Electronic Materials and Photonics
Room Ballroom BC - Session EM-ThP
Electronic Materials and Photonics Poster Session

**EM-ThP-1 Comparison of Experimental Analysis and Theoretical Calculation of the Lattice Dynamics, Phonon and Vibrational Spectra Dynamics of Titanium Nitride and Oxynitride*, Ikenna Chris-Okoro,* *Sheilah Cherono, Wisdom Akande, Swapnil Nalawade, Mengxin Liu, Barbee Brianna, Brooklyn Jenkins, Ghanashyam Gyawali, Bishnu Bastakoti, Shyam Aravamudhan, J. David Schall, Dhananjay Kumar,* North Carolina A&T State University

Titanium nitride (TiN) and its isostructural oxide derivative, Titanium oxynitride (TiNO) has gained interest in industry as a cost-effective alternative material to noble metals and refractory metals with wide range of applications especially in the optoelectronics and plasmonic. However, there still remain some gaps and disagreement in the literature on specific optical and photoelectrochemical properties of TiN and TiNO, due to difficulty and the varying approach in quantifying defects, vacancies, oxidation state and direct impact of impurities in experimental results.

In this study, thin films of TiN and TiNO were synthesized via pulse laser deposition on sapphire. Structural properties of these thin films were investigated using X-ray Diffraction and Reflection (XRD, XRR), X-ray Photoelectron Spectroscopy (XPS), Rutherford backscattering spectrometry (RBS), Raman Spectroscopy and Fourier Transform Infrared Spectroscopy (FTIR). To corroborate our experimental observations, the phonon dispersions and Raman active modes are calculated using the virtual crystal approximation for rutile TiO_2 and rocksalt TiNO and molecular dynamics simulations were used to calculate the phonon density of states. The results shows that the incorporation of nitrogen atoms does not significantly alter the phonon dispersions of rutile TiO_2. However, it results in the emergence of new phonon modes at approximately 7.128 THz (237.65 cm^{-1}) at the Gamma point, which corresponds to the experimentally observed Multi-Photon Phase-MPP (240 cm^{-1}-R). From the experimental and theoretical studies, a multilayer optical model has been proposed for the TiN/TiNO epitaxial thin films for obtaining individual complex dielectric functions from which many other optical parameters can be calculated.

This work was supported by a DOE EFRC on the Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS) via grant # DE-SC0023415. Part of the work has used resources established by the Center for Collaborative Research and Education in Advanced Materials (CREAM) via NSF PREM grant # DMR-425119 PREM.ML and GG are jointly supported by the CEDARS and CREAM projects.

EM-ThP-2 Reliability Improvement for Nanostructured High Power AlGaAs/GaAs Vertical-Cavity Surface-Emitting Semiconductor Lasers*, Gwomei Wu,* Chang Gung University, Taiwan

The objective of this study has been to develop high power 850 nm vertical-cavity surface-emitting laser (VCSEL) using oxidation confinement technique. The active layer consisted of three pairs of $Al_{0.3}Ga_{0.7}As$/GaAs semiconductor nanostructures and it exhibited a photoluminance emission wavelength of 835 nm. Distributed Bragg reflector mirror nanostructures of 40 pairs in n-type and 21 pairs in p-type were designed to confine the resonance. The multi-layered epitaxial wafers were further processed by photolithography techniques. Inductively coupled plasma etching was employed to create the platform during the mesa process. Various non-oxidized aperture sizes have been achieved by a wet-oxidation method. The experimental results showed that the VCSEL device exhibited low threshold current of 0.6-0.8 mA. The optical output power was about 6.0-6.8 mW at the injection current of 6 mA. The slope of efficiency was found to be about 3.2~3.7 mW/mA. The corresponding voltage was in the range of 1.7~2.1 V. On the other hand, an eye diagram could be clearly observed under the high data rate of 25 Gbit/sec. The response frequency was measured at 17.1 GHz at -3 dB, also at the injection current of 6 mA. In addition, a high thermal conducting AlN (~230 W/m-K) dielectric bonding substrate was employed to improve device reliability. The related electro-optical characteristics would be presented and further discussed.

EM-ThP-3 Singlet Fission from Tetracene and Charge Transfer to Metal Halide Perovskites*, Yutong Ren,* *Antoine Kahn,* Princeton University

Metal halide perovskites (HaPs) have garnered widespread interest for light-harvesting and light-emitting applications due to their exceptional optoelectronic properties and relatively simple fabrication methods. However, like with other semiconductors, HaP-based solar cells lose excess energy through thermalization when absorbing photons with energy that exceeds the absorber bandgap.[1] A promising strategy to reduce these losses and improve photon utilization is to exploit singlet fission, whereby a high-energy singlet exciton formed in an adjacent layer splits into two triplet excitons.[2,3] By transferring these triplet excitons into a HaP film engineered with a composition that aligns the absorber's bandgap closely with the exciton energy, one can effectively harvest this otherwise wasted energy. In our work, we demonstrate that singlet fission in the molecular semiconductor tetracene (Tc) efficiently generates triplet excitons[4] that are energetically matched to the bandgap of a Sn–Pb based HaP, offering a viable pathway toward improved device performance.

