An investigation of the nature of dislocation defects in a α-Al_2O_3 thin crystal with LACBED method

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Introduction: The thin crystal of α-Al_2O_3 is often used as a substrate for growing of semi-conductor materials such as GaN. Thus it is required implicitly that this substrate crystal is almost defect free perfect crystal. However we report here observations of dislocation defects in a α-Al_2O_3 used as a substrate, and determination of the nature of the dislocations using LACBED (Large Angle CBED) technique associated with Cherns and Preston's rule (CP's rule) [1,2].

Observations: The dislocations in a thin crystal of α-Al_2O_3 were observed with J2010 (200 kv) TEM microscope. Fig. 1a and b are the bright and the dark field images of **g**($\bar{1}\,\bar{2}$.1) reflection with near the [2$\bar{1}$00] zone axis, respectively. Here the "." in **g**denotes *i=-(h+k).* The α-Al_2O_3 has the corundum structure with the space group R$\bar{3}$c (167) and the cell parameter a=0.4759nm, c=1.299 nm in the hexagonal system or a=0.5127 nm α=55° 16.7 in the rhombohedral system. Fig. 2a shows the LACBED pattern taken for the area containing dislocations in the Fig. 1. We can see the fringe splits of several diffraction lines crossing the dislocation line. Clearly the **g**(24.$\overline{14}$) diffraction line(3-3') is spitted as 4 fringes and the **g**($\bar{1}$ $\bar{2}$.1) diffraction line(2-2') also has 4-fringe split.

Analysis: As seen in Fig. 1 the dislocation lines are perpendicular to the [0001] direction. Therefore the dislocation lines must lie in the (0001) basal slip plane. In this slip plane the Burger vector **b** of the perfect dislocation must be ⅓<11$\bar{2}$0>. Applying the CP's rule to the 4-fringe splitting of **g**(24.$\overline{14}$) diffraction line(3-3') indicates the **b**= -⅓[$\bar{1}$2$\bar{1}$0] only. But for the case of the **g**($\bar{1}\,\bar{2}$.1), the possible

Burger vector would be 2**b**, which is an indication of the double dislocation lines separated by very short distance. To confirm this analysis the corresponding simulations were performed as below. The simulations would give details of the nature of dislocations including the identification of single or double dislocation lines.

Simulations: In the simulations the Bloch wave dynamical theory for the contrast of dislocations [3] and the formulation developed by the author (HSK)[4] were used. The analyzed data given in simulations was follows: the thickness of the specimen is about 130 nm; the orientation of specimen to the beam, near the $[2\bar{1}00]$; the convergent angle of the beam, 0.906°×2 and the specimen height from the convergent point, 0.014 mm. The direction of the dislocation lines, which is best fitted with observations, is about $\frac{1}{3}[01\bar{1}0]$ which is inclined to the surface of the crystal by the angle about 15°. This direction makes the angle of 30° to the **b**-direction, which means a mixed type of dislocation. The simulation results are displayed in Fig. 3a-f for single dislocation. Clearly the fringe splits of diffraction lines are well matched with observations except those of $\mathbf{g}(\bar{1}\,\bar{2}.1)$ and $\mathbf{g}(12.\bar{7})$. However, the simulations of Fig. 3a and b with the double dislocation separated about 10 nm are well agreed with observations. These lines intersect dislocations in the left hand side in Fig. 1. Therefore it is concluded that in Fig. 1 the dislocation line at the left hand side is double dislocation lines while that in the right hand side is single dislocation line.

Discussion: One can see very good agreements between the observed LACBED pattern and their theoretical simulations, as shown in the figures. It is also worthwhile to note that the CP's rule can be, in general, applicable to the relatively complex crystal as this α-Al_2O_3. The magnitude of the **b** of the perfect dislocation in this crystal is a=0.4759 nm, roughly two times larger than those of the usual metals like Aluminum. This fact also means that the energy of the defect formation would be much greater than those of metals. Therefore the dislocation defects in this crystal seem to occur in the synthesizing process with impurities or clustering their own atoms irregularly. This point will be further investigated.

