Positron

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) surface 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_2O_3(iv).[1] The other models such as Ti_2O, missing row and Ti_2O_3(ih) did not reproduce the TRHEPD rocking curve.

4 Conclusions.

TRHEPD has demonstrated that the added Ti_2O_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.

1.H. Onishi and Y. Iwasawa, *Surf. Sci*. **313**, L783 (1994).

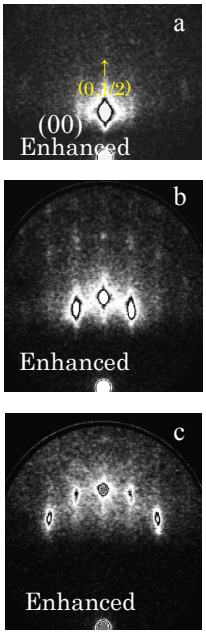

Fig. 1 TRHEPD patterns with
(a) glancing angle= 2.9 ° (total reflection conditions)
(b) glancing angle= 4.0°
(c) glancing angle = 6.0°
We did not observe the bulk reflection in the total reflection conditions(a) while it strongly appears in (b) and (c)

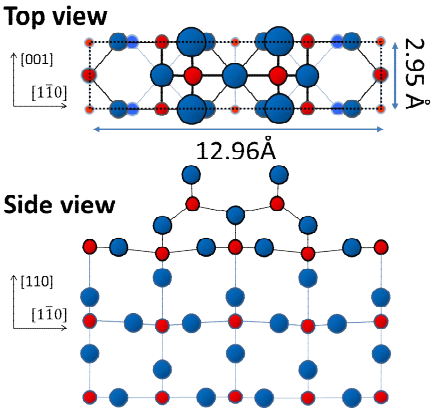

Fig.2 A model structure of added Ti_2O_3(iv).