PCSI

Room Ballroom South - Session PCSI-MoM1

Group-IV Alloy Semiconductors

Moderator: Stefan Zollner, New Mexico State University

8:30am **PCSI-MoM1-1 Crystal Growth and Interface Engineering of Sn-related Group-Iv Alloy Semiconductor for Device Applications**, ***Osamu Nakatsuka***, *Masashi Kurosawa, Shigehisa Shibayama, Mitsuo Sakashita,* Nagoya University, Japan **INVITED**

Sn-related group-IV alloy semiconductors, GeSn and GeSiSn have much attracted on those unique material properties; an indirect-direct transition, a high carrier mobility, a good responsivity for near- and mid-infrared lights, a low growth temperature, a low thermal conductivity, etc. Also, the heterostructures of those alloy semiconductors realize rich energy band engineering for not only the band gap but also the band offsets like group-III-V compound semiconductors. These characters promise improved and/or superior electronic, optoelectronic, andthermoelectric device applications integrated on Si large scale integrated circuit platform.

We have developed the crystal growth technology of epitaxial and polycrystalline Sn-related group-IV alloy semiconductor thin films for device applications. There are some difficulties of the crystal growth of GeSn thin films; the low thermal-equilibrium solid solubility of Sn in Ge as low as 1%, also we have to take care for dislocations and defects with the strain relaxation on Si substrate and the low growth temperature. We need to establish the engineering technology of crystal growth and heterostructure formation with GeSn and GeSiSn to control the electrical properties. Recently, we achieved the thin film growth of a GeSn epitaxial layer with an ultra-high-Sn content over 50%. A key point for realizing such a high Sn content is the lattice-constant engineering of substrate for epitaxial growth. We used a large-lattice-constant substrate of GaSb whose lattice matches to that of $Ge_{0.48}Sn_{0.52}$ to suppress the strain between epitaxial layer and substrate.

We also achieved the heteroepitaxial growth of GeSn/GeSiSn multi layers for providing a double barrier structure. Those realize the carrier confinement structures at the valence and conduction band edges. We demonstrated its effectiveness improving optoelectronic properties enhancing photon-electron response and recently realizing the resonant tunneling diode operating at room temperature.

The development of interface engineering technology on insulator/GeSn and metal/GeSn systems is also a key issue for high-performance devices. In our presentation, we will introduce our recent achievements in an Al_2O_3/GeO_2/GeSn structure for surface passivation[5] and low-resistance NiGe(Sn)/Sb-doped Ge(Sn) contacts for electronic and optoelectronic device applications.

9:10am **PCSI-MoM1-9 Growth Orientation Analysis of Snte Epitaxial Layers on Gaas(001) Substrates by Xrd Pole Figure Measurements**, ***Yingjie Chen***, Department of Electrical Engineering and Bioscience, Waseda University, Japan

SnTe, a representative IV-VI rocksalt compound, exhibits a mirror-symmetry-protected topological crystalline insulator (TCI) phase with confirmed bulk band inversion and surface Dirac states . For the band engineering, high-quality single-domain epitaxial films are crucial. Although the GaAs(001)/ZnTe buffer system enables SnTe growth, it often shows orientation competition and twinning. Hence, x-ray diffraction (XRD) pole figure analysis was used to identify those domains and their relation to growth parameters.

SnTe films were formed on GaAs(001) by molecular beam epitaxy with ZnTe buffer layers. As a representative case, sample A was grown at with a thickness of 0.2 um. Using the X-ray diffraction (XRD) θ-2θ scan, the dominant phase of the layer aligned to the substrate surface was (001). However, this technique alone cannot fully characterize complex microstructures because it is insensitive to orientations that deviate from the substrate normal. To overcome this limitation, we further performed XRD pole-figure analysis, with measuring peaks of GaAs111, SnTe200, and SnTe222 and resolving the three-dimensional configuration. It was confirmed that (001), (011), and (111) oriented domains were included in most layers. The SnTe200 pole figure exhibits (001), (011), (111) oriented domains normal to the substrate surface.The SnTe (111) component became dominant when the SnTe buffer layer was extensively annealed. An insufficient annealing duration enhances the (022) component. These findings provide an experimental basis for fabricating high-quality, single-domain SnTe epitaxial layers and will facilitate device research based on SnTe as a TCI.

