

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, N. 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 ($\alpha\text{-Al}_2\text{O}_3$) (11-20) substrate [1]. Diamond heteroepitaxial layer exhibited the highest crystal quality, such as TDD of $1.4 \times 10^7 \text{ cm}^{-2}$, 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 have established p-type doping on the H-terminated diamond using NO_2 gas [4], and thermal stabilization and gate insulation with ALD 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 $\Omega \cdot \text{mm}$, and extremely high OFF-state breakdown voltage (V_{BR}) of ~ 2568 V. The specific on-state resistance, ($R_{ON,spec}$) was determined to be 7.54 $\text{m}\Omega \cdot \text{cm}^2$, 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, $\sim 40\%$ 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).

11:40am PCSI-TuM2-39 Adsorption and Thermal Evolution of Nitrogen Species on Diamond Surfaces, *Kai Huang*, Guangdong Technion-Israel Institute of Technology, China

Layer-by-layer construction of diamond devices for spin-sensing calls for atomistic understanding of the nitrogen species on diamond surfaces.[1] As motivated by recent spectroscopic measurements (e.g., X-ray photoelectron spectroscopy, high-resolution electron energy loss spectroscopy and temperature-programmed desorption) on diamond surfaces impacted by N_2 plasma,[2] we conducted density functional theory simulations to gain atomistic details into the adsorption and thermal evolution of the resulted nitrogen species, as below.

- Diamond(001)**. We find that nitrogen plasma attacks the C=C dimers on the pristine diamond(001), forming nitrogen-dimers in a horizontal configuration, h- $\text{N}_2(\text{ad})$. [3] The formation of h- $\text{N}_2(\text{ad})$ is capable of resolving some discrepancy in the literature. the desorption of $\text{N}_2(\text{ad})$ on pristine diamond(001) follows a concerted process with a barrier of 0.91 eV. By contrast, there emerges a new state of nitrogen-dimers in a vertical configuration, v- $\text{N}_2(\text{ad})$, in addition to h- $\text{N}_2(\text{ad})$. [4] Consequently, the desorption of $\text{N}_2(\text{ad})$ is altered into a stepwise fashion, giving an overall barrier of 2.36 eV.
- Diamond(111)**. On bare domains of diamond, as represented by the models of C(111)-2x1 and graphite-like C(111), $\text{N}_2(\text{ad})$ is identified as major surface species; the desorption of $\text{N}_2(\text{ad})$ proceeds on both models via a concerted process of breaking two C-N bonds.[5] By contrast, there is evidence of formation of

$(\text{NH})_2(\text{ad})$ via the insertion reaction of N_2 plasma on hydrogenated domains of diamond, as represented by the models of C(111)-2x1-H and C(111)-1x1-H. Interestingly, contrasting dynamics of desorption of $(\text{NH})_2(\text{ad})$ are presented on these two models; that is, via sequential breaking of two C-N bonds on C(111)-2x1-H, and via concerted breaking of both C-N bonds on C(111)-1x1-H.[6]

References

- Jaffe, T.; Attrash, M.; Kuntumalla, M. K.; Akhvediani, R.; Michaelson, S.; Gal, L.; Felgen, N.; Fischer, M.; Reithmaier, J. P.; Popov, C.; Hoffman, A.; Orenstein, M. *Nano Lett.* **2020**, *20*, 3192–3198.
- For example, see Attrash, M.; Kuntumalla, M. K.; Michaelson, S.; Hoffman, A. *J. Phys. Chem. C* **2020**, *124*, 5657–5664.
- Zheng, Y.; Hoffman, A.; Huang, K. *Langmuir* **2021**, *37*, 6248–6256.
- Zheng, Y.; Kuntumalla, M. K.; Attrash, M.; Hoffman, A.; Huang, K. *J. Phys. Chem. C* **2021**, *125*, 28157–28161.
- Kuntumalla, M. K.; Zheng, Y.; Attrash, M.; Gani, G.; Michaelson, S.; Huang, K.; Hoffman, A. *Appl. Surf. Sci.*, **2022**, *600*, 154085.
- Zheng, Y.; Hoffman, A.; Huang, K. *J. Chem. Phys.* **2024**, *160*, 214713

