Deposition of ScAIN thin film using dual-sputtering method

2元スパッタリング法による ScAlN 薄膜の形成

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1. Introduction

High-Sc-content ScAlN thin films have attracted significant attention because of their strong piezoelectric properties. Akiyama et al. found that the piezoelectricity of ScAlN thin films increased monotonically with increasing Sc concentration, r [1, 2]. The piezoelectricity reached a maximum at r = 43 at%, at which the piezoelectric coefficient, d_{33} , was five times that of pure AlN [1, 2]. Hashimoto et al. reported that a surface acoustic wave (SAW) resonator based on the ScAlN/6H-SiC structure exhibited resonance O, anti-resonance Q, and K^2 values of 340, 240, and 4.5%, respectively, at 3.8 GHz [3]. They also reported that a SAW resonator based on the ScAlN/single crystal diamond (SCD) structure exhibited resonance Q, anti-resonance Q, and K^2 values of 520, 130, and 6.1%, respectively, at 3.6 GHz [4]. The Akiyama group showed that the d_{33} of a ScAlN thin film with a high Sc content and wurtzite structure would be much larger than that of the 43 at% Sc film, as calculated by first-principles methods [5]. However, ScAlN thin films typically exhibit a rock-salt rather than a wurtzite structure with increasing Sc content, because ScN has a rock-salt structure at thermal equilibrium [6].

In this report, we studied the deposition of ScAlN thin films using a dual-sputtering method, and used Raman spectroscopy to clarify the deposition conditions needed for films with high piezoelectricity.

2. Experimental

An AlN thin film with a thickness of 50 nm and a *c*-axis orientation was deposited as a seed layer on Fz-Si(100) using an electron cyclotron resonance(ECR) sputtering machine. A dual radio frequency (RF)-magnetron sputtering machine with a 2" Al target and Sc target was employed for the ScAIN thin film. The Sc/Al deposition ratio can be controlled by the power applied to each target. The details of the conditions studied are shown in **Table** **I**. The chemical composition of the ScAlN thin films was determined by X-ray fluorescence spectrometric analysis (XRF). Micro-Raman spectroscopic measurements at an excitation wavelength of 458 nm (Ar-ion laser) and X-ray diffraction were perfomed to characterize the crystal quality of the ScAlN thin films.

Table I. Deposition Conditions

| (A) | Background Pressure | $< 1 \times 10^{-4}$ (Pa) |
|-----|------------------------|---------------------------|
| | Total Gas Pressure | 1.1 (Pa) |
| | Ar Flow | 4.0 (sccm) |
| | N ₂ Flow | 2.0 (sccm) |
| | RF Power for Al target | 75–150 (W) |
| | RF Power for Sc target | 100–150 (W) |
| | Substrate Temperature | 400 (°C) |
| (B) | Background Pressure | $< 1 \times 10^{-4}$ (Pa) |
| | Total Gas Pressure | 0.5 (Pa) |
| | Ar Flow | 1.8 (sccm) |
| | N ₂ Flow | 1.2 (sccm) |
| | RF Power for Al target | 80 (W) |
| | RF Power for Sc target | 100–150 (W) |
| | Substrate Temperature | 580 (°C) |

3. Results and discussion

Figure 1 shows the dependence of the Sc content in the ScAlN thin film on the RF power ratio applied to the Sc target. The Sc ratio in the ScAlN thin film was well controlled by the RF power ratio. When the Sc content was over 33%, the *c*-axis orientation was not obtained. Figures 2 and 3 show micro-Raman spectroscopy results for films prepared under conditions (A) and (B) from Table I. The figures show that, as the Sc content of the ScAlN thin film increases, the peak at ~800 nm⁻¹ of the A1 mode, due to Sc atoms in the A1 sites of the wurtzite structure, shifts to lower frequency for both sputtering conditions. This means that Sc atoms occupy Al sites in the wurtzite structure in the thin film until the Sc content reaches 33%. This phenomenon was also observed for AlGaN thin films [7]. The peak near 700 cm^{-1} for the ScN thin film, ascribed to a cubic structure, is deformed with increasing Al content.

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Fig. 1 Dependence of Sc content in ScAlN thin films on the RF-power ratio under conditions (A) and (B)



Fig. 2 Results of micro-Raman spectroscopy measurements of $Sc_xAl_{1-x}N$ thin films deposited under conditions (A).



Fig. 3 Results of micro-Raman spectroscopy measurements of $Sc_xAl_{1-x}N$ thin films deposited under conditions (B).

4. Conclusions

ScAlN thin films with *c*-axis orientations were deposited by a dual-sputtering machine and characterized by XRF, XRD, and Raman spectroscopy. The results showed that Sc atoms occupied Al sites in the wurtzite structure in the thin films, until the Sc content reached 33%.

We have not yet investigated the piezoelectric properties of the ScAlN thin films because of their high surface roughness. However, we are currently trying to optimize deposition conditions to produce ScAlN thin films that exhibit high piezoelectricity.

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