ALD for Manufacturing
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ALD for Manufacturing Poster Session

AM5-1 Development of MeCpPtMe3 Platinum Process by Rotary Type Reactor Atomic Layer Deposition on Powders*, **Min Jong Kil**, S. Yoon,* Korea Electronics Technology Institute, Korea (Republic of)*; S. Jung,* Gachon University, Korea (Republic of)*; H. Kim,* Korea Electronics Technology Institute, Korea (Republic of)*; T. Kim,* Gachon University, Korea (Republic of)*; H. Kim,* Korea Electronics Technology Institute, Korea (Republic of)

Atomic layer deposition has been widely studied to deposit materials with optimized usage and conformal coating on various applications such as semiconductor, energy storage/conversion devices, and catalyst. However, conventional atomic layer deposition is not suitable for powders or (nano)particles to coat materials with static processes. Therefore, atomic layer deposition for powders is developed in two types: fluidized bed reactor and rotary type reactor. At first, vertical fluidized bed reactor type atomic layer deposition was developed to conformally coat on (nano)particles. However, to develop the excessive usage of precursors in fluidization method, horizontal rotary type atomic layer deposition is developed to optimize the usage of precursor, especially noble metal precursors. To coat materials by powder atomic layer deposition, optimization of precursors and agglomeration/breakage of powders are required to achieve atomic layer deposition mode. In this study, process optimization and powder agglomeration/breakage are solved using rotary reactor type atomic layer deposition with MeCpPtMe3 platinum precursor and oxygen. For process optimization, each step pulse time is controlled with stop valve mode on silicon wafer. Using this optimized process, powder agglomeration/breakage is achieved by controlling ball type, size, and rotation speed. Platinum process optimization is achieved by X-ray reflectometry for thickness and density. Conformal coating on powders is confirmed by transmission electron microscopy and energy dispersive X-ray spectroscopy. This optimized process is applied to the biomass-derived graphene-based carbon to confirm the performance difference between conventional atomic layer deposition and powder atomic layer deposition. These results are expected to be valuable for atomic layer deposition on nanoparticles.

AM5-2 Nanoscale Film Thickness Gradients Printed in Open Air by Spatially Varying Chemical Vapor Deposition*, **Jhi Yong Loke**,* University of Waterloo, Canada

Nanoscale films are integral to all modern electronics. To optimize device performance, researchers vary the film thickness by making batches of devices, which is time-consuming and produces experimental artifacts. We present thin films with nanoscale thickness gradients that are rapidly deposited in open air for combinatorial and high-throughput (CHT) studies. Atmospheric pressure spatial atomic layer deposition reactor heads are used to produce spatially varying chemical vapor deposition rates on the order of angstroms per second. We printed ZnO and Al2O3 films with nm-scale thickness gradients in as little as 45 seconds and performed CHT analysis of a MIM diode and perovskite solar cell. By testing 360 Pt/Al2O3/Al diodes with 18 different Al2O3 thicknesses on a single substrate, we identified a thicker insulator layer (6.5 to 7.0 nm) for optimal diode performance than has been reported previously. An Al2O3 thin film encapsulation layer was deposited by atmospheric pressure chemical vapor deposition (AP-CVD) on a perovskite solar cell stack for the first time and a convolutional neural network was developed to analyze the perovskite stability. The rapid nature of AP-CVD enables thicker films to be deposited at a higher temperature than is practical with conventional atomic layer deposition. The CHT analysis showed enhanced stability for 70 nm encapsulation films.

AM5-5 Measurements and Prediction Model for the Evaporation of Bis(diethylamino)silane*, **Seung-Ho Seo**, E. Shin, Y. Lee, D. Kim, H. Shin,* GO Element, Korea (Republic of)*; C. Kim, W. Lee,* Sejong University, Korea (Republic of)

In ALD and CVD processes, the evaporation rate of the precursor affects the growth rate of the thin film. Therefore, a sufficient amount of the precursor must be continuously supplied to the reactor, and it is important to measure and predict the amount of precursor supply in an actual ALD system. The amount of precursor supply varies depending on the structure and temperature distribution of the precursor delivery system including the canister, the type of precursor, and the flow rate of the carrier gas. Recently, a nondispersive infrared (NDIR) gas analyzer was installed in the canister outlet pipe to measure the partial pressure of a Ta precursor, and the evaporation amount of the precursor was calculated [1]. However, in order to accurately predict precursor evaporation, it is necessary to measure the precursor partial pressure and temperature inside the canister.

In the present study, we measured the evaporation amount of a liquid silicon precursor, bis(diethylamino)silane (BDEAS), under various conditions and presents a model to predict the evaporation amount of the precursor. In order to accurately understand the evaporation characteristics, we measured the pressure and the temperature inside the canister were measured, not in the delivery line. We also measured the evaporation amount of BDEAS in real-time using an ultrasonic level sensor installed at the bottom of the canister. To predict the evaporation amount of the liquid precursor, the evaporation coefficient was calculated using the Hertz-Knudsen-Langmuir equation. The predicted evaporation amount of the precursor agreed well with the measurement result. The construction of the precursor evaporation prediction model is expected to be used to optimize the precursor delivery system design and the ALD process condition.

