Revealing the atomic structure of bcc {112}/<111> twin boundaries by aberration-corrected STEM

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The atomic configuration of the bcc {112}/<111> twins has been studied mainly via electron diffraction giving grounds to the existence of a ω hexagonal phase [1-3]. This finding has been disputed by attributing the extra reflections in the diffraction patterns to double diffraction and streaking [4]. With respect to this outlook, the current study shows the atomic structure of bcc {112}/<111> twins in a high-carbon steel and provide experimental and simulation - based evidence of the nature of the double-diffracted beams observed in these. Fig. 1a shows a bright-field image of a twinned region with a diffraction pattern (Fig. 1b) acquired from the region marked by the red circle in Fig. 1a. The diffraction pattern is indexed as a bcc lattice observed from the [110] zone axis (red), bcc {112}/<111> twins (yellow) and double-diffracted spots (green). In Fig. 1c, dark-field (DF) TEM imaging using the $0\bar{1}1$ reflection from the twins delineates the location of the twin. Similarly, when the diffracted spot closest to the 000 spot (in green in Fig. 1b) is used to form a DF TEM image, a similar image to the twins is produced (Fig. 1d). However, it is self-evident that the regions producing the double-diffracted beams are different and narrower than the twins. The red-green-blue (RGB) mix of the two images shows this clearly, with the twins appearing in red and the regions that produce the double-diffracted beams in green (Fig. 1e). Moreover, the intensity profile shown in Fig. 1f shows that the regions producing the double-diffracted exist to the sides of the twins with some overlap, confirming that the bcc {112}/<111> twins in this steel are not atomically sharp and that an overlap of two crystals produces the diffracted spots.

Aberration-corrected scanning transmission electron microscopy (STEM) imaging confirmed that the {112}/<111> twin boundaries are not sharp. Fig 2a shows a high angle annular dark-field (HAADF) STEM image with several twins. The Fourier transformation in the inset also shows the double-diffracted spots and that the effect is contained in an incoherently formed image. Fig. 2b shows an atomic scale HAADF STEM image where a Moire superposition can be clearly observed at the twin boundary (TB); thereby confirming its imperfect nature. This shows that the TB is not sharp as proposed in Fig. 2c, but rather that it is a step-wise boundary in the [110] direction which results in the projected atomic structure shown in Fig. 2d. Fig. 2e shows a superposition of the atomic structure with the experimental image showing a perfect match. Fig. 2f shows the TB cross section along the $[\bar{1}11]$ direction, with the left crystal in blue and the right crystal in red.

The step-wise TB along the [110] direction provides a full explanation of the electron diffraction analysis and refutes the existence of the ω-phase. These results show that atomically flat TB in bcc high-carbon steels may be less stable than this step-wise boundary; either due to boundary energy, alloying effects or C segregation. These possibilities need to be systematically explored further.

References

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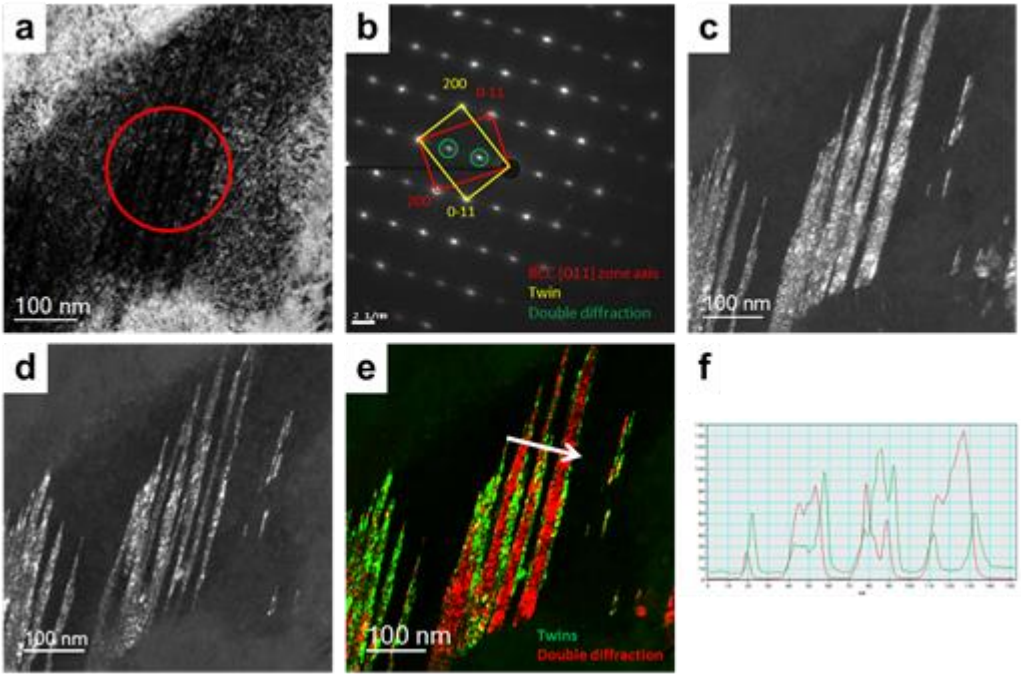

