Surface Science 604 (2010) 1614–1618

Contents lists available at ScienceDirect

Surface Science

journal homepage: www.elsevier.com/ locate/susc

Characterization of epitaxial MgO growth on Si(001) surface

Tadashi Abukawa *, Shunsuke Sato, Youta Matsuoka

Institute for Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

ARTICLE INFO

Article history:
Received 20 May 2010
Accepted 8 June 2010
Available online 12 June 2010

Keywords:
RHEED
Single crystal epitaxy
Semiconductor-insulator interfaces
MgO
Si(001)

ABSTRACT

MgO epitaxial growth on a Si(001) surface by ultrahigh-vacuum molecular beam epitaxy was investigated. Epitaxial orientation and crystalline quality were characterized based on the three-dimensional reciprocal map obtained by Weissenberg RHEED. The epitaxial orientation and crystallinity were strongly dependent on the initial condition of the substrate. When MgO was deposited on a clean Si(001) surface at room temperature a MgO(001) film grew on the Si(001) substrate with two in-plane orientations:MgO[110]//Si [100] and MgO[100]//Si[100]. This is the first observation of MgO epitaxy with the former orientation, which has a smaller mismatch than the latter orientation. When the substrate was exposed to O_2 or thermally oxidized, the latterorientation predominantly grew on the substrate. Deposition of Mg on the substrate also produced the latter orientation. These results imply that nucleation sites on the initial substrate play an important role in determining the epitaxial orientation.

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1. Introduction

Integration of magnetic devices with silicon technology is an important topic in advanced electronics. However, problems such as strong metal/semiconductor intermixing and the generally high lattice mismatch between 3d ferromagnetic layers and substrates have lead to buffer layers being investigated. MgO has been used for buffer layers on Si(001) because it has many favorable properties including the ability to function as a diffusion barrier, a high thermal stability and good electrical insulation properties. However, it suffers from a large mismatch in the lattice constant with Si(001) and from a high thermal expansion [1–5]. In addition, crystalline MgO forms a very effective tunnel barrier layer in tunnel magnetoresistance (TMR) junctions (e.g., Fe(001)/MgO(001)/Fe(001) [6–8]. These junctions usually use single-crystal MgO(001) as the substrate. Thus, TMR junctions could be integrated on silicon wafers if it were possible to grow high-quality MgO(001) layers on Si(001) substrate.

MgO growth on Si substrates was initially studied with a view to producing a buffer layer for ferroelectric thin films on Si [1–4]. Masuda et al. used MgO buffer layers to grow lead–zirconate–titanate (PZT) films on Si(001) substrates [1]. MgO was deposited by pulsed laser deposition (PLD) on H-terminated Si(001) in a vacuum of 10^{-5} Pa and in O_2 ambient. Amorphous MgO films were obtained in a vacuum of 10^{-5} Pa, whereas epitaxial MgO(001) films were formed at O_2 pressures of 13 and 40 Pa at a substrate temperature of 720 K. However, the initial oxide layer on Si(001) degraded the MgO films. Chen et al. also reported a dependence of oxygen pressure on MgO growth on Si(001) [2–4]. They varied the oxygen pressure in the range 10^{-5} to 1 Pa and found that good crystalline MgO(001) films could be obtained for oxygen pressures in the range 10^{-2} to 1 Pa at a substrate temperature of 870 K. Ning et al. observed an amorphous SiO_2 layer and a misoriented MgO layer at the interface by cross-sectional TEM [5]. They suggested that the misoriented layers were necessary to reduce the large mismatch between MgO and the substrate. Although PLD is generally used to grow MgO buffer layers on Si substrates, electron-beam evaporation has been used to grow a thin MgO barrier for TMR junctions [6,7].

