

Bravais Lattice of TiAl Determined from a Single Electron Backscatter Diffraction Pattern

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A typical electron backscatter diffraction (EBSD) pattern shows abundant crystallographic information. It contains tens of Kikuchi bands (which corresponds to the diffracting lattice planes), the intersections of whose traces form hundreds of Kikuchi poles (or called zone axes). The positions of the zone axes as well as the diffracting source of the EBSD pattern can give the directions in a Bravais lattice. The edges of most Kikuchi bands appear blurred (poor contrast) and hence the band width measurement often suffers from obvious errors, whereas the positions of Kikuchi poles which are concurrently constrained by several traces can be located easier with less error.

EBSD combined with energy dispersive spectroscopy in scanning electron microscopy is a widely used method for phase identification. This method first need to know chemical composition as a prerequisite for limiting the scope of possible candidates, then the EBSD pattern is indexed according to the Bravais lattice of these candidates one by one, and finally the best match is chosen to be the result of the phase identification. However, this method might be no longer applicable convincingly when a) the crystal structure is unavailable in a database (e.g., unknown crystals prepared under some extreme experimental conditions); b) various polytypes of a crystalline compound exist especially when their diffraction patterns appears quite similar; c) a crystal has been described by different unit cells which might be crystallographically equivalent, even though they are available in a database. In above exceptional cases, three-dimensional reconstruction of the Bravais lattice becomes irreplaceable for correct phase identification. In this paper, we demonstrate the process of determining the Bravais lattice of TiAl (which has different structural descriptions, refer to the exceptional case b) by using a single EBSD pattern.

Figure 1a shows an experimental EBSD pattern recorded from a TiAl crystal. The green lines represent the traces of Kikuchi bands. The band widths (partially marked in the figure) are used to perform the Bravais-lattice determination. Some bands (diffracting lattice planes) have high-order interferences, and thus their widths may be defined differently. If define the band widths by the black arrows (shown in Figure 1a), the determination result is face-centered cubic with $a = 0.4021$ nm. The maximum discrepancy between the measured and calculated positions of all zone axes is 5.6 pixels. If the band widths are defined by the white arrows (also shown in Figure 1a), the determination result is primitive tetragonal with $a = 0.2842$ nm, $c = 0.4029$ nm. The maximum discrepancy between the measured and calculated positions of all zone axes can lower to less than 0.01 pixel. For the same Kikuchi band with different orders of interferences, since the narrower band widths correspond to shorter reciprocal vectors which are critical to reconstruct the reciprocal cell with smaller volumes, the narrowest band width must be defined to reconstruct the smallest reciprocal primitive cell. For this reason, the primitive tetragonal determined by using narrower band widths is a more reasonable result.

The reported crystal structure of TiAl has a space group P4/mmm, with two possible unit cells [1, 2]: 1) $a_1 = 0.28373$ nm, $c_1 = 0.40591$ nm; and 2) $a_2 = 0.401867$ nm, $c_2 = 0.406542$ nm. Figures 1b and 1c

depict these two unit cells. In fact, both describe the same crystal structure. If tiny discrepancy between the unit cell constants are neglected, the basis vectors a_1 , c_1 and a_2 , c_2 have the following correspondence:

$$a_1 = (a_2 + b_2)/2, \quad b_1 = (-a_2 + b_2)/2, \quad c_1 = c_2$$

By comparing Figures 1b and 1c, it is obvious that the Bravais lattice shown in Figure 1b is more reasonable, in which the lattice point consists of one Ti atom and one Al atom. The determined Bravais lattice and lattice constants from the EBSD pattern shown in Figure 1a agrees well with the reported experimental result [3].

References:

[1] T. Novoselova *et al*, Mater. Sci. Eng., A **371** (2004), p. 103.

[2] K.-D. Liss *et al*, Metals **6** (2016), p. 165.

