SAND2023-07750C

Structural and Chemical Inhomogeneity of Interface Underlying Nonideal Electrical Behavior in Au/β-Ga_2O_3 Contacts

Stephen D. House[1,2,3*], Luke A.M. Lyle[4,5,6], Judith C. Yang[1,2,7,8], Lisa M. Porter[4]

[1.] Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, United States
[2.] Environmental TEM Catalysis Consortium (ECC), University of Pittsburgh, Pittsburgh, PA, United States
[3.] Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM, United States
[4.] Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, United States
[5.] Electronic Materials and Devices Department, Applied Research Lab, Pennsylvania State University, University Park, PA, United States
[6.] Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA, United States
[7.] Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA, United States
[8.] Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, United States

* Corresponding author: sdhouse@sandia.gov

The ultrawide bandgap (4.7-4.9 eV) of β-Ga_2O_3, in addition to its range of shallow n-type dopants (Si, Sn, Ge) and commercially-available melt-grown substrates, have garnered significant interest for power electronics and UV photodetector applications. Investigations of electrical contacts to this semiconductor provide an understanding of the interplay between fundamental material properties and the metal/semiconductor interfaces that form the building blocks of larger-scale, widely employed devices, such as Schottky barrier diodes and power MOSFETS. In addition, the high temperatures, electric fields, and current densities present in the applications for which β-Ga_2O_3 is most attractive necessitates the development of thermally stable contacts able to withstand these conditions. However, in studies of Schottky and Ohmic contacts to various orientations of β-Ga_2O_3, some metals exhibited chemical reactions in the as-deposited state (e.g., Ti [1-3], Cr [4]) or at elevated temperatures (e.g., Pd [5], Ni [6,7]). Such reactions have significant impacts on the electrical and thermal properties of devices.

In a prior study [8] of this system, we observed that as-deposited Au/(100) β-Ga_2O_3 Schottky contacts exhibited higher ideality factors than Ni contacts to the same substrate and processed identically. The peculiarities of the electrical behavior of the Au/Ga_2O_3 contacts suggested that undesirable chemical and/or structural changes may have occurred, leading to local variations in the Schottky barrier height. This presentation discusses our investigation [9] of the nanoscale structure and chemistry of the Au/β-Ga_2O_3 interface and their correlation with the inhomogeneous electrical properties.

Single crystals of (100) β-Ga_2O_3 grown by the Czochralski method were first characterized by Hall effect, X-ray diffraction (XRD) and atomic force microscopy (AFM) prior to metal deposition via electron beam evaporation. Ohmic contacts using Ti/Au (20/100 nm) metallization were formed and annealed for 5 min at 400 °C followed by deposition of Au or Ni Schottky contacts in diameters of 500, 250, 125, and 62.5 μm. The as-deposited state of the Au/(100) β-Ga_2O_3 contact structures, with no heat treatment, was used

in all subsequent characterization. Current Density-Voltage (J-V) and Capacitance Voltage (C-V) measurements were conducted to characterize the electrical properties. Atomic-resolution high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and energy-dispersive X-ray spectroscopy (EDS) were employed to reveal the interfacial structure and chemistry of the contacts. Lift-out samples for TEM were prepared from using a Focused Ion Beam (FIB) and NanoMill.

The quantitative TEM analysis provided direct evidence of the inhomogeneous interfacial microstructure and chemistry, believed to be associated with the nonideal J-V characteristics and Schottky barrier heights. Specifically, it revealed a chemical reaction occurring at the Au/Ga_2O_3 interface, forming "humps" of defected Ga_2O_3 at the interface, leading to a significant increase in RMS roughness (1.77-2.86 nm) compared to the original semiconductor surface (0.8 nm). These humps formed by the asymmetric diffusion of Ga and O into the Au contact, leaving behind a layer of nanovoids 5-20 nm below the interface. This was confirmed both through EDS composition profiles and direct HAADF-STEM visualization of interstitial migration. The resulting post-deposition structure is summarized in Figure 1. These results suggest that even in non-annealed conditions, nano-scale interfacial chemical reactions can significantly impact the electrical characteristics of β-Ga_2O_3 contacts, and highlight the necessity of high-resolution studies for establishing stable metallization schemes. [10]

