Thin Films
Room Naupaka Salon 5-7 - Session TF-WeE

Emerging Topics: Growth and Properties of Electronic Materials, 2D Layers, and Metallic-glass Thin Films

Moderator: Ludvik Martinu, Polytechnique Montréal, Canada

5:40pm **TF-WeE-1 Recent Development of Biocompatible Thin Film Metallic Glasses and High Entropy Alloy Coatings**, *B. Lou,* Chang Gung University, Taiwan; ***Jyh-Wei Lee***, *S. Ho,* Ming Chi University of Technology, Taiwan, Republic of China; *Y. Yang,* National Taipei University of Technology, Taiwan; *J. Chu,* National Taiwan University of Science and Technology, Taiwan **INVITED**

Biomedical Ti, Ti-6Al-4V alloys, and 316L stainless steels are widely used in biomedical devices for various parts of the human body. It has been reported that the corrosion and erosion-corrosion failures of such biomedical implants are very critical. Therefore, the surface modification of these implants is important for improving their corrosion resistance and extending their surface lifetime. Recently, thin film metallic glass (TFMG) and high entropy alloy films (HEAF) have been intensively studied due to their good physical and mechanical properties, such as high strength and excellent corrosion resistance. The applications of biocompatible TFMGs and HEAFs as surface modification coatings on the biomedical Ti, Ti-6Al-4V alloys, and 316L stainless steel have become an important research topic.

In this work, several Zr-, Ti-, Fe- and W-based TFMGs, TiZrNbTaFe, and TiZrNbTaMo HEAFs were fabricated using the magnetron sputtering method through the collaborative work of several research groups in Taiwan. The in-vitro and in-vivo studies of these biocompatible TFMGs and HEAFs were explored. The application of TFMGs on the surface of surgical instruments, such as dermatome and endodontic files were discussed. For the in-vivo animal study, the TiZrNbTaFe HEAFs coated cp-Ti implants were inserted into the femur of Sprague–Dawley rats. The surrounding bone volumes of implants were examined by a micro–computed tomography after 4- and 12-weeks implantation. The tensile pull-out test wasperformed together with the histological analysis to investigate the bone tissue regeneration and bone tissue adhesion ability. Better osseointegration ability and biocompatibility were found for of the HEAF coated cp-Ti implants. Some possible applications of biocompatible TFMGs and HEAFs on biomedical instruments were also proposed in this work.

6:20pm **TF-WeE-3 Influence of Relatively High Density Background Carriers on Photo-Dember Effects at the Surfaces of *n*-type and *p*-type InSb Single Crystals Observed with the Use of Terahertz Time-Domain Spectroscopy: A Study on Ultrafast Photogenerated Carrier Diffusion**, ***Hideo Takeuchi***, Osaka Metropolitan University (formerly Osaka City University), Japan; *T. Sumioka,* Osaka City University, Japan

Carrier-diffusion phenomena are essential issues on electronic and optoelectronic semiconductor devices. Ultrafast optical spectroscopy, which progresses with the development of femtosecond pulse-laser technology, is effective to investigate transient carrier diffusion. Terahertz electromagnetic waves, which are emitted from surfaces of narrow gap semiconductors with the use of illumination of femtosecond laser pulses, provide information on the photogenerated carrier diffusion process, the so-called photo-Dember effects. The photo-Dember effects result from the difference in a diffusion coefficient connecting with mobility between electrons and holes [1]. The diffusion-coefficient difference builds up transient polarization producing the terahertz wave. In a typical narrow gap semiconductor, InSb, the emission process of the terahertz wave is dominated by the photo-Dember effects. We, here, point the fact that the earlier terahertz time-domain spectroscopic works in InSb was focused on lightly doped samples [2]. It is reasonable to assume that the diffusion process is strongly influenced as the background carrier density is increased. This is because the mobility depends on the carrier density [3]. Accordingly, for verifying the above assumption, it is meaningful to clarify the characteristics of the terahertz wave emitted from the InSb crystals with the relatively high background carrier density. In the present work, we investigated the terahertz-wave emission from *n*-type and *p*-type InSb single crystals with relatively high major carrier density of 2 x 10^{17} cm^{-3}. We observed the terahertz wave originating from the photo-Dember effects in the *p*-type InSb crystal. In contrast, we found that the terahertz wave originating from the photo-Dember effects disappears in the *n*-type InSb crystal. According to Ref. 2, the photo-Dember voltage V_D is proportional to $\ln[1+\{(b+1)\Delta n/(bn_0+p_0)\}]$, where n_0 and p_0 is background electron and hole densities, respectively, and b is the ratio of the electron mobility to hole mobility: $\mu_e/\mu_h \approx 100$. In addition, the quantity Δn is the photogenerated electron density. It is apparent that, in highly doped InSb crystal, bn_0 is much larger than p_0, which reduces the photo-Dember voltage V_D. We, therefore, attribute the origin of the observed difference between the n-type and p-type InSb crystals to the fact that the photo-Dember voltage is suppressed in the case where the background electron density is relatively high.