Fig. 1. **a**. TEM image of a twinned region along the [110] zone axis. **b**. Selected area diffraction pattern from the red circle shown in **a** along the [110] zone axis where the twins can be easily identified. **c**-**d**. DF TEM images formed using the $0\bar{1}1$ twin spot and the first double diffracted spot (marked with a green circle) respectively. **e**. Colour mix image of e (red) and d (green) **f**. Intensity profile from the black arrow in e.

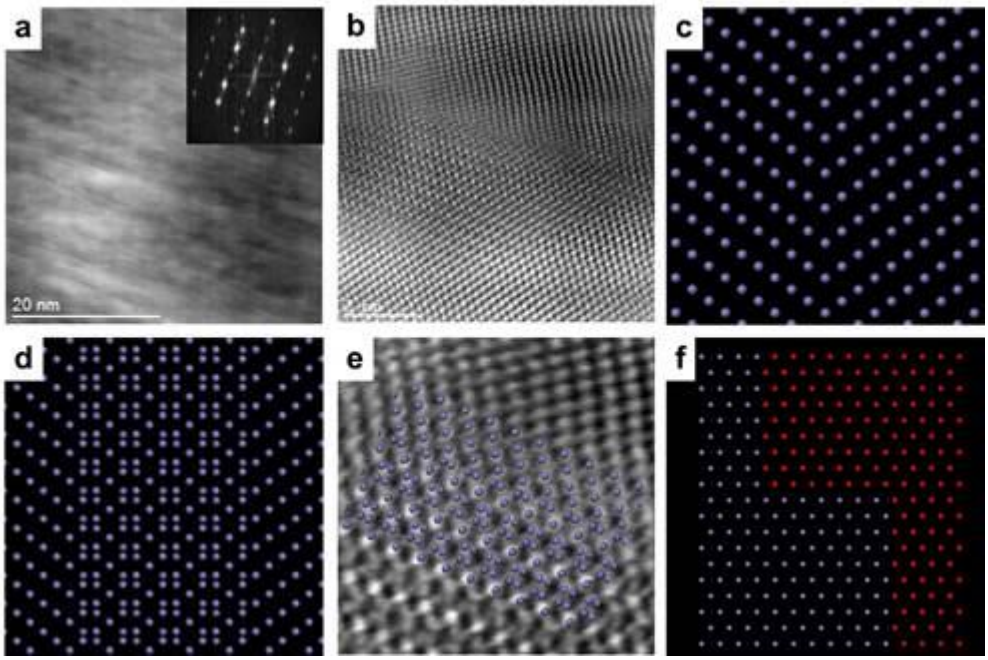

Fig. 2. **a**. HAADF STEM image of a twinned region, with the inset showing the FFT of the image. **b**. atomic resolution HAADF STEM image of a TB. **c**-**d**. Atomistic models of a perfect TB and a step-wise TB. **e**. Atomic resolution HAADF STEM image of a TB with a superimposed model of the step-wise TB in d. **f**. Cross-section of the TB shown in d viewed from the $[\bar{1}11]$ direction with the left crystal shown in blue and the right crystal shown in red.