Previous studies have reported that MgO(001) films grow on Si (001) substrates with an in-plane epitaxial orientation of MgO[100]// Si[100] (see Fig. 1(a) and (b)) [1–5]. Since the lattice constants of MgO and Si are4.21 Å and 5.43 Å, respectively, there is a lattice mismatch of −22.5% for this orientation. It is interesting to consider why the MgO[100]//Si[100] orientation is preferred to the MgO[100]//Si[110] orientation in which the MgO orientation is rotated 45° in-plane (see Fig. 1(c)). The surface unit cell length of the Si[110] direction is 3.84 Å so that the lattice mismatch is +8.8% for this orientation. Although 8.8% is still a large mismatch, it is considerably smaller than −22.5%. In this study, we realize MgO[100]//Si[110] epitaxy and we investigate the reason of the preferred orientation.

The main purpose of this study is to investigate the effect of deposition conditions on the initial epitaxial orientation and quality of MgO films grown on Si(001). Unlike most previous studies that used PLD in a high vacuum, we grow MgO films using an electron-beam evaporator in an ultrahigh-vacuum (UHV) MBE system. The crystal structures and morphologies of the epitaxial films were investigated by Weissenberg reflection high-energy electron diffraction (W-RHEED) [9–12], in which hundreds of RHEED patterns are measured at different azimuthal anglesof the sample. A three-dimensional (3D) reciprocal

* Corresponding author.
E-mail address: abukawa@tagen.tohoku.ac.jp (T. Abukawa).

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doi:10.1016/j.susc.2010.06.003

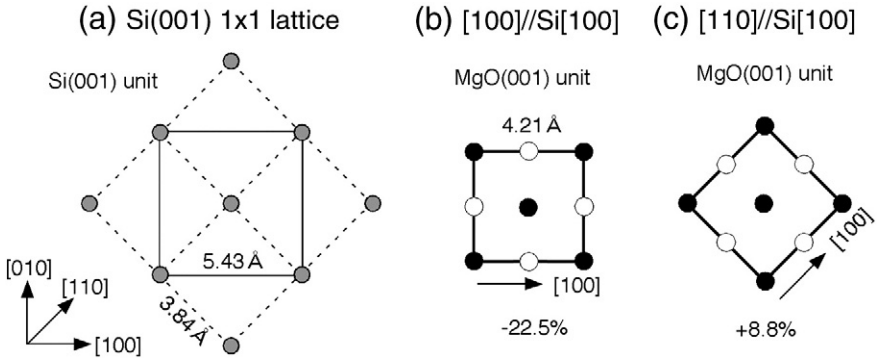

Fig. 1. Schematic diagrams of crystal (001) lattices: (a) Si(001) substrate lattice; (b) MgO(001) lattice with MgO[100]//Si[100] orientation; (c) MgO(001) lattice with MgO[100]//Si[110] orientation.

map can be obtained by W-RHEED, whereas only a section of the reciprocal map is projected in a single RHEED pattern. W-RHEED is highly advantageous for characterizing films because the crystal structure and morphological information can be immediately obtained from the 3D reciprocal pattern [10].

2. Experimental

Experiments were mainly performed using the UHV azimuthal-scan RHEED system shown in Fig. 2. It consists of an electron gun, an energy filter, a phosphor screen, a five-axis sample manipulator and an electron-beam evaporator for MgO deposition. Polar and azimuth rotations of the sample manipulator were motorized. The energy filter was used to remove inelastically scattered electrons, which generally disturb the diffraction pattern. It is a high-pass energy filter and consists of three spherical retarding grids, which were constructed in accordance with the procedure given in Ref. [13]. The filter has an energy resolution of 4 eV at a primary electron energy of 10 keV. The primary beam energy for RHEED measurements was 10 keV in the present study. The energy-filtered RHEED patterns were displayed on the phosphor screen and were captured by a CCD video camera.

A mirror-polished Si(001) wafer (0.004 Ωcm, As doped) with dimensions of $25\times3\times0.6$ mm^3 was used as the substrate. The sample was resistively heated and the sample temperature was measured by infrared and optical pyrometers. A clean Si(001) 2×1 surface was prepared by flashing at 1500 K for 5 s followed by annealing at 1250 K for 2 min in an UHV.