[1] H. Dember, Z. Phyik vol. 32, 554 (1931), 856 (1931), vol. 33, 207 (1932).
[2] P. Gu *et al*., J. Appl. Phys. vol. 91, 5533 (2002).
[3] S. Watanabe, J. Phys. Soc. Jpn. vol. 50, 1049 (1981).

6:40pm **TF-WeE-4 Theoretical Analysis on Alternative Pathway for Low Temperature Atomic Layer Deposition of Nitrides**, *J. Lee, S. Lee,* ***Bonggeun Shong***, Hongik University, Republic of Korea

Atomic layer deposition (ALD) enables various advantages in deposition of thin films such as excellent step coverage and conformality. ALD is composed of alternative cycles of metal precursors and counter-reactants, whose self-limiting chemical reactions on the substrate surfaces determine the process conditions for the deposition. For example, in ALD of titanium nitride (TiN), TiCl4 with NH3 is most commonly used; however, temperatures as high as 500 °C is often required in such process to decrease the contamination of the TiN films by Cl. High thermal budget is often an issue also for other nitride ALD processes in general. Recently, a new recipe for TiN ALD is reported to simultaneously decrease both the deposition temperature and the Cl contamination, by introducing a H2S pulse between TiCl4 and NH3 reactants [1]. In this study, we conducted a theoretical analysis on comparing conventional versus alternative pathways for nitride ALD, using density functional theory (DFT) calculations. It was found that introduction of H2S may decrease the activation energy of the ligand exchange reaction by N for some elements, but not for all nitride species. Our study may be utilized toward development of the new efficient method for ALD of nitride thin films with lower thermal budget.

[1] ACS Appl. Electron. Mater. 2021, 3, 999.

7:00pm **TF-WeE-5 Morphology and Statistics of Wet-Etched Gallium Oxides (Doped and Undoped) Deposited by RF Magnetron Sputtering**, ***Jazmyne Smith***, *A. Adedeji,* Elizabeth City State University

Gallium oxide is an ultra-wide energy gap, transparent semiconductor with many potential applications including high power electronics and opto-electronics device fabrications. Doped and undoped gallium oxide thin films were deposited on 2-inch silicon substrates by RF-magnetron sputtering with 200 W rf-power, at substrates temperature of 570°C, chamber pressure of 10 milli-torr, and in Ar/O_2 gas mixtures. Wet etching was achieved with phosphoric acid at elevated temperature. Etch rates of the films were determined with micron sizes circular structures defined by photolithography and diced. Etch rates greater than 180 nm/min were measured with contact profiler. Surface morphology, roughness and atomic composition of etched layers were monitored with Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and Atomic Force Microscopy (AFM). Statistical analysis of the etch rate, issues associated with wet-etching gallium oxide and its sensitivity to dopants and deposition conditions is discussed.

7:40pm **TF-WeE-7 Spectroscopic Evidence of Highly Correlated Electrons in VSe_2**, *T. Yilmaz, E. Vescovo,* National Synchrotron Light Source II, Brookhaven National Lab; *J. Sadowski,* Center for Functional Nanomaterials, Brookhaven National Lab; ***Boris Sinkovic***, University of Connecticut

We present detailed high-resolution angle-resolved photoemission experiments on thin VSe_2 films grown on single-layer graphene (Gr) and highly ordered pyrolytic graphite (HOPG) substrates under various conditions. The surface electronic structure of optimally grown film on HOPG hosts three distinct features: presence- of the energy gap at the Fermi level, a high-temperature spectral kink in the dispersion of the band close to the Fermi level and appearance of the quasiparticle peak in EDC spectra in vicinity of the Fermi level. These observations combined indicate strong electronic correlation that are usually attributed to the presence of the superconducting state. Temperature evolution of the quasiparticle peak and the Fermi gap also follow the trend observed in high-Tc superconductors. Namely, progressive quenching of the quasiparticle peak, which persists up to ~100 K, and presence of the Fermi gap at higher temperatures, vanishing at ~150 K. These observations will aid the future

efforts to induce the high-temperature superconductivity in transition metal dichalcogenides as well as understanding the physics of high-Tc superconductors in general.

