Epitaxial growth of CaN_xH_y thin films using reactive magnetron sputtering

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[Introduction] Calcium compounds combined with nitrogen and hydrogen (CaN_xH_y) are promising catalysts for the production of ammonia, which is an important industrial chemical such as fertilizers [1,2,3]. To precisely understand the mechanism of such catalytic reactions, it is required to prepare well-defined surfaces with smooth and highly-oriented structures. For this purpose, epitaxial thin films can provide an ideal platform. However, due to its chemical instability, there has been no report on the thin film fabrication. In this study, we introduce our approach to fabricate CaN_xH_y epitaxial thin films using reactive magnetron sputtering.

[Experiment] CaN_xH_y thin films were deposited on MgO(100) substrates using reactive magnetron sputtering. A Ca metal plate (1 inch) was used as a target material. Substrate temperature was set to 300°C and RF power of 30 W was supplied. During the deposition, Ar, N_2 and H_2 gases were introduced to the growth chamber with flow rates of 10, 5 and 5 sccm, respectively. The total pressure was set to 1.0 Pa. The deposition time and typical film thickness was 1 hour, and 160 nm respectively. Note that the thickness was measured in air using stylus profiler. The structural properties of thin films were characterized by X-ray diffraction (XRD) using a custom-built Ar-filled cell to avoid atmospheric air.

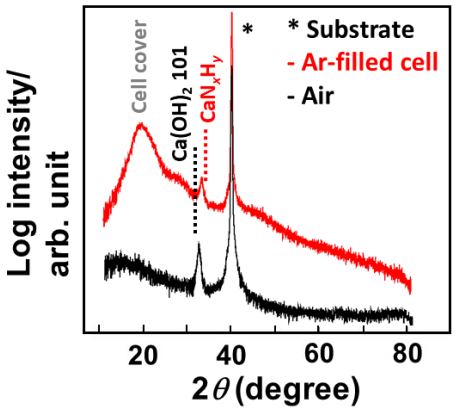

Fig 1: XRD patterns of the obtained thin films in Ar-filled cell and Air.

[Results and discussion] Figure 1 shows XRD patterns of the CaN_xH_y films. Whereas $Ca(OH)_2$ 101 was observed in air at the $2\theta = 34.0°$, only a single peak at $2\theta = 34.8°$ was observed using the Ar-filled cell (upper). This peak corresponds to the reflection of $Ca(NH_2)_2$ 200 or CaNH 200. To confirm the epitaxial relationship between the substrate and thin film, pole figure measurements for the diffraction at $2\theta = 50°$ and $\psi = 45°$ ($Ca(NH_2)_2$ 204 or CaNH 220) were carried out (Fig. 2b). Four-fold spots were observed with identical in-plane rotational angles (ϕ) as those of MgO 220, indicating epitaxial thin films were successfully fabricated. In the presentation, we will report further identification processes for the chemical composition of CaN_xH_y.

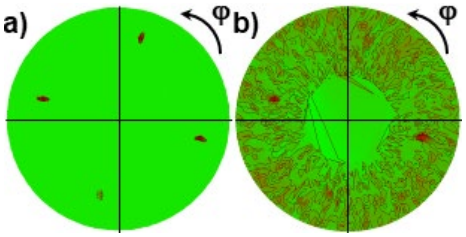

Fig 2: Pole figures of the a) MgO 220 and the b) $Ca(NH_2)_2$ 204 or CaNH 220 at $2\theta = 50°$ and $\psi = 45°$.

References

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