



# Atomically controlled surfaces with step and terrace of $\beta$ -Ga<sub>2</sub>O<sub>3</sub> single crystal substrates for thin film growth

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## ABSTRACT

The surface of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (1 0 0) single crystal grown with floating zone method was treated by chemical-mechanical-polishing (CMP) for 30–120 min followed by annealing in oxygen atmosphere at temperature 600–1100 °C for 3–6 h. The evolution of the step arrangement was investigated with reflection high energy electron diffraction and atomic force microscopy. Atomically smooth surfaces with atomic step and terrace structure of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates were successfully obtained after just CMP treatment as well as CMP treatment and post annealing at 1100 °C for 3 h. The uniform step height was 0.57 nm, and smooth terrace width was 100 nm, where the misorientation angle was about 0.36°. The obtained atomically smooth surface provides a potential application for the high-quality epitaxial film growth.

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## 1. Introduction

The substrates for atomically controlled flat surfaces are required in order to grow the high-quality film and enhance the epitaxial thin film growth on substrate surfaces. Since surface crystallinity and surface reconstructions of substrate materials can affect the quality of the epilayers, understanding substrate-preparation techniques and characterization of the substrate surfaces have been increasingly important. Sapphire surface morphology is known to be dependent on the annealing protocol, and atomic steps were obtained by annealing at high temperature in an electric furnace [1–3]. Yoshimoto et al. reported on an atomically flat surface of the sapphire (0 0 0 1) surface after annealing at 1000 °C for 1 h [1]. Besides  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>, atomically smooth surfaces of ZnO substrates have also been achieved using high temperature annealing [4,5]. These ultrasurface smooth surfaces were considered to be formed due to the migration and the evaporation of atoms on the surface to minimize surface energy during annealing. Therefore, annealing process was thought to be effective and needed to control the surface morphology and reconstruction required for film growth substrates.

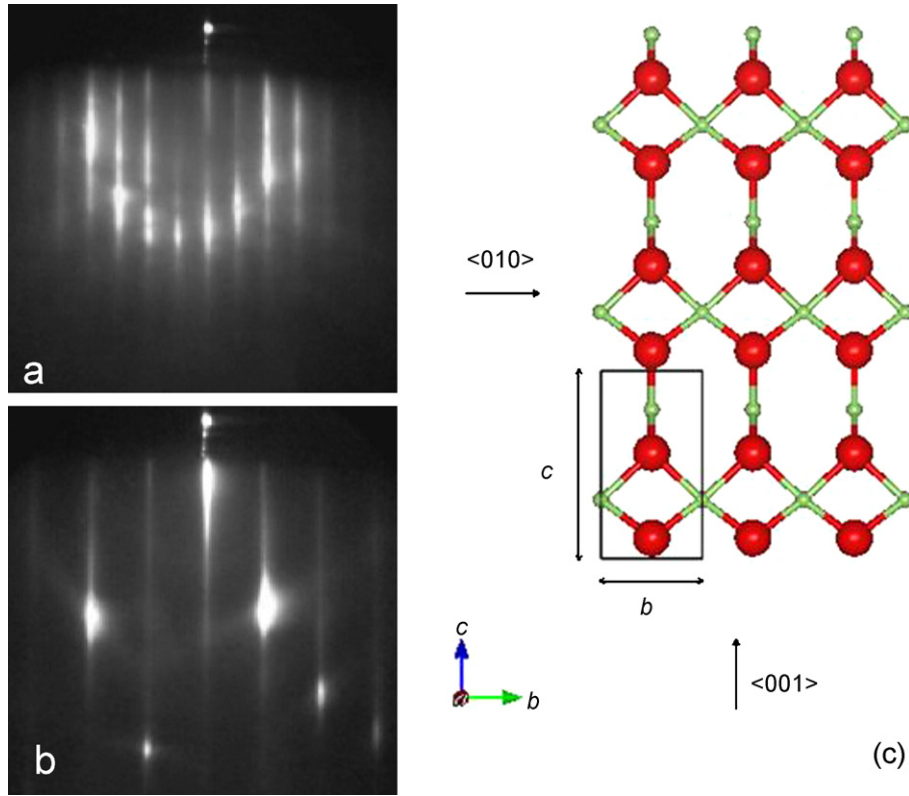
$\beta$ -type gallium sesqui-oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) is a transparent conducting oxide with a band gap of around 4.7–4.9 eV, and has a transparency from the visible into the UV region [6]. Using these unique properties,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> single crystal has been applied to a substrate for the epitaxial growth of GaN-based films growth, because  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> comprises both the properties of high transparency and electrical conductivity required as a substrate for vertical current structure of light emitting diode or laser diode [7,8]. So far, however, there has been no report on investigation of the nanoscaled surface structure of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates.

