99.9wt.%) and Al-W (55.92wt.%). The alloy was melted in a water-cooled copper crucible inside the vacuum induction skull melting (ISM) furnace and
cast into a cylindrical ingot with a diameter of 112 mm and a height of 220 mm. The macrostructure produced by this process consists of columnar grains growing from the surface towards the central part of the ingot, as shown in Fig. 1.

**Fig. 1: Macrostructure of as-cast Ti-46Al-0.5W-0.5Si alloy**

Flat tensile specimens and single-edge-notched (SEN) specimens were cut from this as-cast ingot with an electric discharge machine, perpendicular to and parallel to the axial direction of the longitudinal section of the ingot, respectively. The gauge section of the flat tensile specimens was 6 mm in width, 2 mm in thickness and 18 mm in gauge length. The single-edge-notched (SEN) specimens were 2 mm in width, 4 mm in thickness and 20 mm in length, and were notched to a depth of 2 mm and a width of 0.2 mm.

All specimens were polished before testing. The tensile tests and fracture toughness tests were carried out at room temperature using an INSTRON 5500R testing machine at a strain rate of $5 \times 10^{-4} \text{s}^{-1}$. Fracture toughness tests were carried out by three point bending. In order to analyze the initiation and propagation of cracks, attention was focused on the region adjacent to the fracture zone and the notch root. Fracture surface observations were carried out by an FEI Quanta 200F scanning electron microscope (SEM). Micro-crack observations were carried out by backscatter electron (BSE) analysis, and the compositions of various microstructural constituents were determined by energy dispersive X-ray spectroscopy (EDS).

### 2 Results

#### 2.1 Silicides in as-cast Ti-46Al-0.5W-0.5Si alloy

Figure 2 show the BSE micrographs of the as-cast Ti-46Al-0.5W-0.5Si alloy at different locations. The micro segregation area appears different colors due to different average atomic numbers in composition. The microstructure mainly consists of fully lamellar of $\alpha_2$ and $\gamma$ phases. The microstructures observed from the section parallel and perpendicular to the growth direction of the columnar grains are shown in Fig. 2(a) and (b), respectively. Some bright reticular structures and several dark grey regions are observed within the structure of $\alpha_2/\gamma$ lamellar. The bright reticular structures mainly concentrate in dendrite core, as clearly shown in Fig. 2(b), which exhibits dendritic morphology. Semi-quantitative energy dispersive X-ray spectroscopy (EDS) analysis shows that these regions are rich in W and poor in Al. Dark grey structure concentrates in the inter-dendritic regions [as shown in Fig. 2(a)] or along the boundaries of the grains [as shown in Fig. 2(b)]. In order to further analyze the microstructure of the dark grey regions, the image at a higher magnificent is shown in Fig. 2(c). Several light grey clusters with irregular shape are

**Fig. 2: Silicides in as-cast Ti-46Al-0.5W-0.5Si alloy: (a) Silicides in the columnar grains or along the boundaries observed from the section parallel to the growth direction of the columnar grain; (b) Silicides along the boundaries observed from the section perpendicular to the growth direction of columnar grain; (c) Silicides in the grain; (d) Silicide formed from liquid during the late stage of the solidification**
embedded in the dark grey regions. EDS indicates that these clusters contain much higher Si content and lower Al content. They are considered as primary silicides. In order to further analyze the silicide formation, the shrinkage holes near the axis of the ingot (Point A in Fig. 1) have been studied, and its BSE micrograph is showed in Fig. 2(d). The primary phases contain higher W content show a dendritic arm morphology, as can be seen in the lower right portion of Fig. 2(d). It is also shown in the same figure that the inter-dendritic dark grey regions, which form at the end of the solidification of this alloy, contain higher Al and Si content and lower W content. When the contents of silicon and aluminum in the remaining liquid at the interdendritic areas are big enough, the eutectic reaction \( L \rightarrow \gamma + \xi \) would take place. Figure 2(d) indicates the formation of \( \gamma + \xi \) near the shrinkage (appeared as black holes) during the last stage of the solidification that lacks liquid metal supply.