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9:15am **PCSI-MoM1-10 Infrared Ellipsometry from 300 K to 10 K for 30 nm α-Sn Films**, ***Jaden R. Love***, *Carlos A. Armenta, Atlantis K. Moses, Jan Hrabovsky, Stefan Zollner,* New Mexico State University*; Aaron N. Engel, Chris J. Palmstrom,* University of California at Santa Barbara

α-Sn is the low-temperature phase of tin that crystallizes in an FCC diamond-like lattice structure. MBE was used to grow 30 nm thick α-Sn films on bulk undoped single side polished InSb (100) substrates [3]. The α-Sn layer on sample AE225 was grown on an Indium rich c(8x2) reconstruction and the α-Sn layer on sample AE227 was grown on an Antimony rich c(4x4) reconstruction. It has been shown that the band occupancy of α-Sn is strongly influenced by the preparation methods [2,4].

Due to relativistic effects in heavy atoms, the Γ_7^-band maximum is negative for α-Sn.There is a degeneracy at Γ and a curvature inversion of the light hole band. The degeneracy and inversion lead the Γ_8^{+v} band to appear as a valence band and the Γ_8^{+c} band to appear as a conduction band. Consequently, intervalence band transitions are allowed from the Γ_7^-band into the Γ_8^{+v}band. The oscillator strength of this transition, $\tilde{E}_0$, depends on the occupancy of each band and is influenced by changing the concentration of acceptor or donor ions in the α-Sn lattice. Growth on an Indium rich interface leads to higher concentrations of acceptors that cause the oscillator strength of the $\tilde{E}_0$ transition to increase. $\tilde{E}_0$ is observable using infrared spectroscopic ellipsometry and has been recorded previously at 0.41 eV [2,4].

We use temperature dependent Fourier Transform Infrared Spectroscopic Ellipsometry to measure intrinsic and n-type doped 30 nm thick α-Sn layers grown on InSb (100) substrates from 300 K to 10 K. We model the dielectric function at all temperatures using a basis spline (b-spline) polynomial. Using the oscillator strength of the $\tilde{E}_0$ transition we find the integrated peak intensity after a linear background subtraction and determine the hole density at each temperature by applying the Thomas-Reiche-Kuhn f-sum rule [5]. The results for the intrinsic and n-type doped samples are compared to experimental data for 70 nm α-Sn layers on InSb and CdTe substrates collected previously by [2]. We compare the experimental results to literature values obtained by using degenerate Fermi-Dirac carrier statistics [1]. We find that the carrier density is strongly influenced by substrate preparation.

[1] S. Zollner. J. Vac. Sci. Technol. B 42 (2024), p. 022203.

[2] R. A. Carrasco et al. Appl. Phys. Lett. 113 (2018), p. 232104.

[3] A. N. Engel et al. Phys. Rev. Mater. 8 (2024), p. 044202.

[4] R. A. Carrasco et al. Appl. Phys. Lett. 114 (2018), p. 06102.

[5] M. Altarelli et al. Phys. Rev. B 6 (1972), p. 4502.

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9:20am **PCSI-MoM1-11 Implications for Sigesn Growth from the Surface Science of Sn on Si**, ***Caitlin McCowan***, *Evan Anderson, Ezra Bussmann,* Sandia National Laboratories*; Damien West, Yunfan Liang, Shengbai Zhang,* Rensselaer Polytechnic Institute

SiGeSn is a promising alloy for optoelectronic applications due to having a simpler path for integration into silicon semiconductor manufacturing than compound semiconductors. A direct bandgap has been predicted theoretically, but has not been definitively observed experimentally. This discrepancy is thought to result from the atoms in the lattice not forming a random alloy, but exhibiting short range order. Curiously, SiGe has the same underlying atomic- and mesoscopic-scale forces, i.e. bonding and strain, but is a random alloy. The goal of this research is to understand what is driving short range ordering in SiGeSn alloys. We collected data with scanning tunneling microscopy (STM), analyzing growth in a step-by-step fashion where sub-monolayer Sn is deposited on to a Si(100) substrate, and then annealed. Step-by-step tuning of growth and annealing variables can be analyzed *in situ* with STM.

