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Thin Films Division
Room On Demand - Session TF-Invited On Demand
Thin Film Invited On Demand Session

TF-Invited On Demand-1 Inherent Selective Atomic Layer Deposition Strategies and its Applications, ***Rong Chen,*** Huazhong University of Science and Technology, China **INVITED**

The chemical principal and mechanisms that enable selective atomic layer depositions are gaining rapid growing interests, which have unlocked attractive avenues for the development of novel nanostructures by depositing atoms at desired surface locations. It has found versatile applications in emerging fields beyond semiconductor industry. Yet with the continuing downscaling, it is important to expand approaches for selective ALD with atomic scale precision on nanoscale features. The self-driven selective growth is needed, modifiying specific surface down to atoms, to enable unprecedented capability of tuning the structure-property relationship for emerging applications. In this talk, the inherent selective atomic layer deposition processes will be discussed, including defects modification, selective growth on desired heterogeneity regions, including terraces, step edges, phases etc. of the same material. By choosing the precursors with proper ligands activity, steric hindrance etc., terraces or step edges selectivity can be achieved. The method could control the decoration sites and growth orientations to obtain preferred exposure properties. The developed facet-selective ALD has been used in oxidation of benzyl alcohol to enhance the selectivity and yield of target benzaldehyde products. The selective deposition on the step edges also enhance the nanoparticles' stability under aging treatment, that prevent the atoms at edges from gasifying. The surface originally has local and subsurface irregularity in the lattice matrix, include vacancies, dangling bonds etc. Relies on precursors' preferential adsorptions on those sites, single atoms fabrication can be achieved for highly active CO oxidation catalysis. The selective deposition also enables the defects passivation for photoluminescence applications. The surface defect sites of CsPbBr3 quamtums dots are selectively passivated that the nonradiative decay is effectively suppressed, and extends the exciton lifetime as well as the fluorescence quantum yield. It is a great expansion of ALD beyond semiconductor industry, and helps bridge high accuracy and robustness of bottom up nanofabrication.

TF-Invited On Demand-7 Free-Standing Nanoengineered Functional Oxides Thin Films, *P. Salles, I. Caño,* ICMAB-CSIC, Spain*; R. Guzman,* School of Physical Sciences and CAS Key Laboratory of Vacuum Physics ; University of Chinese Academy of Sciences, China*; W. Zhou,* School of Physical Sciences and CAS Key Laboratory of Vacuum Physics, University of Chinese Academy of Sciences, China*;* ***Mariona Coll,*** ICMAB-CSIC, Spain **INVITED**

Complex oxides are of great interest for their rich variety of chemical and physical properties including magnetism, ferroelectricity, multiferroicity, catalytic behavior, and superconductivity. Up to date, the preparation of crystalline complex oxide thin films has been mainly limited on substrates that can stand high temperature thermal treatments and on single crystal substrates when epitaxial growth is pursued. These requirements dramatically limit their applicability excluding the possibility to prepare many artificial multilayered architectures to investigate emergent phenomena that arise in thin films and at their interfaces. To tackle this bottleneck, herein, we will present a facile and sustainable chemical route to prepare water-soluble epitaxial $Sr_3Al_2O_6$ thin films to be used as sacrificial layer for future free-standing epitaxial complex oxide manipulation. Two solution processes are put forward based on metal nitrate and metalorganic precursors to prepare dense, homogeneous and epitaxial $Sr_3Al_2O_6$ thin films that can be easily etched by milli-Q water. [1] Thorough investigation of the precursor-solvent compatibility, thermogravimetric analysis and film crystallization is performed. Additionally, we demonstrate the viability of $Sr_3Al_2O_6$to subsequently prepare and transfer a wide variety of atomic layer deposited functional oxides (Al_2O_3, Co_3O_4, Fe_2O_3, $CoFe_2O_4$, $BiFeO_3$) on arbitrary substrates ranging from flexible polymers to silicon substrate. This robust and low-cost procedure could be adopted to prepare a wider family of thin film compositions to fabricate artificial heterostructures and 2D materials with monolayer by monolayer control to go beyond the traditional electronic, spintronic, and energy storage and conversion devices.

