

## The Atomic Interfacial Structure between $\alpha_2$ and $\gamma$ Phases within a TiAl Alloy in Lamellar Form

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Due to the attractive properties such as high strength-to-weight ratio and excellent high temperature creep and oxidation resistance, TiAl-based alloys with fully lamellar microstructure have been widely applied in producing aerospace and car engines [1-3]. The distribution of  $\alpha_2$  and  $\gamma$  phases, strongly affected by their interface, plays an important role in determining their mechanical properties at high temperature [4-6]. Although many researchers have investigated it by transmission electron microscopy [4, 7], the atomic interfacial arrangement and the chemical bonding nature have not been fully clarified. Therefore, we aim on analysing of the detailed interfacial structure in TiAl alloys.

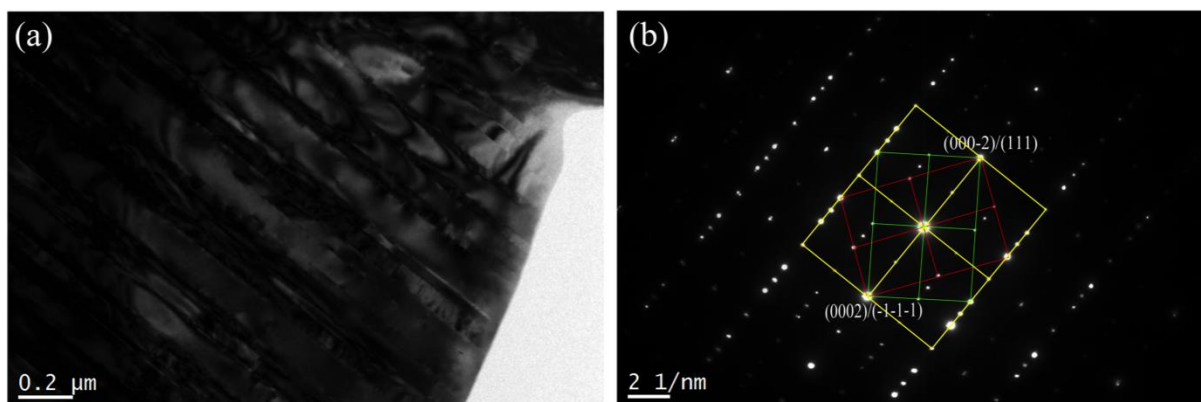
We studied TiAl-based alloys synthesized by arc melting (at China Iron and Steel Research Institute Group). The lamellar structure was achieved by the heat treatment including 1340 °C for 0.5 h, 1 h and 2 h followed by air cooling. The microstructure morphology was studied by the optical microscopy and scanning electron microscopy. The samples were mechanically polished and etched by the aqueous reagent of 2% hydrofluoric acid and 10% hydrogen nitrate prior to the optical characterization. The TEM samples were prepared by the twin-jet electro-polishing technique with an electrolyte of 4% perchloric acid. The detailed atomic structure was investigated using a JEOL ARM200F Scanning Transmission Electron Microscopy (STEM) with a probe corrector.