References

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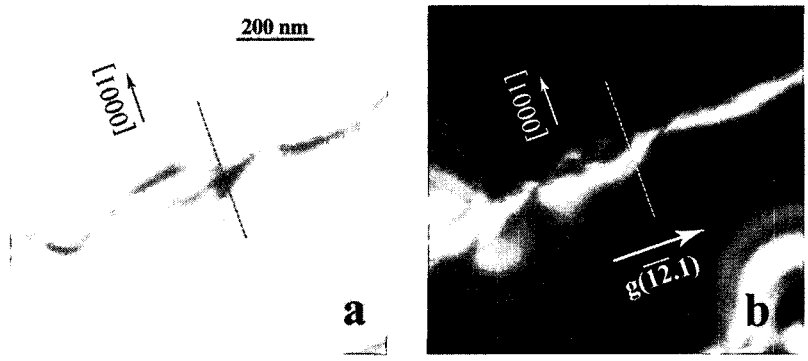

Fig. 1. The (a) and (b) are the bright field image and the dark field image of the dislocations, respectively, with the orientation near the[2$\bar{1}$00]. The dotted lines are for the boundary of the double/single dislocations.

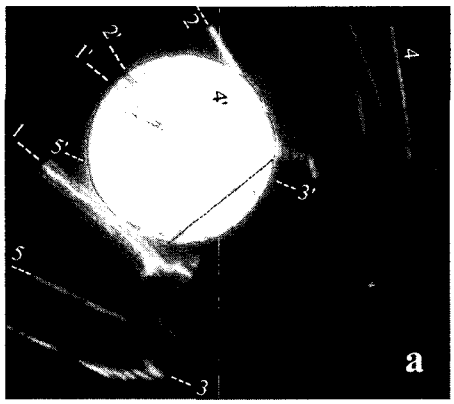

Fig. 2a. The LACBED pattern taken for the area containing dislocations in the Fig. 1, with the orientation near the [2$\bar{1}$00]. The straight dotted line in the (0000) disk is for dislocations.

The 1'-1 lines: the g(12.$\bar{4}$).

The 2'-2 lines: the g($\bar{1}\,\bar{2}$.1).

The 3'-3 lines: the g(24.$\bar{14}$).

The 4'-4 lines: the g($\bar{2}\,\bar{4}$.$\bar{4}$).

The 5'-5 lines: the g(12.$\bar{7}$).

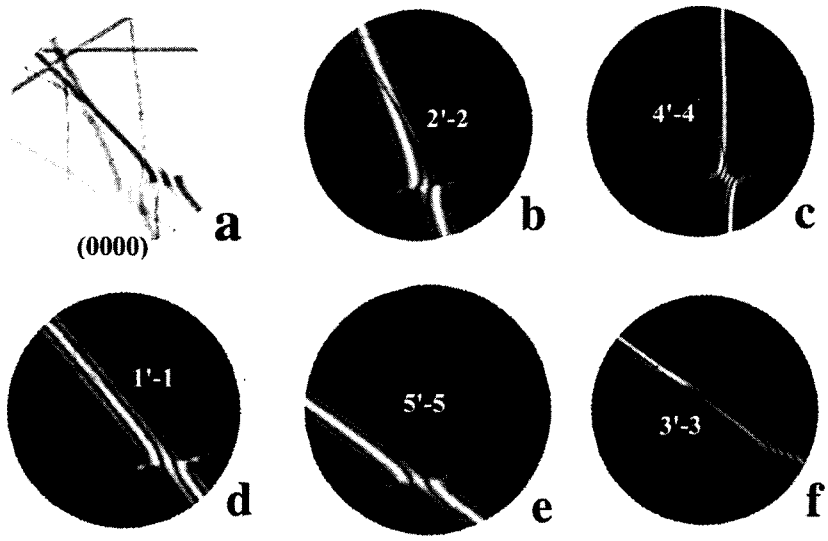

Fig. 3. The simulations of the LACBED pattern using 16 diffraction beams for the single diffraction line. (a) : the (0000). (b): the g($\bar{1}\,\bar{2}$.1). (c): the g($\bar{2}\,\bar{4}$.$\bar{4}$). (d): the g(12.$\bar{4}$). (e): the g(12.$\bar{7}$). (f): the g(24.$\bar{14}$). It should be noted that the fringe splits of the diffraction lines are well matched with observations in Fig. 2a, except for the case of (b) and (e).

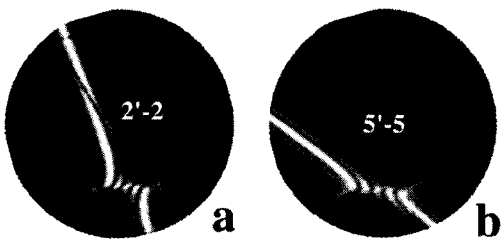

Fig. 3. The simulations with the double dislocations separated by 10 nm. The (a) is for the g($\bar{1}\,\bar{2}$.1) disc, whose fringe pattern is well agreed with the observation of (2'-2) line splitting in Fig. 2a. The (b) is for the g(12.$\bar{7}$) disc simulated with the double dislocations.