PCSI

Room Ballroom South - Session PCSI-MoM1

Semiconductor Heterostructures (Growth, Nanostructures & Interfaces) I

Moderator: Kirstin Alberi, National Renewable Energy Laboratory

8:30am **PCSI-MoM1-1 Mechanisms and Applications for Remote Epitaxy of Heusler Compounds**, ***Jason Kawasaki,*** University of Wisconsin - Madison **INVITED**

Remote epitaxy on monolayer graphene is promising for synthesis of highly lattice mismatched materials, exfoliation of free-standing membranes, and re-use of expensive substrates. However, due to contaminants at the transferred graphene/substrate interface, other mechanisms such as pinhole-seeded lateral epitaxy often dominate rather than the intrinsic growth via remote interactions [1]. I will describe our understanding of the synthesis science of remote epitaxy, focusing on III-V semiconductors and Heusler compounds [1,2]. I will also show how exfoliated free-standing membranes of rare earth Heusler compounds can be used to tune (flexo)magnetism and novel superconductivity [3,4]

[1] S. Manzo, et. al.,Nature Commun., 13, 4014 (2022). https://doi.org/10.1038/s41467-022-31610-y

[2] D. Du et. al., Nano Lett. 22, 21, 8647 (2022). https://doi.org/10.1021/acs.nanolett.2c03187

[3] D. Du, et. al., Nature Commun., 12, 2494 (2021). https://doi.org/10.1038/s41467-021-22784-y

[4] D. Du, e. al. APL, 122, 170501 (2023). https://doi.org/10.1063/5.0146553

9:10am **PCSI-MoM1-9 UPGRADED: High-Mobility Two-Dimensional Electron Gas with Quantized States in Polar-Discontinuity Doped $LaInO_3/BaSnO_3$ Heterostructure Grown by Molecular Beam Epitaxy**, *G. Hoffmann,* Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin, Germany*; A. Hartl,* Paul Scherrer Institut, Switzerland*; M. Zupancic,* Leibniz-Institut für Kristallzüchtung, Germany*; A. Riaz,* University College London, UK*; V. Strocov,* Paul Scherrer Institut, Switzerland*; M. Albrecht,* Leibniz-Institut für Kristallzüchtung, Germany*; A. Regoutz,* University College London, UK*;* ***Oliver Bierwagen,*** Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin, Germany

Transistor applications of semiconducting oxides require, both high room-temperature electron mobilities (μ_{RT}) and high charge carrier densities (CCDs), ideally realized with a two-dimensional electron gas (2DEG). So far, prototype oxide 2DEG systems have either high μ_{RT} but limited CCD such as modulation-doped $(Al_xGa_{1-x})_2O_3/Ga_2O_3$, or a high CCD but low μ_{RT} such as the polar-discontinuity doped $LaAlO_3/SrTiO_3$ interface. Interfacing the more suitable, wide-bandgap, nonpolar semiconductor $BaSnO_3$ (BSO), having high bulk μ_{RT} (up to 320 cm^2/Vs), with polar $LaInO_3$ (LIO) is predicted to create and confine a 2DEG with CCD up to $2x10^{14}$ cm^{-2} for the SnO_2/LaO interface termination.

We demonstrate the adsorption-controlled growth of the LIO[1] on BSO heterostructure by molecular beam epitaxy using a shutter sequence to control the SnO_2/LaO interface termination. The films were analyzed by reflection high-energy electron diffraction (RHEED) [Figs. 1(a) and 1(b)], x-ray diffraction, atomic force microscopy (AFM) [Fig. 1(c)]. The interface structure is investigated by cross-sectional transmission-electron microscopy. The formation of the quantized 2DEG at their interface is confirmed by capacitance-voltage (CV) [Fig. 1(d)] and angular-resolved photo-electron spectroscopy (ARPES) [Fig. 1(e)]. Van der Pauw-Hall measurements confirm CCD>$10^{13}$$cm^{-2}$ and μ_{RT}>100cm^2/Vs.

[1] G. Hoffmann et al., Phys. Rev. Mater. **7**, 084606 (2023).