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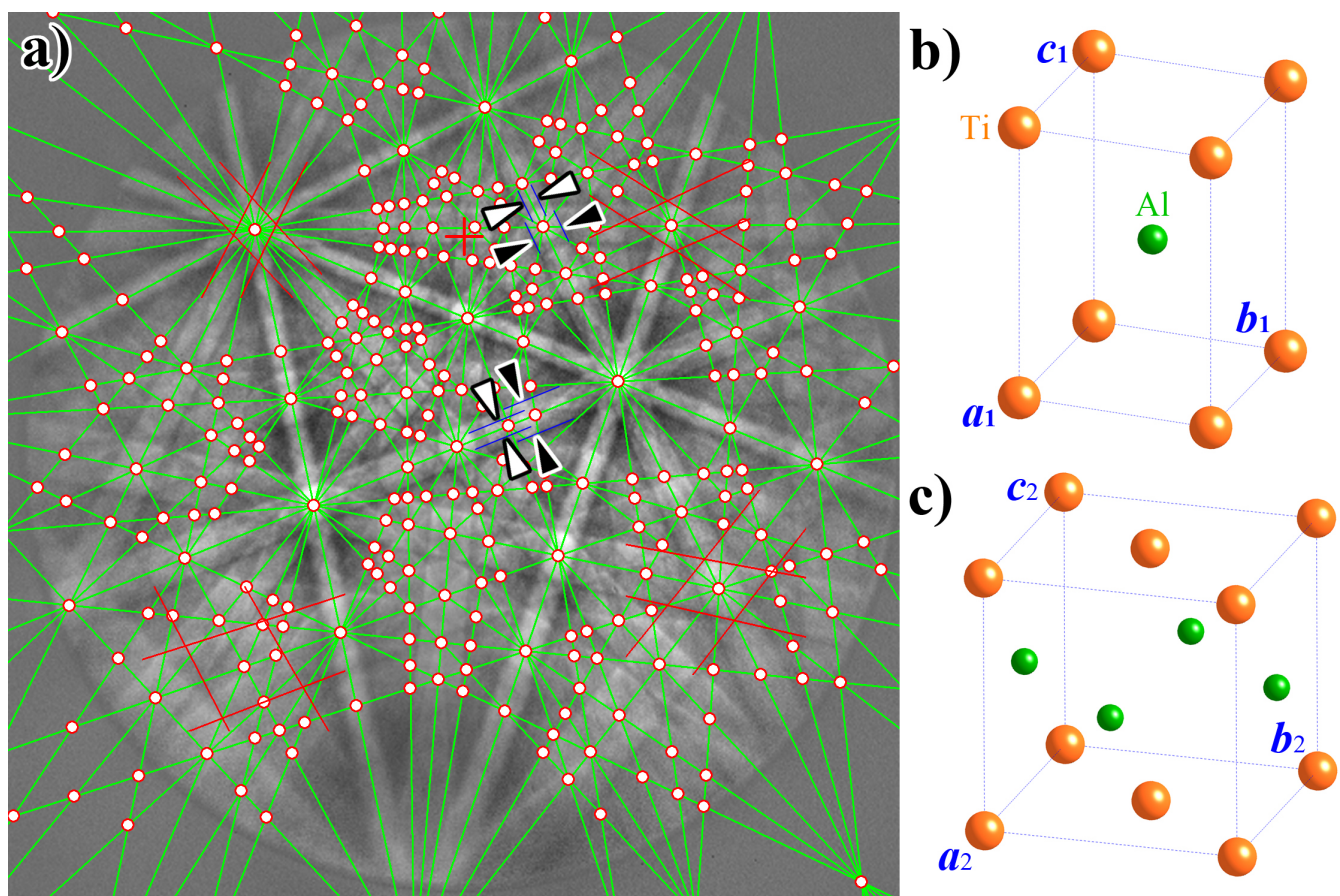


Figure 1. EBSD pattern and reported unit cells of TiAl: a) EBSD pattern collected with 20 kV. The red cross indicates the pattern center. b) Body-centered tetragonal crystal structure, c) A tetragonal unit cell very close to the cubic.