PCSI
Room Keahou I - Session PCSI-TuM2
Wide Bandgap Materials II

Moderator: Joel Varley, Lawrence Livermore National Laboratory,

11:00am **PCSI-TuM2-31 Diamond High Power and Voltage MOSFETs: Inch-Sized Wafer Growth, Doping, Static and Dynamic Characteristics**, ***MAKOTO KASU***, *Niloy Chandra Saha,* Saga University, Japan **INVITED**

Diamond possesses an ultrawide bandgap energy of 5.47 eV, a breakdown field of >10 MV/cm), higher thermal conductivity (22 W/cmK), and higher electron and hole mobilities (4500 and 3800 cm^2/Vs, respectively) than GaN and SiC. Therefore, diamond is considered to be the most capable candidate for the power semiconductor device application. Diamond single-crystal substrates have been limited to sizes of 4 mm. Diamond heteroepitaxial growth has not been achieved because of a large difference in coefficients of thermal expansion between diamond and foreign substrate materials. Recently, we have demonstrated a two-inch-diameter diamond wafer grown on Ir/sapphire (a-Al_2O_3) (11-20) substrate [1]. Diamond heteroepitaxial layer exhibited the highest crystal quality, such as TDD of $1.4x10^7$ cm^{-2}, and XRCFWHM of 98 arcsec [2]. We clarified diamond's nucleation process on Ir/sapphire surface by AFM, TEM, and EDS [3]. For diamond p-channel MOSFETs, so far impurity doping into diamond has not been successful because of extremely high activation energy. But we haveestablished p-type doping on the H-terminated diamond using NO_2 gas [4], and thermal stabilization and gate insulation withALD Al_2O_3 layer [4]. We have fabricated diamond MOSFET (Fig. 1) demonstrating high drain current density (I_D)of 0.68 A/mm, a low ON-state resistance of 50 Ω·mm, andextremely high OFF-state breakdown voltage (V_{BR}) of −2568 V. The specific on-state resistance, ($R_{ON,spec}$) was determined to be 7.54 mΩ·cm^2, and the maximum available power, i.e., BFOM (= $V_{BR}^2/R_{ON,spec}$) has been obtained to be 874.6 MW/cm^2 (Fig. 2), the highest ever in diamond, ~40% of GaN's top value [5]. Further, we demonstrated fast turn-on (t_{on}) and turn-off (t_{off}) switching times of 9.97 ns and 9.63 ns, respectively [6]. The first stress measurement was performed, showing 190 h of stable operation under a DC gate bias and drain bias stress [7]. No evident degradation in I_D was observed throughout the stress period; the gate current (I_G) increased after 83 h of stress due to the charge injection into the Al_2O_3 layer, although it did not influence the I_D.

[1] M. Kasu, Jpn. J. Appl. Phys. **56**, 01AA01 (2017). [2] S. -W. Kim, M. Kasu et al., Appl. Phys. Express **14**, 115501 (2021). [3] M. Kasu et al., Dia. Rel. Mater. **126**, 109086 (2022). [4] M. Kasu et al., Appl. Phys. Express 5, 025701 (2012). [5] N. C. Saha, M. Kasu, et al., IEEE Electron Dev. Lett. **43**, 777 (2022). [6] N. C. Saha, M. Kasu, et al., IEEE Electron Dev. Lett. **44**, 793 (2023). [7] N. C. Saha, M. Kasu, et al., IEEE Electron Dev. Lett. **44**, 975 (2023).

11:45am **PCSI-TuM2-40 Atomic and Electronic Structure Prediction for Heterostructural Interfaces with Ultra-Wide Gap Materials** , ***Stephan Lany,*** *Sharad Mahatara,* 15013 Denver West Pkwy

First-principles calculations can be an invaluable tool for modeling of interface properties. However, such calculations require detailed knowledge of the atomic structure, which is often not known experimentally. This is especially true for heterostructural interfaces between materials with different bulk crystal structures. Thus, interface atomic structures are often constructed by making plausible assumptions but without confirmation that the structure actually represents a free energy minimum. Atomic force relaxation alone is generally insufficient, because it only yields a local total energy minimum. A more rigorous approach requires the sampling of the configuration space. In general, we distinguish commensurate and incommensurate interfaces, where the former display a 1:1 matching of the in-plane primitive cell lattice vectors whereas the latter require construction of a coincidence site lattice for the matching of two 2D supercells. As an example of a commensurate heterostructural interface, we consider the case of wurtzite AlGaN alloys on rocksalt TaC (111) substrates, where the lattice matching of the hexagonal interface primitive cell occurs at high Al compositions for ultra-widegap applications. Using an algorithm for systematic enumeration of the stacking sequences promoting the transition from the rocksalt to the wurtzite structure, we perform high-throughput density functional theory calculations for energy minimization. Subsequent electronic structure calculations for the most favorable structures reveal the band alignment, Schottky barrier, and electronic interface density of states. We will further discuss the outlook for other substrate/film combinations and the case of incommensurate interfaces.