9:30am **PCSI-MoM1-13 Enabling Direct-Write Fabrication of Low Dimensional Micro- and Nanostructures on Supported and Suspended Substrates**, ***Irma Kuljanishvili,*** Saint Louis University

Low-dimensional nanomaterials, such as one-dimensional (1D) or two-dimensional (2D) systems, assembled in vertical or lateral arrangements, often lead to enhanced properties and new functionalities. Nanotubes, nanowires (NWs), and 2D layered structures (graphene and graphene like materials) are emerging as key building blocks for the next generation devices and emerging technologies. Practical implementation of such nanomaterials necessitates their successful incorporation with well-established processes for fabricating electronic and/or mechanical devices. While preparing layered architectures usually involves multi-step fabrication processes but relies on mask-assisted fabrication techniques. Here, we present a methodology for the controlled and selective preparation of nanostructures such as 1D NWs on 2D materials-substrates in various controlled geometric assemblies by employing direct write patterning (DWP) of custom ink precursors on supported or suspended architectures for subsequent chemical vapor deposition (CVD) synthesis.Our two-step fabrication approach enables simple and flexible routes to produce various architectures in a precisely controlled fashion. Location-specific materials synthesis provides access to as-grown interfaces and rapid testing of materials' quality, crystallinity, chemical composition, etc.

9:35am **PCSI-MoM1-14 Silicon (111) - Aluminum (111) - Amorphous Alumina: Asymmetric Quantum Well and Band Alignment**, ***Hanran Jin,*** University of Texas at Austin, China*; A. Demkov,* University of Texas at Austin

Thin single crystal films of Al can be epitaxially grown on Si(111) [1]. When taken out of ultra-high vacuum, Al oxidizes and forms a quantum well structure Si-Al-Al_2O_3. Theoretical calculations can shed light on finding the band alignment across the hetero-structure and its electronic and optical properties. However, one needs to build a structural model. The structure of Al on Si(111) has been experimentally determined via the electron microscopy by McSkimming et al. [1]. The Al layer is found to be (111) oriented, with a linear ratio of 3 Si to 4 Al atoms along the interface. Using this information, we construct a periodic model of Si-Al interface and perform density functional theory (DFT) calculations to find the relaxed structure, layer-projected density of states, and planar averaged potential across the interface. From there, we find the band alignment using the valence band offset from the bulk averaged potential. When aluminum metal is exposed to air, a several nanometers thick layer of alumina rapidly forms [2]. This oxide layer is amorphous. We simulate the structure of amorphous alumina using ab-initio molecular dynamics with the melt-and-quench technique [3]. This amorphous alumina can then be directly combined with the previous system to form an asymmetrical quantum well, where the well states and band alignment can be directly obtained from the DFT calculations.

[1] McSkimming, B. M., Alexander, A., Samuels, M. H., Arey, B., Arslan, I., & Richardson, C. J. (2016). Metamorphic growth of relaxed single crystalline aluminum on silicon (111). J. Vac. Sci. & Technol. A **35**, 021401 (2017).

[2] Jeurgens, L. P., Sloof, W. G., Tichelaar, F. D., & Mittemeijer, E. J. Growth Kinetics and mechanisms of aluminum-oxide films formed by thermal oxidation of aluminum. Journal of Applied Physics, **92**, 1649 (2002).

[3] Gutiérrez, G., asnd Johansson, B. Molecular dynamics study of structural properties of amorphous Al_2O_3. Physical Review B **65**, 104202(2002).

9:40am **PCSI-MoM1-15 Silicene Ribbons: Synthesis, Electronic and Geometric Structure at the Atomic Scale**, *A. Costine,* University of Virginia*; Z. Gai,* Orak Ridge National Laboratory*;* ***Petra Reinke,*** University of Virginia

Silicene is a 2D material which poses significant challenges in synthesis and device integration but offers unique electronic properties which are not yet fully understood. Challenges remain in silicene synthesis on non-metallic substrates and the control of buckling. The degree of in-plane buckling is tied to the emergence of a Dirac point and intriguing quantum phases have been predicted.[1-4]In our previous work we discovered a new pathway to silicene synthesis using h-$MoSi_2$ (0001) surfaces as templates,[5]and we present here the formation of silicene nanoribbons on the same surface, and measure their geometric and electronic structure with STM and STS at 77 K. Our work promises a new pathway to create silicene layers and nanoribbons with molecular beam epitaxy directly on silicon wafers.