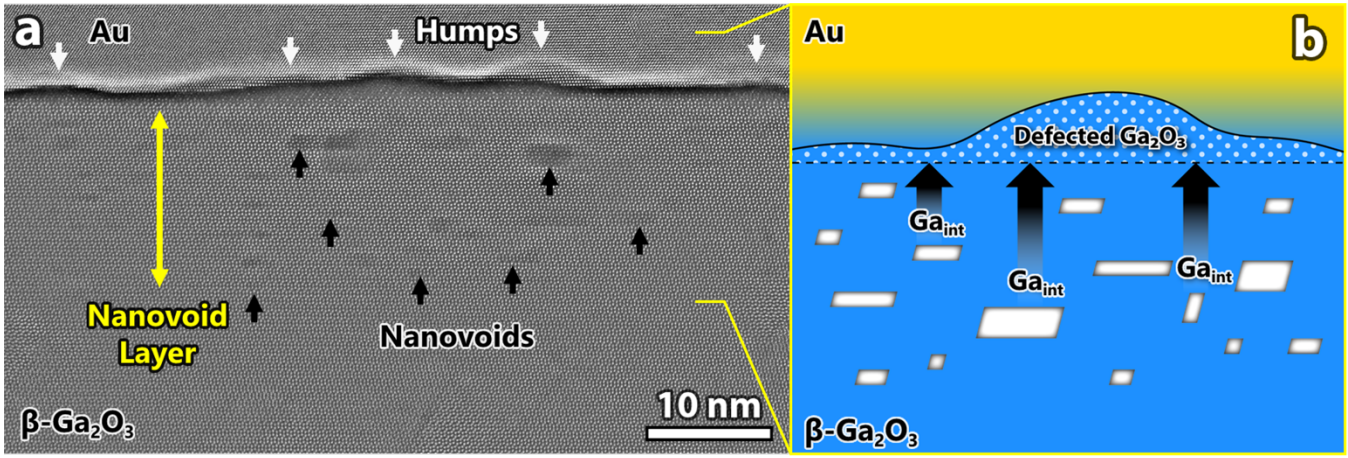

Figure 1. (a) Representative atomic-resolution HAADF-STEM overview image – high-pass filtered for ease of visualization – and (b) schematic of the Au/(100) β-Ga_2O_3 interface, showing the primary structural changes arising from the chemical reaction.

References:

[1] L Lyle, et al., APL Materials **9** (2021), p.061104
[2] M-H Lee and R Peterson, APL Materials **7** (2019), p.022524
[3] M-H Lee and R Peterson, ECS Journal of Solid State Science and Technology **8** (2019), p.Q3176
[4] H Aller, et al., Nano Letters **19** (2019), p.8533
[5] C Hou, et al., IEEE Transactions Electron Devices **68** (2021), p.1791
[6] M Labed, et al., ACS Applied Electronic Materials **3** (2021), p.3667
[7] H Kim, et al., Journal of Materials Chemistry C **7** (2019), p.10953
[8] L Lyle, et al., Journal of Vacuum Science and Technology A **39** (2021), p.033202
[9] L Lyle† and S House†, et al., ACS Applied Electronic Materials **4** (2022), p.4471

[10] LAML and LMP acknowledge funding from the Air Force Office of Scientific Research under award numbers FA9550-18-1-0387 and FA9550-21-1-0360. The work was partially performed in the framework of GraFOx, a Leibniz-Science Campus partially funded by the Leibniz Association. Zbigniew Galazka (Leibniz-Institut für Kristallzüchtung) is thanked for providing β-Ga_2O_3 wafers, and Kunyao Jiang (Carnegie Mellon University) for assisting with AFM characterization.
SDH acknowledges support from National Science Foundation award number CMMI-1905647. The ECC is supported by the University of Pittsburgh and Hitachi High Technologies. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.