11:50am **PCSI-TuM2-41 Si Diffusion Into Self-Organized GaN Nanocolumns Grown on Si(111) by RF-MBE**, ***Tohru HONDA***, *Naoki GOTO, Yuto HOSOYA, Takeyoshi ONUMA, Tomohiro YAMAGUCHI,* Kogakuin University, Japan

The small-size micro-LED displays requests micrometer-scale pixels. The monolithic fabrication of GaN-based LEDs (monolithic integration) is also interesting for high-dense integration. In a view of the optical isolation of integrated LEDs, GaN nanocolumns grown on Si is interesting for the monolithic integration, because threading dislocations in them can be reduced (filtering effect) [1]. However, Si atoms will be diffused into the GaN nanocolumns. In this study, these carrier concentrations as a function of the amount of a Mg dope (compensation of electron carrier) are estimated using Raman spectra.

GaN nanocolumns (NCs) was grown on the substrate using plasma-assisted molecular beam epitaxy (RF-MBE). The growth time was 60 min., the growth temperature was 1020 °C, the Ga flux was 9.0×10^{-7} Torr, the N_2 flow rate was 2.0 ccm, and the RF power was 400 W. In a case of a Mg dope, its beam equivalent flux of 5.7×10^{-9}Torr was adopted. Raman spectra of GaN nanocolumns were observed using a 532-nm-line of YAG: Nd. The modes of E2 and LO-phonon-plasmon coupled (LOPC) modes [2] are shown in Figs. 1 and 2. The peak shift of E2 modes means the amount of strain in the layers. The strain in GaN NCs grown on Si is free compared with that in GaN layers grown on sapphire by MOVPE. It means that the NCs have the low dislocation densities due to “filtering effect” [1]. On the other hand, a very weak peak of the LOPC mode was observed form the GaN NCs. This means to the high electron carrier concentration in GaN NCs. The LOPC mode in carrier compensated GaN NCs using a Mg dope (Mg concentration was estimated using a local vibration mode) is also observed. A clear LOPC peak was observed. These peak positions indicate that the Si concentration in GaN NCs is approximately 100 ppm.

[1] H. Sekiguchi et al., APEX, **1**, 124002 (2008). [2] H. Harima et al., J. Cryst. Growth, **189/190**, 672 (1998).

11:55am **PCSI-TuM2-42 Realization of Smooth Surface and Interface in Mist CVD Growth of Rocksalt structured-MgZnO/MgO MQWs**, ***Hiroyuki Aichi,*** *Takeyoshi Onuma,* Kogakuin University, Japan

Rocksalt (RS) structured-$Mg_xZn_{1-x}O$ alloys have bandgap energies ranging from 2.45 to 7.78 eV [1,2]. They are candidate materials for deep and vacuum ultraviolet light emitters. Our group has grown atomically flat single-crystalline RS-$Mg_xZn_{1-x}O$ films on (100) MgO substrates using the mist chemical vapor deposition (mist CVD) method [3]. The CL spectra at 300 K exhibited the shortest near-band-edge emission peak at 187 nm. The RS-$Mg_xZn_{1-x}O$/MgO for x≥0.6 was confirmed to have type-I band alignment by the X-ray photoelectron spectroscopy measurements [4]. This study reports on growths of RS-$Mg_xZn_{1-x}O$/MgO multiple quantum well (MQW) structures by the mist CVD method.

RS-$Mg_xZn_{1-x}O$/MgO MQW structures were grown on (100) MgO substrates at 725°C. Magnesium acetate tetrahydrate and zincacetate dihydrate were used as source precursors. The x in the well layer was controlled by molar ratio of magnesium($[Mg]^L$ = [Mg]/([Mg]+[Zn])) in the sourcesolution. The structure consisted of a 30-nm thickMgO cap layer, 10 periods of MQW composed of 3-nm-thick RS-$Mg_{0.73}Zn_{0.27}O$ well and 10-nm-thick MgO barrier, and a 200-nm-thick MgO buffer layer.

As shown in Fig. 1, the structure exhibited atomically-flat smooth surface morphology with root mean square (RMS) roughness of 0.30 nm. Thevalue is comparable to those obtained for the RS-$Mg_xZn_{1-x}O$ single layers [3]. As shown in Fig. 2, distinct observationof the +1st, 0th, -1st, and -2nd order satellite peaks impliesrealization of excellent interface flatness and periodicity. Furthermore, cross-sectional STEM image showed a well-defined layered structure with abrupt interfaces.

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[1] T. Onuma *et al*., Appl. Phys. Lett. **119**, 132105 (2021). [2] A. Segura *et al.*, Appl. Phys. Lett. **83**, 278 (2003). [3] K. Ogawa *et al*., Jpn. J. Appl. Phys. **63**, 02SP30 (2024). [4] M. Matsuda *et al*., The 41th Electronic Materials Symposium, We1-11 (2022).

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