In this study, we investigate the electronic structure of Sn–Pb-based HaP films and their interfaces with Tc using ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES). Based on the work by Nagaya et al.,[5] we introduce a second molecular donor, zinc phthalocyanine (ZnPc), at the interface to engineer a more staggered energy alignment between Tc and the perovskite film, thereby promoting an energetically more favorable sequential electron transfer plus formation of a charge transfer (CT) state ($ZnPc^+$ - HaP^-). UPS/IPES measurements suggests that the CT state lies approximately between the Tc triplet energy and the HaPenergy gap, which is favorable for triplet transfer. Complementary photoluminescence (PL) and time-resolved PL (tr-PL) measurements provide guidance for selecting alternative donors with deeper or shallower HOMO levels to replace ZnPc and further refine the interfacial energetics. Moreover, optoelectronic characterization reveals insights into undesirable charge carrier recombination pathways at the organic/HaP interface. Collectively, our results underscore the potential of singlet fission to enhance the efficiency of perovskite solar cells and reduce the cost of the energy that they generate.

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2. Smith, M. B. & Michl, J. *Chem. Rev*. **110**, 6891–6936 (2010).

3. Yost, S. R. et al. *Nat. Chem*. **6**, 492–497 (2014)

4. Geacintov, N., Pope, M. & Vogel, F. *Phys. Rev. Lett.* **22**, 593–596 (1969).

5. N Nagaya et al., arXiv preprint arXiv:2407.21093 (2024)

EM-ThP-4 Nano-Optical Imaging of Plasmon Polaritons in Kagome Metal*, Guangxin Ni,* Florida State University

Scanning near-field Nano-Optical imaging is an invaluable resource for exploring new physics of novel quantum materials. Surface plasmon polaritons and other forms of hybrid light-matter polaritons provide new opportunities for advancing this line of inquiry. In particular, nano-polaritonic images obtained with modern scanning nano-infrared tools grant us access into regions of the dispersion relations of various excitations beyond what is attainable with conventional optics. In this talk, I will discuss this emerging direction of research with example from layered kagome metals and the interesting story from light-matter coupling.

EM-ThP-5 Enhancing ILT with StyleSwin: Reducing Mask Complexity While Preserving Edge Fidelity*, Bosuk Kang,* *Eunil Park,* Sungkyunkwan University (SKKU), Republic of Korea

In semiconductor manufacturing, lithography is a critical process in which the mask (reticle) plays an essential role in accurately transferring patterns. Although Inverse Lithography Technology (ILT) offers a powerful way to optimize masks, it typically incurs high computational costs. To address this challenge, deep learning (DL)–based ILT models have been actively explored, with one notable example, Litho-GAN, reporting a 190× speedup in mask generation compared to traditional methods.

However, many recently proposed GAN-based DL-ILT approaches still encounter limitations due to convolution's restricted receptive field, which can fail to capture sufficient global context and instead focus on local patterns, thereby increasing mask complexity. In response, we introduce an ILT model leveraging the Double Attention mechanism in StyleSwin. By effectively handling both global and local information, our approach maintains the required accuracy while significantly reducing mask complexity.

This study employs LithoBench, a benchmark dataset for evaluating DL-based ILT models. LithoBench contains about 140,000 pattern samples, used to train and assess multiple DL-ILT methods. Its results indicate that the GAN-based DAMO ILT model attains the highest performance. Building on that, we replaced the Deconvolution block in DAMO ILT with the

Transformer-based GAN model, StyleSwin, and developed a modified architecture.

In this work, we replaced the Deconvolution layers in DAMO ILT with StyleSwin Transformer blocks. Specifically, the target pattern context extracted via five convolution layers and four residual connections is fed into three stages of StyleSwin blocks to generate an optimized mask. Each stage contains two double-attention blocks that incorporate a style-latent vector. For evaluation, we used the same MetalSet (metal line patterns) dataset employed in previous studies.

Compared to DAMO ILT, which achieved state-of-the-art (SOTA) results in the LithoBench framework, our proposed model maintains the same edge placement error (EPE=5.2) while reducing the shot count by about 15. By incorporating learnable style-latent injections and double attention at each stage, the model introduces controlled noise at the global pattern level, thereby lowering local mask complexity without sacrificing accuracy. These findings suggest that our method can offer valuable insights for future DL-based ILT applications, potentially enhancing not only accuracy but also mask fabrication processes.

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