The lamellar structure, consisting of  $\alpha_2$  (Ti<sub>3</sub>Al, DO<sub>19</sub>) and  $\gamma$  (TiAl, L1<sub>0</sub>) phases, was successfully synthesized through the above approaches. The lamellar spacing increases with increasing annealing time. A well-defined orientation relationship of  $\{111\}_\gamma // (0001)_{\alpha_2}$  &  $\langle 1-10 \rangle_\gamma // \langle 11-20 \rangle_{\alpha_2}$  was additionally confirmed using the selected area diffraction (SAD) technique (see Figure 1). There are always three sets of diffraction patterns co-existing within the same regions. The diffraction labeled by the yellow rectangle in figure 1 is from  $\alpha_2$  phase. The other two diffraction patterns, indicated by the red and green rectangles, belong to  $\langle 011 \rangle_\gamma$  and  $\langle 1-10 \rangle_\gamma$ , respectively. The atomic arrangement of  $\gamma$  phase viewed along  $\langle 011 \rangle_\gamma$  and  $\langle 1-10 \rangle_\gamma$  is different (see the STEM-high-angle annular dark-field (HAADF) images in figure 2 (b) and (c)) due to the ordered L1<sub>0</sub> structure with a slightly larger c axis. Although the c axis is not equivalent to the other two axes in  $\gamma$  structure, the c/a ratio is only in the range of 1.01-1.03 depending on the Al content. As shown in the STEM-HAADF images in figure 2,  $\alpha_2$  phase has brighter Z-contrast compared to the  $\gamma$  phase. Viewed from  $\langle 11-20 \rangle_{\alpha_2}$ , the Ti column has slight brighter contrast compared to the Ti-Al column. The interface between  $\alpha_2$  and  $\gamma$  phase is atomic sharp, as shown in figure 2 (d) and (e). In addition, we always detected the twinning (figure 2 (e)) and pseudo-twinning (figure 2(f)) of  $\gamma$  phase viewed along  $\langle 011 \rangle_\gamma$ . The pseudo-twinning refers as the mirror structure of  $\gamma$  phase forming at sides of  $\alpha_2$  phase with a dimension of ~2 nm.

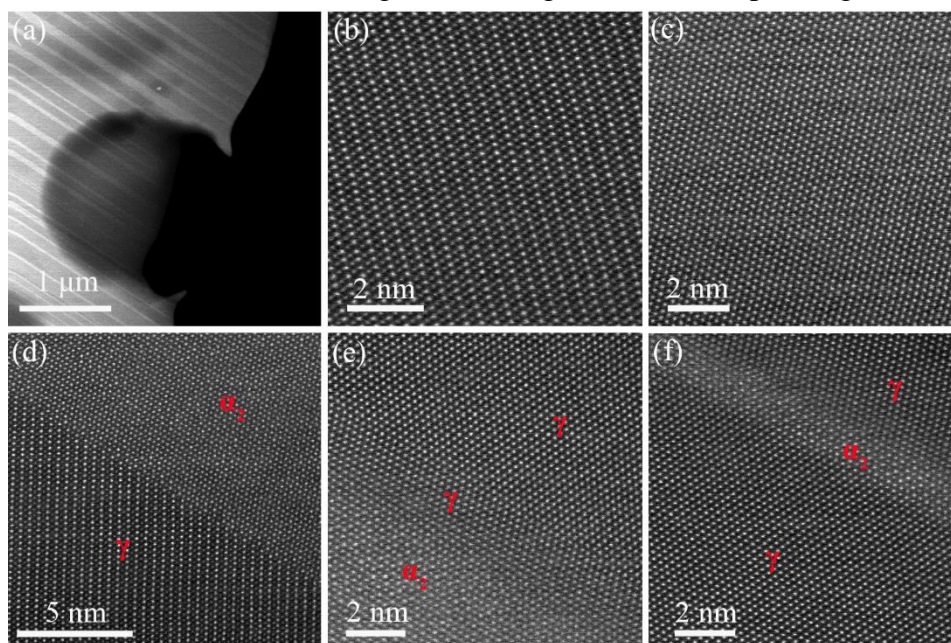
The detailed atomic arrangement of the  $\alpha_2/\gamma$  interface is currently under investigated by atomic resolution STEM and electron energy-loss spectroscopy techniques (EELS). Different atomic models can be built to study their interface energy by applied first principles computation.

## References:

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**Figure 1.** The lamellar structure. (a) the bright field image (b) the corresponding diffraction pattern.



**Figure 2.** The atomic structure of lamellar microstructure. (a) the low magnification HAADF image (b)-(c) shows the atomic structure of  $\gamma$  phase when the beam is parallel to  $\langle 1-10 \rangle_\gamma$  and  $\langle 011 \rangle_\gamma$ , respectively (d) the interface of  $\gamma$  and  $\alpha_2$  (e)-(f) the twinning and pseudo-twinning, respectively.