8:00pm **TF-WeE-8 Exploring the Magnetoelectric Coupling at the Composite Interfaces of $BaTiO_3/CoFe_2O_4/BaTiO_3$Heterostructures*, Venkata Puli,*** Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; R. Katiyar,* University of Puerto Rico*; A. Reed, M. McConney,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; S. Heidger,* Air Force Research Laboratory, USA, United Arab Emirates

Magnetoelectric multiferroic biphase system with robust ferroelectric and ferromagnetic response at room temperature would be ideally suitable for microelectronic and memory devices and spintronic applications.Multiferroic magnetoelectric $BaTiO_3$-$CoFe_2O_4$-$BaTiO_3$ (BTO/CFO/BTO) heterostructures thin films were synthesized by pulsed laser deposition (PLD) on Pt(111)/TiO_2/SiO_2/Si substrate. High quality PLD thin films were grown by thermal annealing at 750 °C at oxygen partial pressure of 100 mTorr for 1 hour. Crystal quality and phase formation was monitored using X-ray diffraction (XRD), Raman measurements. XRD and Raman spectra examinations confirm the growth of polycrystalline heterostructures and coexistence of both perovskite BTO and spinel CFO phases in heterostructures at room temperature. X-ray diffraction (XRD) patterns and Raman spectroscopy confirms Scanning electron microscopy (SEM) was used to characterize the grain growth and thickness of the heterostructures. The surface quality/rms roughness values of the films were determined by atomic force microscopy (AFM). In order to obtain robust ME coupling at room temperature, we studied the $BaTiO_3$-$CoFe_2O_4$-$BaTiO_3$ (BTO/CFO/BTO) tri-layer structure as a representative FE/FM/FE system. We report the ferroelectric, magnetic and ME properties of BTO/CFO/BTO trilayer nanoscale heterostructures having dimensions 140/80/140 nm, at room temperature. The presence of perovskite BTO and inverse spinel CFO peaks in the PFM and MFM measurements confirmed the ferroelectric and magnetic nature of these films at nanoscale. These nanostructures exhibit low loss tangent, large saturation polarization (Ps ~ 99.86 $\mu C/cm^2$), magnetization (Ms ~ 51.48 emu/cm^3) and a strong magnetoelectric coupling coefficient of~274 mV/cmOe at a bias feld of +90 Oe, at a frequency of 1 kHz at room temperature revealing them as potential candidates for nanoscale multifunctional applications.

8:20pm **TF-WeE-9 Structural stability of 2D II-V compounds*, Lucia Guadalupe Arellano Sartorius,*** The University of Electro-Communications (UEC Tokyo) and Instituto Politécnico Nacional, Mexico*; T. Suga, T. Hazama, T. Takashima,* The University of Electro-Communications (UEC Tokyo), Japan*; M. Cruz Irisson,* Instituto Politécnico Nacional, Mexico*; J. Nakamura,* The University of Electro-Communications (UEC Tokyo), Japan

In recent years, a variety of two-dimensional materials has been investigated and used for the development of new devices. Recently, it has been theoretically revealed that III-V compound semiconductor ultrathin films can exist stably. This structure has been shown to be different from that of a three-dimensional bulk. The ionic and covalent bond formation is thought to contribute to stability. Most of the two-dimensional materials discovered have been obtained as components of three-dimensional crystals that form layered structures, such as graphene. For example, compounds III-VI ultrathin films, which have been synthesized experimentally, are semiconductors with a layered structure in the three-dimensional bulk. Recently, it was reported that three-dimensional ZnSb with a layered structure can be made by electrochemical treatment of ZnSb, an II-V compound semiconductor. It was also theoretically suggested that ZnSb ultrathin films, can exist stably. However, the structural stabilization mechanism of compounds II-V ultrathin films has not been clarified. In this paper, we propose novel 2D materials, II-V compounds with the double bilayer (DB) structure (BeP, BeAs, BeSb, ZnP, ZnAs, ZnSb, CdP, CdAs, and CdSb) through the systematic analysis of electronic properties and phonon stabilities. Two types of DB stacking fashions were identified, which originate from the size effect due to the difference in the size of group II and group V atoms. The structural stabilities of these materials were systematically explained using indices employed in discussions of the stability of surface structures of compound semiconductors so far, the electron counting (EC) model, and the bond orbital (BO) model. It was found that the surface dangling bonds disappeared and stabilized with a semiconducting electronic state. In the III-VI, strong covalent bonds and lone pairs are formed and in group II-V, covalent bonds do not form as strongly as in group III-VI, and the structure changes depending on the difference in atomic radius between group II and group V atoms. However, in addition to the formation of covalent bonds, the ionic interaction between the bilayers is also thought to contribute to the stabilization of the system. In particular, it was shown that the relationship between atomic arrangement and electronic structure could consistently explain thermodynamical stability and stacking fashions.

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