*Author for correspondence: kai.huang@gtit.edu.cn [mailto:kai.huang@gtit.edu.cn]

11:45am PCSI-TuM2-40 Atomic and Electronic Structure Prediction for Heterostructural Interfaces with Ultra-Wide Gap Materials, *Stephan Lany, S. 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 AlGaIn 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, N. GOTO, Y. HOSOYA, T. ONUMA, T. 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 $^\circ\text{C}$, 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

Tuesday Morning, January 21, 2025

other hand, a very weak peak of the LOPC mode was observed from 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, T. 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 $x \geq 0.6$ 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 ($[Mg]^+ = [Mg]/([Mg]+[Zn])$) 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).

12:00pm PCSI-TuM2-43 Si-Integrated Epitaxial BaTiO₃ for Ultra-Low Loss, Efficient Modulators in Silicon Photonics, Alex A. Demkov, A. Posadas, A. Raju, D. Wasserman, The University of Texas at Austin

The integration of optical components with traditional silicon technology, known as integrated silicon photonics (SiPh), is experiencing explosive growth. It offers many advantages such as lower power consumption, higher speed, and higher bandwidth when compared to the traditional CMOS-based information technology [1,2]. Electro-optic (EO) modulators are among the key active photonic components of SiPh, they can modulate either the amplitude or the phase of light. The operation of some of the most promising high frequency EO modulators is based on the linear EO effect, commonly referred to as the Pockels effect [2]. The linear EO effect constitutes the change in the refractive index of a material in response to an external electric field. Silicon is transparent below 1.1 eV and demonstrates extremely low optical loss, around 0.1 dB/m that is ideal for integrated photonic devices with applications in optical communications, optical neuromorphic and quantum computing, however, Si doesn't exhibit linear EO effect [3]. Barium titanate BaTiO₃ (BTO) is an emerging material in SiPh with one of the largest known linear electro-optic coefficients. However, in BTO-based devices, high optical losses are consistently observed, typically an order of magnitude larger than those observed in lithium niobate. I will show that the origin of optical loss in BTO waveguides is non-absorptive and is caused by internal interfaces, aka planar defects such as e.g., ferroelectric domain walls. I will then discuss monolithic barium titanate photonic structures fabricated from BTO grown epitaxially by RF-sputtering on silicon-on-insulator substrates. Three types of test structures will be discussed: simple cut-back structures, high-Q ring resonators, and high-Q racetrack resonators. The record low loss of our monolithic barium titanate waveguide structures enables the demonstration of high-Q resonators with quality factors of $Q > 100,000$. The low loss of the barium titanate photonic structures, coupled with

barium titanate's large non-linear optical response offers a path to compact and high efficiency barium titanate photonic devices and structures for high-speed modulation, optical computing, and non-linear applications. This research is supported by a Multidisciplinary University Research Initiative from the Air Force Office of Scientific Research (AFOSR MURI Award No. FA9550-22-1-0307).

Author Index

Bold page numbers indicate presenter

— A —

Aichi, Hiroyuki: PCSI-TuM2-42, **2**

— D —

Demkov, Alex A.: PCSI-TuM2-43, **2**

— G —

GOTO, Naoki: PCSI-TuM2-41, **1**

— H —

HONDA, Tohru: PCSI-TuM2-41, **1**

HOSOYA, Yuto: PCSI-TuM2-41, **1**

Huang, Kai: PCSI-TuM2-39, **1**

— K —

KASU, MAKOTO: PCSI-TuM2-31, **1**

— L —

Lany, Stephan: PCSI-TuM2-40, **1**

— M —

Mahatara, Sharad: PCSI-TuM2-40, **1**

— O —

Onuma, Takeyoshi: PCSI-TuM2-42, **2**

ONUMA, Takeyoshi: PCSI-TuM2-41, **1**

— P —

Posadas, A.B.: PCSI-TuM2-43, **2**

— R —

Raju, A.: PCSI-TuM2-43, **2**

— S —

Saha, Niloy Chandra: PCSI-TuM2-31, **1**

— W —

Wasserman, D.: PCSI-TuM2-43, **2**

— Y —

YAMAGUCHI, Tomohiro: PCSI-TuM2-41, **1**