[1] P. Salles, M.Coll et al. Adv. Mater. Interf, (2021), 8, 2001643

TF-Invited On Demand-13 A Comparative Study on the Heteroleptic Ti Precursors for ALD of TiO_2: DFT Calculations and ALD Experiments, *H. Kim, R. Hidayat, S. Kim, J. Kim, Y. Choi,* ***Won-Jun Lee,*** Sejong University, Korea (Republic of) **INVITED**

Titanium oxide (TiO_2) has been an attractive material with interest for various applications, including photocatalysts, optical coatings, and the high-permittivity dielectrics of DRAM capacitors. The atomic layer deposition (ALD) technique is used to deposit thin films with excellent step coverage, accurate thickness control, and excellent film quality. The most common precursors for the ALD of TiO_2 were tetrakis(dimethylamido)titanium (TDMAT) and titanium tetraisopropoxide (TTIP). However, they showed low ALD temperatures because of their insufficient thermal stability. In general, the higher the deposition temperature, the better the physical and electrical properties of the dielectric film. Therefore, Ti precursors with better thermal stability and reasonable reactivity are requested. The thermal stability of the Group 4 metal (Ti, Zr, Hf) precursors can be improved by introducing a "spectator ligand," cyclopentadienyl (C_5H_5, Cp). Stabilizing ability of the Cp ligand can be further enhanced by Me-substitution [1]. In the present work, we compared the thermal stability and reactivity of heteroleptic Ti precursors by density functional theory (DFT) calculations and the ALD experiments. Thermolysis reactions of precursors were simulated, and the ALD temperature windows and the film densities were investigated. The surface reactions of the precursors were simulated, and the saturation dose and step coverage were investigated. Compounds with a different "spectator ligand," such as Cp, Me_5Cp, or linked amido-Cp, were compared. Compounds with different "actor ligands," dimethylamido or methoxy, were also compared. The introduction of a linked ligand or Me_5Cp enhanced the thermal stability compared to introducing a Cp ligand, and the precursor with methoxy ligands showed better reactivity than the precursor with dimethylamido ligands.The underlying mechanisms for better stability or reactivity were described by DFT simulation.

[1]J.-P. Niemelä et al.,Semicond. Sci. Technol. 32 (2017) 093005.

TF-Invited On Demand-19 Refractive Index Control of Highly Anisotropic 2D Materials, *J. Caldwell,* ***Mingze He,*** Vanderbilt University **INVITED**

Two-dimensional materials are inherently anisotropic – with strong bonding in-plane and weak bonding out-of-plane. Consequently, their optical properties are birefringent, particularly at frequencies of the optically active infrared phonons. At these frequencies, the strong optical anisotropy results in hyperbolicity, where the permittivity tensor along at least one axis is negative, while at least one is positive. Hexagonal boron nitride (hBN) is an exemplary material in this regard. Materials which exhibit hyperbolicity can support volume-confined polaritonic modes, which have a wavelength much shorter than that of light in free space. Such spatially compressed modes have important implications for IR technologies, as they may be utilized to create planar meta-optics that are much more compact than the current state of the art. In particular, 2D materials can be used to realize metasurfaces, capable of shaping both nearfield- and far field light waves for a broad range of applications.

Conventional metasurface designs use geometrically fixed structures, or materials with excessive propagation losses, thereby limiting their potential applications. Here demonstrate that this can be overcome through the realization of a reconfigurable hyperbolic metasurface comprising a heterostructure of isotopically enriched hexagonal boron nitride (hBN) in direct contact with the phase-change material (PCM), such as single-crystal vanadium dioxide (VO2) or GST. Here, the metallic and dielectric domains in PCM provide spatially localized changes in the local dielectric environment that modify the polariton wavelength supported in hBN by a factor of 1.6. Using this platform, we demonstrate the first reduction to practice of in-plane HPhP refraction, and the means for launching, reflecting and transmitting of HPhPs at the PCM domain boundaries. Ultimately, this phenomenon can be used to create planar refractive optics, such as lenses or waveguides, but on length scales far below the diffraction limit. Further, my employing doped semiconductor materials with controllable plasma frequencies, such direct control of hyperbolic polaritons can also be obtained via modification of the free carrier density of the underlying semiconductor

TF-Invited On Demand-25 Microscopic Mechanisms and Applications for Remote Epitaxy of Iii-vs and Heusler Compounds, ***Jason Kawasaki,*** University of Wisconsin - Madison **INVITED**

Remote epitaxy, i.e., epitaxial growth through a semi lattice-transparent monolayer material such as graphene, has emerged as a promising alternative that circumvents some of the limitations of conventional

epitaxy directly on a crystalline substrate. However, the microscopic mechanisms for remote epitaxy remain unclear, in particular, the role of point and extended defects in graphene. In this talk, I will describe our understanding of the mechanisms based on in-situ electron diffraction, photoemission, atomic force microscopy, and photoemission electron microscopy (PEEM). I will begin with experiments on the model system GaAs on graphene/GaAs (001), grown by molecular beam epitaxy (MBE), and describe recent efforts for the growth of Heusler compounds on graphene-terminated Al2O3 (0001). I will also describe one particularly promising application: our observation of strain-induced magnetism in rippled Heusler membranes that are exfoliated from graphene [1]. This work was supported by the ARO (W911NF-17-1-0254), AFOSR (FA9550-21-1-0127), DARPA (0011940523), and NSF (DMR-1752797).

[1] D. Du, et. al. arXiv:2006.10100 (2020)

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