Atomic scale analysis of the Sn:Si surface gives insight into what drives ordering of group IV alloys. Our data shows Sn deposited on Si forms 2x1 dimer chains, but, unlike Si deposited on Si, they don't pack closely together due to steric repulsion. After annealing, Sn both assembles into

islands at the surface as well as incorporates into the topmost layer of Si atoms in the substrate, but with a 3x2 periodicity (Fig 1). The change implies an interaction between the local strain inherent to the dimer rows, bonding, and steric repulsion. Sn coverage, annealing time, and annealing temperature collectively change the appearance of structures above the atomic scale – e.g. the length of the chains. Meanwhile, only the long-range periodicity of these features is dictated by the strain. Atomic positions from the experimental data will be compared to predictions from modeling.

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9:25am **PCSI-MoM1-12 Pressure-Dependent Photoluminescence of a Gesn/Sigesn Single Quantum Well at 10 K**, ***Meghan Worrell,*** New Mexico State University

The 10 K photoluminescence (PL) properties of a GeSn/SiGeSn single quantum-well (SQW) heterostructure are measured as a function of hydrostatic pressure applied using a diamond anvil cell (DAC) from 0 to ~0.5 GPa. With increasing pressure, the PL peak exhibits a consistent blueshift with a clear reduction in intensity beyond ~0.5 GPa due to PL quenching. The PL peak energy increased linearly with pressure, resulting in a pressure coefficient of approximately 48 meV/GPa. By fitting the PL energy shift against strain calculated using the Murnaghan equation, the hydrostatic deformation potential is evaluated as −3.5 ± 0.1 eV. The strain in the GeSn/SiGeSn structure is evaluated using high-resolution X-ray diffraction (XRD) and reciprocal space mapping (RSM) along both (004) and (224) directions. These measurements allowed precise determination of in-plane and out-of-plane lattice constants for the quantum well, buffer, and barrier layers. Using these lattice parameters, the hydrostatic and shear strain components are calculated for each layer in the heterostructure, enabling determination of the band edge alignment as a function of strain. The results provide insights into band structure engineering in GeSn/SiGeSn QWs and demonstrate their tunable optical properties under external pressure.

9:30am **PCSI-MoM1-13 Group IV Alloy Short-Range Order and Fluctuation Effects on Quantum Electronics**, ***Ezra Bussmann,*** Sandia National Laboratories **INVITED**

Recent progress with spin quantum computing and lasers in group IV (Si, Ge and Sn) alloy heterostructures revealed alloy fluctuations and correlations that have appreciable influence on materials electronic properties [1-3]. This has inspired high-fidelity studies exploring fluctuations and short-range order across group IV alloys [3-5]. Here, short-range order (SRO) denotes atomic neighborhood correlations between alloy elements site-to-site on the diamond-type crystal lattice, whereas fluctuation denotes neighborhood statistical variations from mean composition. I will describe experiments to detect subtle nanosize alloy fluctuations and SRO, and theory and models to explain their origins and outsized effect on single-particle states for qubits in SiGe and electronic bands in SiGeSn. For electron spin qubits in SiGe heterostructures, alloy fluctuations modify splittings separating qubit states from other excited states, allowing state mixing and quantum leakage paths [3].In SiGeSn, SRO correlations emerge above background alloy fluctuations, and this SRO is predicted to modify electronic band parameters, electronic and thermal transport, and materials design [2]. I will describe ongoing work to measure and isolate these effects and to design and control alloy fluctuations and SRO as an electronic engineering degree-of-freedom. The talk will highlight advances around the group IV epitaxial material community, through collaborations in the *Center for Manipulation of Atomic Ordering for the Manufacture of Semiconductors* (*μATOMS*) a recently funded *Energy Frontier Research Center*, and my teams work on fluctuations affecting qubit variability in SiGe materials [5].

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[2] Cao, B. *et al*., ACS Appl. Mater. & Interfaces **12**, 57245 (2020).

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