MgO was evaporated from the electron-beam evaporator onto Si (001) substrates under several different conditions. MgO depositions up to 60 ML were investigated in the present study. ML corresponds to the surface atomic density of the MgO(001) surface. Typical deposition rate was 1.0 ML/min, which was measured by a quartz thickness monitor. The films were characterized by W-RHEED and Auger electron spectroscopy (AES).

W-RHEED measurements were performed by rotating the surface over 45° from the [110] incidence to [100] incidence of the substrate, taking advantage of the C_{2v} symmetry and the double-domain structure of the substrate. The rotation interval was 0.1°, which is sufficiently fine for a continuous survey of reciprocal space. Over 450 RHEED patterns were obtained in a single azimuthal scan. After RHEED measurements, selected samples were transferred in air to a scanning electron microscope chamber, and their morphology was observed.

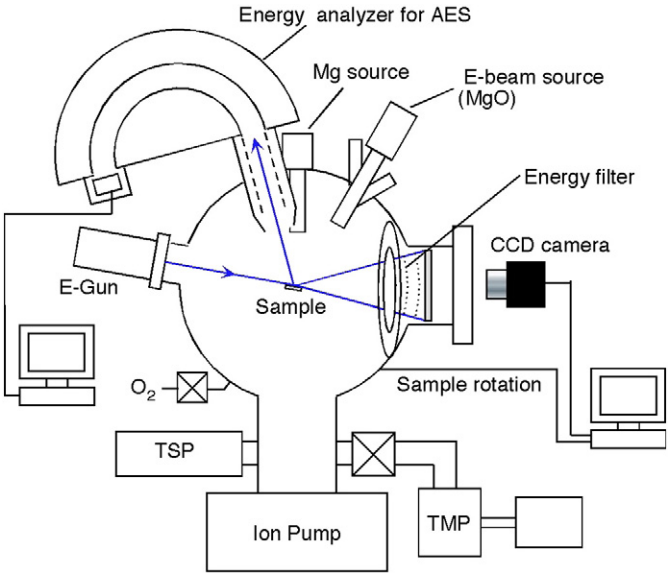

Fig. 2. Schematic drawing of MBE growth chamber with Weissenberg RHEED and AES system.

3. Results

In previous studies, MgO was deposited on heated substrates with temperatures of 720–870 K [1–5]. In the present study, we deposited MgO on substrates at room temperature (RT) and at temperatures of 670 K and 870 K. Fig. 3 shows AES spectra for films grown at these three temperatures. The Mg KLL to O KLL intensity ratio for RT deposition agrees with that expected for MgO. Mg KLL decreased and O KLL and Si KLL increased at high-temperature deposition, indicating the formation of SiO_2 on heated substrates. A RHEED pattern with a high

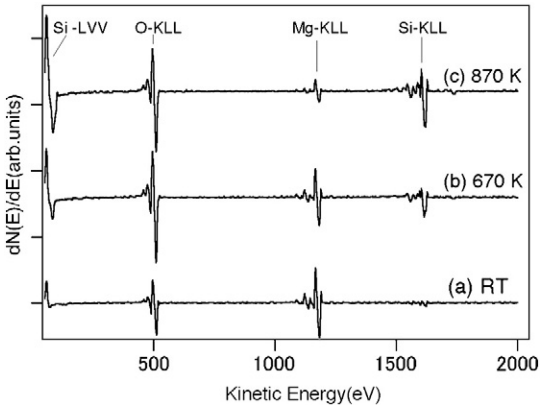

Fig. 3. AES spectra from (a) MgO (60 ML) deposited on a clean substrate at RT, (b) MgO (120 ML) deposited on a clean substrate at 670 K and (c) MgO (120 ML) deposited on a clean substrate at 870 K.

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