2.2 Crack initiation and propagation of the tensile specimens

It is worth noting that the lamellar orientation obtained by the preparation methods in this study is approximately perpendicular to the growth direction of columnar grains in Ti-46Al-0.5W-0.5Si alloy, as shown in the Fig. 2(a). According to the cutting methods used in this study, the loading axis of the tensile specimens is either perpendicular or parallel to the lamellar orientation. The microstructures adjacent to the fracture zone of the two previously mentioned tensile specimens have been investigated to analyze the initiation of the micro-cracks. The micro-cracks were found near the silicide clusters, as shown in Fig. 3. The microstructures with the loading axis approximately perpendicular to the lamellar orientation are shown in Fig. 3(a) and (b). The cracks easily initiate and propagate along the lamellar interface, which is considered as a weak link in the fully lamellar microstructure of \( \gamma \)-TiAl alloys \(^{11}\). Crack 1 in Fig. 3(a) is an evidence of this mechanism. However, a larger and deeper crack named Crack 2 along the silicide in Fig. 3(a) indicates that the interface between the clusters of silicides and the \( \alpha_2/\gamma \) lamellar is probably weaker than that of \( \alpha_2 \) and \( \gamma \) layers.

When the loading axis is parallel to the lamellar orientation, the cracks easily initiate and propagate in a trans-lamellar mode in binary \( \gamma \)-TiAl alloys. For the as-cast Ti-46Al-0.5W-0.5Si alloy, the micro-cracks tend to initiate at the silicide clusters in the grain [shown in Fig.3(c)] and at the grain boundary [shown in Fig.3(d)] when their length directions of the silicide clusters are approximately perpendicular to the loading axis, and the micro-cracks tend to propagate along the silicides. In summary, the cracks propagate in a trans-lamellar mode.

It is also worth noting that because silicides are generated randomly in the process of solidification with irregular shapes, they always have a relative length direction. Silicide A and Silicide B in Fig. 3(b) have different length directions. The length direction of Silicide A is approximately perpendicular to the loading axis, and that of Silicide B is approximately parallel to the loading axis. Crack 3 initiates and propagates along the Silicide A, while no cracks were found near Silicide B.

Comparing the tensile specimens with the loading axis parallel to and perpendicular to the lamellar orientation, the micro-cracks are both more likely to initiate and propagate along the long edge of the silicides with their length direction perpendicular to the loading axis. This kind of silicide is most likely to become the crack source.
On the other hand, when an advancing crack meets a cluster of silicides, of which the long edge is perpendicular to the direction of crack propagating, it will be restrained in front of the silicide cluster. The restrained crack would continue to propagate only by increasing the applied load, as shown in Fig. 4.

![Fig. 4: Crack propagation of the tensile specimen: (a) Crack propagation restrained at the cluster of silicide with the elongated cluster structure approximatively parallel to the loading axis; (b) Magnification of (a)](image)

### 2.3 Crack initiation and propagation of the notch specimens

When compression forces are applied to a notch specimen in the three-point bending test, the notch root will subject to tensile stress, as shown at the bottom of Fig. 5. Letters D to F represent silicides, and numbers 4 to 9 represent cracks. Initiating at the most reasonable point of the notch root, Crack 4 in Fig. 5(a), hardly propagates due to the direction of tensile stress parallel to the lamellar orientation. However, Crack 5 on the right side of the notch root, initiating along the interface of $\alpha_2/\gamma$ lamellar, is easier to propagate than Crack 4. Crack 5 propagates along the grain boundary of Grain 1 and Grain 2, which is an easier growing path than the trans-lamellar path of Crack 4. One might think the main crack will grow into the direction of Crack 6. However, the existing of the silicide cluster in the top right corner of the micrograph provides an advancing path. Crack 6 stops due to the difficult trans-lamellar propagating mode. The main crack propagates along the long edge of Silicide E and a new Crack 7 develops. It is noted that the main crack will not propagate along Silicide D due to the improper direction of the long edge.

Crack 8 and Crack 9 in Fig. 5(b) both initiate directly from the notch root in an inter-lamellar mode because the direction of tensile stress is perpendicular to the lamellar orientation. They stop in front of Silicide F because the direction of its long edge is perpendicular to advancing cracks.

