Revisit of a TiO$_2$ rutile (1x2) structure
by TRHEPD (Total-reflection high-energy position diffraction)

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1 Introduction

TiO$_2$ is one of the most important catalyst materials. It is used as catalyst supports and photocatalysts. In order to understand the catalytic properties, TiO$_2$(110) rutile single crystal surfaces have often been studied by means of various surface science techniques. The TiO$_2$(110) surfaces show a (1 × 2) reconstruction. Although several models have been proposed upto now, which model structure is the most appropriate is still under debate.

Positron diffraction is a surface sensitive technique. Owing to its positive charge, its total reflection occurs and it cannot penetrate into the bulk. In this work we applied TRHEPD (Total-reflection high-energy positron diffraction) technique to the structure analysis of the TiO$_2$(110)-(1 × 2) surface to confirm the surface structure.

2 Experiment

TiO$_2$ (110)-(1 × 1) surface was produced after the cleaning and annealing cycles for several times. The (1 × 2) structure was grown after 30 min 1100 K annealing.

TRHEPD measurements were carried out at room temperature. The TRHEPD rocking curve was analyzed using a RHEED program.

3 Results and Discussion

Figure 1 shows the TRHEPD pattern of TiO$_2$(110)-(1 × 2) surface. Figure 1(a) shows the RHEPD pattern with an incidence angle less than critical angle. No strong peaks corresponding to the bulk spots were observed, while the patterns obtained with high incident angle show strong peaks corresponding to the bulk diffraction (Fig. 1(b), (c)) which are observed in a conventional RHEED. The half index spots in Fig.1 (a) with the total reflection condition represent the TRHEPD surface sensitivity.

Figure 2 shows the most well fitted model structure which was proposed by Onishi and Iwasawa as added Ti$_2$O$_3$(iv).$^1$ The other models such as Ti$_2$O, missing row and Ti$_2$O$_3$(ih) did not reproduce the TRHEPD rocking curve.

4 Conclusions.

TRHEPD has demonstrated that the added Ti$_2$O$_3$(iv) model is the most appropriate for the TiO$_2$(110)-(1 × 2) surface. We are now conducting theoretical calculation based on this model structure.


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Fig. 1 TRHEPD patterns with
(a) glancing angle = 2.9° (total reflection conditions)
(b) glancing angle = 4.0°
(c) glancing angle = 6.0°
We did not observe the bulk reflection in the total reflection conditions(a) while it strongly appears in (b) and (c)

Fig. 2 A model structure of added Ti$_2$O$_3$(iv).