Single crystal form induced diversity interface structures in TiO2 (B)/anatase dual-phase nanocomposites

Supplementary Materials

1. TEM BF images and corresponding SAED patterns of TB nanofibers listed in Table 1.

Table 1 in the manuscript text illustrate 8 TB nanofibers with different diameters and SCFs. Besides the images of nanofibers with the number of No. 3 and No. 5 shown in Fig. 2, the TEM BF images and corresponding SAED patterns for the rest 6 nanofibers are illustrated in Fig. S1 (a)-(l). Note all the nanofibers have been divided into two categories with $\{100)$ and $(001\}$ SCF respectively. It is also worth to mention that the spots located between $(00l\}$ and $(02l\}$ series of spots in $\{100)$ SCF correspond to the combination of anatase and other impurities. These spots do not belong to the same set of SAED patterns with TB as they are not located at the repeating reciprocal points.

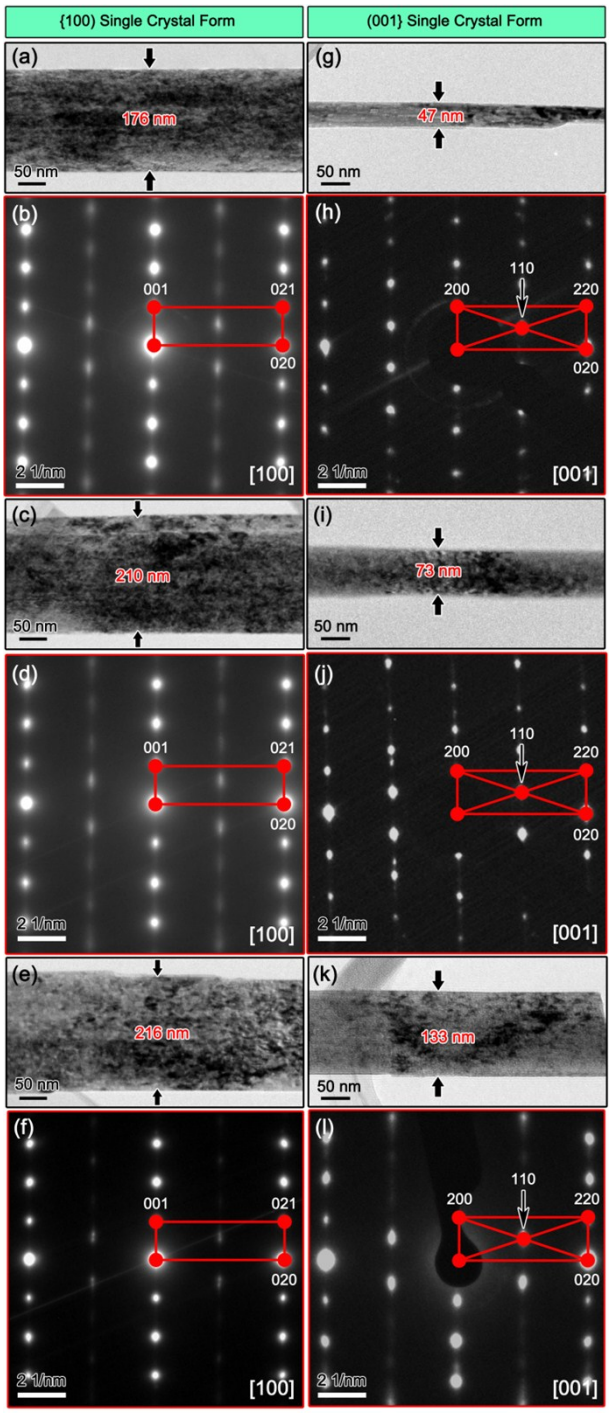

Fig. S1 The TEM BF and corresponding SAED patterns of TB nanofibers with $\{100)$ (a)-(f) and $(001\}$ SCF (g)-(l). The differences in the SAED patterns under $[100]$ and $[001]$ zone axes are the existence of (110) and $(\bar{1}10)$ spots with the angle of 35.7°. Also, the spots located between $(00l\}$ and $(02l\}$ series of spots in $\{100)$ SCF correspond to the combination of anatase and other impurities.