In the present study, the high-quality  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates for epitaxy are described in terms of smooth surfaces with atomically step and terrace structure, and the effect of chemical-mechanical-polishing (CMP) as well as CMP and post annealing on the surface morphology of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (1 0 0) substrate was examined for the first time.

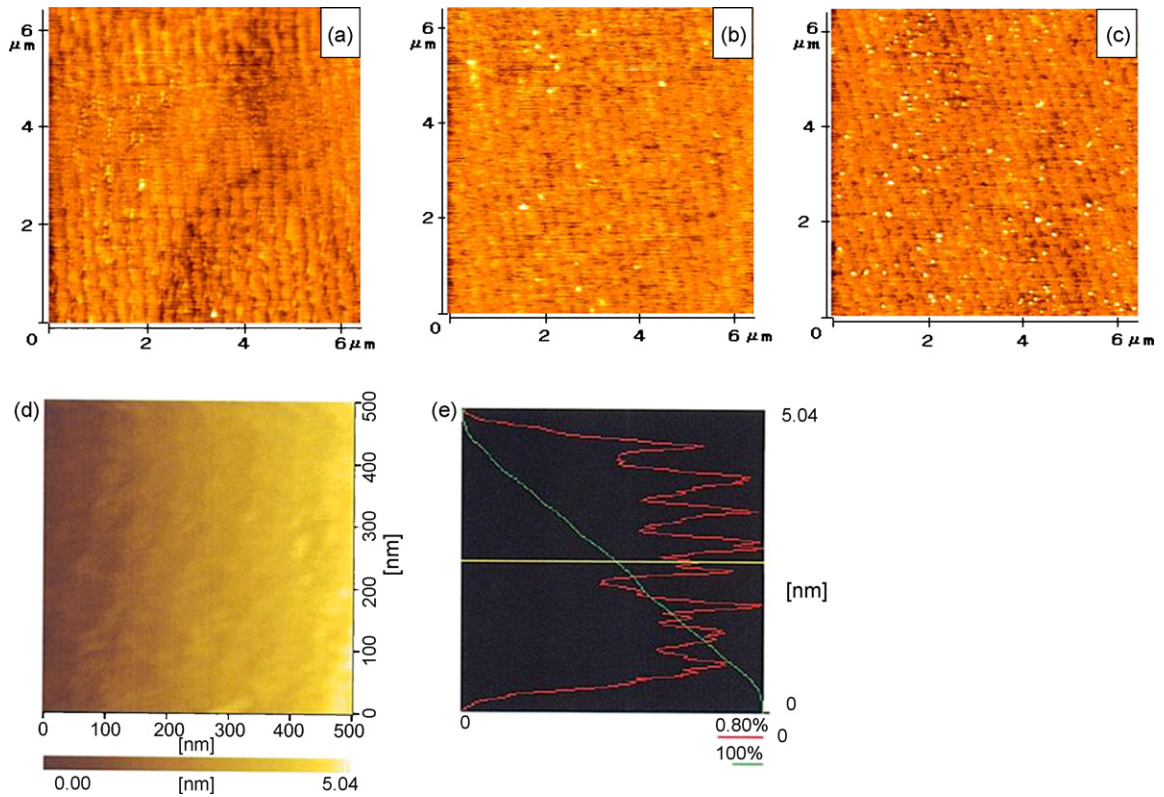
## 2. Experimental

Undoped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> single crystals were grown using floating zone method. The detail of fabricating procedure is described in our previous paper [8]. As-grown single crystals were cut along (1 0 0) plane, and its surfaces were mechanochemically polished to the wafers. The sample size was approximately 8 mm × 8 mm × 0.4 mm. Post annealing was performed at temperature between

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**Fig. 1.** RHEED patterns from  $\beta\text{-Ga}_2\text{O}_3$  (1 0 0) surfaces after CMP treatment for 30 min and subsequent wet etch treatment. The direction of incident electron beam is parallel to (a) (0 1 0)  $\text{Ga}_2\text{O}_3$ , and (b) (0 0 1)  $\text{Ga}_2\text{O}_3$ , respectively. (c) Schematic illustration of  $\beta\text{-Ga}_2\text{O}_3$  (1 0 0) surfaces, where the large balls and small balls indicate oxygen atom and gallium atom, respectively. Rectangular shows unit cell, and arrow indicates the direction of the incident electron beam.



**Fig. 2.** AFM images of  $\beta\text{-Ga}_2\text{O}_3$  (1 0 0) surfaces after CMP treatment with various times and scan sizes. Scan size is  $6 \mu\text{m} \times 6 \mu\text{m}$  for (a)–(c), and  $500 \text{ nm} \times 500 \text{ nm}$  for (d). CMP treatment time is (a) 30 min, (b) 180 min, (c) 240 min, and (d) 30 min, respectively. (e) Height distribution profile of (d) after rotating the terrace gradient horizontally.

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