The h-$MoSi_2$ (0001) crystallites are synthesized on Si(100) by deposition of a thin Mo film with electron beam evaporation, and subsequent annealing to form well-defined crystallites with 15 - 120 nm in diameter. Nanoribbons cover the entire surface for all "flat top" silicide crystallites with (0001) surfaces. Several surface reconstructions present intermediate superstructures, and are precursors for the nanoribbons. The STM images in Fig. 2 illustrate the geometric structure of the nanoribbons which are 1.8 nm in width and separated by a distinct groove of roughly a single atomic row in width. Models of the nanoribbon's geometric structure will be discussed. The atoms located at the ribbon edge appear brighter which is likely due to density of states (DOS) modulation by edge states. Characteristic defects are seen in the ribbons and express identical STM. The average DOS (dI/dV) measured with STS is indicative of a Dirac type electronic signature with a V-type dip around E_F, and the position dependent DOS across the ribbons allows to identify the Dirac type regions.

We will discuss all aspects of electronic and geometric structure of the nanoribbons including electronic confinement, and localized Dirac type signatures. In addition, point defects, and long range deformations induced by strain are addressed and inform our structural models.

[1] C. Grazianetti et al.. ACS Nano **11**, 3376-3382 (2017). [2] C.-C. Liu et al.. Physical Review Letters **107**, 076802 (2011). [3] A. Molle et al. Chemical Society Reviews **47**, 6370-6387 (2018). [4] H. J. W. Zandvliet. Nano Today **9**, 691-694 (2014). [5] C. Volders et al. Nano Letters **17**, 299-307 (2017).

9:45am **PCSI-MoM1-16 Spontaneous Growth of Silver on Si(001) Tuned by Substrate Temperature***, **Xiaohang Huang**, K. Huang,* Guangdong Technion - Israel Institute of Technology, China

The development of semiconductor technology features miniaturization of device that approaches the physical limit, i. e., nanostructure of a few atoms and/or molecules. It has been aimed that one could use nanostructures to fabricate functional devices at will. For the system of silver on Si(001), there is a rich collection of nanostructures as revealed in our recent works [1, 2], serving as the candidates to test this aim.

In this work, we examined the spontaneous growth of silver on Si(001) held at 109 to 298 K by scanning tunneling microscopy. As shown in Figure 1, the dimension of the formed silver depends on the substrate temperature during the deposition. That is, silver is formed predominantly as zero-dimensional (0D) objects at less than 120 K, one-dimensional (1D) objects at 120-200 K, and two-dimensional (2D) objects at 200-270 K. These observations are linked to the anisotropic migration of the key intermediate of silver tetramer, as supported by density functional simulations; the barriers are calculated as 0.24 eV along Si-rows, and 0.68 eV across Si-rows [2]. A schematic of the growth dynamics is sketched in Figure 2.

[1] K. Huang, X. Huang, J. Nogami, Phys. Chem. Chem. Phys. 7, 23 (2021).

[2] X. Huang, A. Hoffman, K. Huang, J. Phys. Chem. C. 18, 126 (2022)

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Author Index

Bold page numbers indicate presenter

— A —
Albrecht, M.: PCSI-MoM1-9, 1
— B —
Bierwagen, O.: PCSI-MoM1-9, **1**
— C —
Costine, A.: PCSI-MoM1-15, 1
— D —
Demkov, A.: PCSI-MoM1-14, 1
— G —
Gai, Z.: PCSI-MoM1-15, 1
— H —
Hartl, A.: PCSI-MoM1-9, 1
Hoffmann, G.: PCSI-MoM1-9, 1
Huang, K.: PCSI-MoM1-16, 2
Huang, X.: PCSI-MoM1-16, **2**
— J —
Jin, H.: PCSI-MoM1-14, **1**
— K —
Kawasaki, J.: PCSI-MoM1-1, **1**
Kuljanishvili, I.: PCSI-MoM1-13, **1**
— R —
Regoutz, A.: PCSI-MoM1-9, 1
Reinke, P.: PCSI-MoM1-15, **1**
Riaz, A.: PCSI-MoM1-9, 1
— S —
Strocov, V.: PCSI-MoM1-9, 1
— Z —
Zupancic, M.: PCSI-MoM1-9, 1