2. Twins and anti-phase boundary in TB nanofibers.

The HRTEM image taken along $[110]$ zone axis of TB nanofibers with $\{100)$ SCF is shown in Fig. S2 (a). Seeing from the figure, it is found that the anti-phase boundaries (shown in the square) and twins (shown in the circle) are coexisted inside the nanofiber. By carrying out the Inverse Fast Fourier Transform (IFFT) by using all the diffraction spots of the figure, the IFFT image illustrating the detailed structures of the anti-phase boundaries and twins is shown in Fig. S2 (b). It is noticed that the anti-phase boundary is parallel to $(1\bar{1}0)$ plane, while twin plane is confirmed to be (001). By indexing the SAED pattern in Fig. 3 (g), the twin features can be obtained by performing a reflection operation with the mirror plane of (001). The extended defects in TB nanofibers are commonly found all around the fibers, suggesting a very low formation energy of the stacking faults. Also, the twin features can only be observed along the zone axes with the index of $< hk0]$ as (001) is the twin plane in TB. Therefore, it can be speculated that the nanofibers with $(001\}$ SCF have less chance to form twins than that of $\{100)$ SCF as (001) plane is the main facet in the nanofiber. With only a pair of parallel facets in the nanofiber, it is quite difficult to generate twins inside.

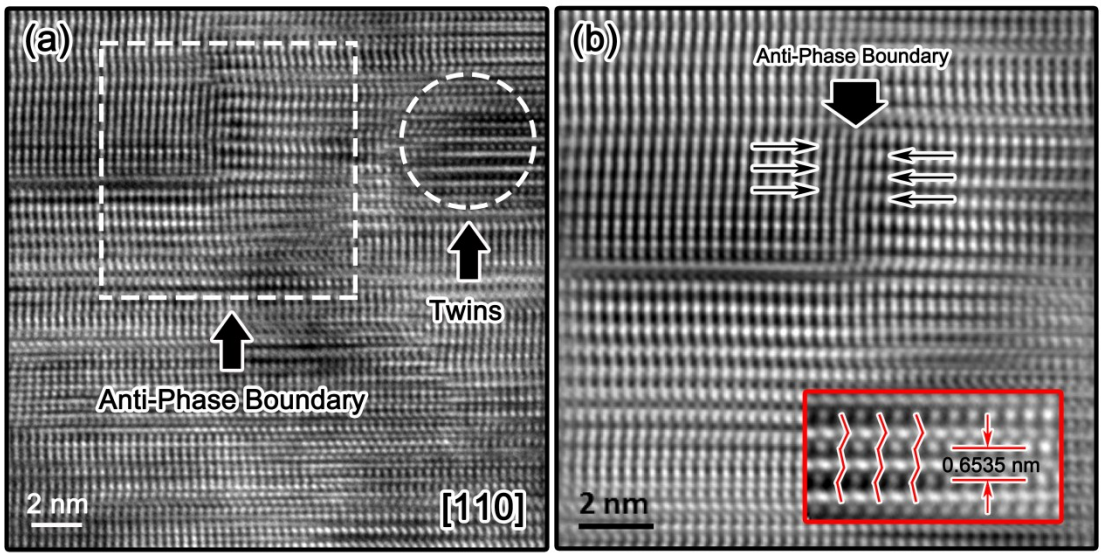

Fig. S2 (a) The HRTEM image of TB nanofibers with $\{100)$ SCF containing anti-phase boundary and twins. (b) The IFFT image generated by using all the diffraction spots in (a) indicate the parallel of (020) for the anti-phase boundary and the (001) twin plane for the twins.