![Fig. 5: Crack propagation of the notch specimens: (a) The main crack propagating along the boundary and cluster of silicide with the long edge approximatively perpendicular to the tensile stress; (b) Micro-cracks stopped at the cluster of silicide with the long edge approximatively parallel to the tensile stress](image)

### 2.4 Fracture surface observation

Figure 6 shows the fracture surface of a fractured tensile specimen. It can be seen that there are several grooves or cavities in the thin layers of $\alpha_2/\gamma$ lamellar. An inclusion is also observed in one of the grooves. This inclusion is identified as silicide, whose analytical EDS result is given in Fig. 6(b). From the fracture morphology, it is easy to understand that other silicide particles, which embedded in the $\alpha_2/\gamma$ lamellar before the tests, have been stripped from the layers and held in the other part of the fracture specimen. It is apparent that the interface between the silicide and its matrix ($\alpha_2/\gamma$ lamellar or $\gamma$ phase) is a weak link.
3 Discussion

For Ti-46Al-0.5W-0.5Si alloy, the fast solidification due to the use of water-cooled copper crucible and the low solubility of Si leads to the formation of silicides at the inter-dendritic regions during the last stage of the solidification. The existence of large silicide clusters leads to the discontinuous lamellar structure. The silicides generated at random in the process of the solidification have irregular strip shapes with relative length directions. In the schematic illustration of Fig. 7 and Fig. 8, the strip objects A to E represent silicides, numbers 1 to 3 represent cracks.

The interface between the silicide clusters and the $\alpha/\gamma$ lamellar is the weakest connection under the tensile stress for as-cast Ti-46Al-0.5W-0.5Si alloy. Whether the cracks propagate along the silicides largely depends on the angles between the length directions of silicides and the loading axis. Similarly, whether the advancing cracks stop in front of the silicides depends on the angles between the length directions of silicides and the crack growing directions.

Figure 7 shows the process of the crack initiation and propagation of a specimen with lamellar planes approximately perpendicular to the loading axis. It is easy for the cracks to initiate and propagate at Silicide A due to that the length direction of the silicide is perpendicular to the loading axis. It is difficult for the cracks to initiate and propagate at Silicide B due to that the improper angle between the length direction...
of the silicide and the loading axis, as shown in Figs. 7(a) and (b). Larger tensile stress can make the crack grow along the lamellar interface in the adjacent Grain 1 of Fig. 7(c). When this advancing main crack meets Silicide B, whose length direction is perpendicular to the crack growing direction, it will be stopped in front of Silicide B.

Figure 8 illustrates the process of crack initiation and propagation of a specimen with lamellar planes parallel to the loading axis. For Ti-46Al-0.5W-0.5Si alloy, cracks would probably initiate at silicide (Crack 1), or at the grain boundaries (Crack 2), or in the grain (Crack 3), as shown in Fig. 8(a). The micro-crack can propagate when larger tensile stresses are applied, as shown in Fig. 8(b). Crack 1 can easily propagate along the interface between the Silicide C and the $\alpha / \gamma$ lamellar, but will be difficult to propagate across lamellar. Crack 2 tends to propagate along the boundary, which is an easier advancing channel. Crack 3 propagates difficultly in a trans-lamellar mode due to lamellar planes parallel to the loading axis. When it meets Silicide E, whose length direction is perpendicular to the crack growing direction, it will stop in front of Silicide E.

In this studied alloy, though the content of silicon is very low, its effect on the mechanical properties cannot be negligible. In summary, the existence of irregular blocky silicides is detrimental to the toughness and ductility properties of the Ti-46Al-0.5W-0.5Si alloy. To eliminate these effects, appropriate heat treatment technology should be employed.

4 Conclusions

(1) The as-cast microstructure of the $\gamma$-TiAl based Ti-46Al-0.5W-0.5Si alloy is composed of fully $\alpha / \gamma$ lamellar. The primary silicides have irregular strip shapes existing within the grains and at the grain boundaries.

(2) When the loading axis is perpendicular to the length direction of the silicides, cracks easily initiate and propagate along the interface of the silicides and the $\alpha / \gamma$ lamellar, which is considered as the weakest juncture. Instead, when the loading axis is parallel to the length direction of the silicides, it is much more difficult for the cracks to initiate at silicides.

(3) Irregular silicide clusters can offer resistance to crack growth when the crack growing direction is perpendicular to the length direction of the silicides.

References


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