Growth of high purity CVD-grown *h*-BN using B_2H_6 and NH_3

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Two-dimensional (2D) van der Waals semiconductors have been proposed as emerging devices for many applications owing to atomically smooth interfaces with free dangling bonds. Among various 2D materials, hexagonal boron nitride (*h*-BN) is expected for deep ultraviolet light-emitting devices [1,2], and gate dielectric layer for graphene transistors [3]. In order to realize wafer-scale mass production of CVD-grown *h*-BN toward various semiconductor device applications, impurity control is extremely important. However, there are few reports regarding residual impurities in CVD-grown *h*-BN thin films. In this presentation, crystal growth and properties of CVD-grown *h*-BN on Al_2O_3 substrate using two different boron precursors (trimethyl boron: TMB and diborane: B_2H_6) and two different wafer susceptors (SiC-coated graphite and BN-molded susceptor) are discussed.

The BN thin films were grown on 2-inch α-Al_2O_3 (0001) substrates using AIXTRON Close Coupled Showerhead® (CCS) 3×2" reactor [4,5]. The susceptor temperatures (T_g) were varied from 1400°C to 1160°C. Alternating supply of boron and nitrogen precursors was applied. The film crystallinities are determined by variable angle spectroscopic ellipsometry (VASE), atomic force microscopy (AFM), secondary ion mass spectrometry (SIMS), high-resolution X-ray diffraction (HRXRD), Raman scattering spectroscopy, and cathodoluminescence (CL) spectroscopy.

Arrhenius plots of growth rates for the BN layer on Al_2O_3 substrates reveal the activation energies of B_2H_6 (0.97 eV) and TMB (0.29 eV), which relate to the surface reactions. The residual atomic concentrations of Si (2.6×10^{16} cm^{-3}), C (3.4×10^{18} cm^{-3}), and O (2.0×10^{17} cm^{-3}) in BN are obtained using B_2H_6 and BN-molded susceptor. These concentrations are approximately two orders magnitude lower than those using TMB and SiC-coated graphite susceptor (Si: 9.4×10^{17} cm^{-3}, C: 2.1×10^{20} cm^{-3}, O: 1.6×10^{19} cm^{-3}). The CL spectrum from the BN layer using B_2H_6 and BN-molded susceptor has 5.5 eV as a broad peak and 4 eV as several peaks. The free excitonic recombinations at the higher energy emission (5.79 eV) is owing to the reduction in residual impurities. The imaginary part of dielectric functions for the *h*-BN layers is derived from VASE [6]. The absorption coefficient of 1×10^4 cm^{-1} is observed in the energy range below 5 eV only when using the SiC-coated graphite susceptor, which is most probably in associated with Si contamination in the BN layer. The negligible absorption coefficient when using the BN-molded susceptor presents high purity *h*-BN signature.

References

[1] Watanabe K et al. Direct-bandgap properties and evidence for ultraviolet lasing of hexagonal boron nitride single crystal. Nat. Mater. 2004; 3: 404-409.
[2] Taniguchi T and Watanabe K. Synthesis of high-purity boron nitride single crystals under high pressure by using Ba–BN solvent. J. Cryst. Growth 2007; 303: 525-529.
[3] Dean CR. Boron nitride substrates for high-quality graphene electronics. Nature Nanotechnol. 2010; 5: 722-726.
[4] Yamada H et al. Comparative Study of Boron Precursors for Chemical Vapor-Phase Deposition-Grown Hexagonal Boron Nitride Thin Films$_3$. Phys. Stat. Sol. A 2020; 2000241.
[5] Yamada H. Reduction in residual impurities in CVD–grown hexagonal boron nitride thin films. Phys. Status Solidi B 2023; 2200352.
[6] Yamada H et al. Dielectric functions of CVD–grown boron nitride from 1.1 to 9.0 eV by spectroscopic ellipsometry. Appl. Phys. Lett. 2021; 118: 112101.