[1] B. A. Sperling et al., J. Vac. Sci. Technol. A 37, 060907 (2019).

AM5-6 Interface Modification of Bismuth by Atomic Layer Deposition: Enhanced Thermoelectrical Performance*, **Shiyang He**, A. Bahrami, K. Nielsch,* Leibniz Institute for Solid State and Materials Research, Germany

Interfaces of phase boundaries play a critical role in the carrier/phonon transport in thermoelectric materials. It remains a big challenge to control over both chemical composition and dimension of interfaces precisely by traditional approaches. Herein, a strategy of interfaces modification based on powder atomic layer deposition (PALD) is introduced to accurately control and modify the phase boundaries of pure Bismuth (Bi). To demonstrate the effect of this strategy, ultrathin layer of Al_2O_3 is uniformly deposited on Bi particles. It is observed that 5 cycles deposition of Al_2O_3 significantly scattered the phonons and 10% reduction on thermal conductivity in Bi-Al_2O_3 system can be achieved. Owing to the carrier scattering in the Bi-Al_2O_3 system, the electrical conductivity decreased from 5700 S/cm to 4500 S/cmfor 5 cycles coated Bi. However, the Seebeck coefficient increases from -69 μV/K to -78 μV/K which results in high power factor. Thanks to the precisely interface modification, a maximum *zT* of 0.13 with 5 cycles deposition of Al_2O_3 at 300 K is obtained, which is 11.2% higher compared with that of pure Bi. As a powerful interfacial modification strategy, PALD-based approach can be extended to other thermoelectric material system simply, which may contribute to the development of high-performance thermoelectric materials.

AM5-9 Low Resistivity Titanium Nitride Thin Film Fabricated by Atomic Layer Deposition on Silicon*, **Cheng-Hsuan Kuo**,* UC San Diego, Taiwan*; V. Wang, z. zhang, H. Kashyap, A. Kummel,* UC San Diego

Titanium nitride (TiN) thin films areutilized as the diffusion barriers for Co and W metal layers as well as the gate metal barrier in CMOS and memory devices due to their low resistivity and good electrical conductivity. TiN is also used as a coating for hard disk drives[1].Low resistivity TiN has been deposited in commercial devices by plasma enhanced ALD (PEALD) and by physical vapor deposition. However, for high aspect ratio features, deposition by thermal ALD is needed because of the high conformality of the thermal ALD process and for back-end compatible deposition below 350 °C.Previously Wolf *et al.* demonstrated that at 400 °C, ALD of TiN with $TiCl_4$ and N_2H_4 resulted in a film with a resistivity of 500 mohm-cm[2].In this work, it is shown that the resistivity can be decreased below 200 mohm-cm when deposited at 300 °C - 350 °C by reducing the oxygen in the films.

Titanium tetrachloride ($TiCl_4$) and anhydrous hydrazine (Rasirc, Brute Hydrazine[Ò]) were employed as the precursors with ultra-high purity nitrogen purge gas. To produce low resistivity films, a turbo molecular drag pump (Edwards EPX) was employed to maintain a high compression ratio during ALD pulsing. The TiN ALD chamber was connected to an *in-vacuo* Auger electron spectrometer (RBD Instruments), which was used to determine the atomic composition of ALD TiN after 50 cycles of deposition. Pulse lengths and purge times were optimized at sample temperatures of 300 °C and 350 °C on HF-cleaned Si (100) or degreased SiO_2; the optimized pulse times were 300 ms for $TiCl_4$ and 2400 ms for N_2H_4. Surface morphology was measured by *ex-situ* atomic force microscopy (AFM). To determine resistivity, four-point probe (Ossila) measurements were performed on TiN thin films on degreased SiO_2 substrates. Scanning electron microscopy (SEM), ellipsometry, and X-ray reflectivity (XRR) were used to measure TiN film thicknesses.

AM5-12 Morphology-Controlled MoS_2 by Low-Temperature Atomic Layer Deposition, ***Chengxu Shen**, M. Raza, P. Amsalem, T. Schultz, N. Koch, N. Pinna,* Humboldt-Universität zu Berlin, Germany

Two-dimensional (2D) transition metal dichalcogenides (TMDs) such as MoS_2 are materials for multifarious applications such as sensing, catalysis, and energy storage.[1] Due to their peculiar charge-transport properties, it is always desired to control their morphologies from vertical nanostructures to horizontal basal-plane oriented smooth layers.[2] Due to the high conformality, atomic layer deposition (ALD) exhibits promising potential in the precise control of the thickness and morphologies of the deposited layers, especially for the preparation of complex nanostructure.[3]

In this work, we established a low-temperature ALD process for MoS_2 deposition using bis(t-butylimino)bis(dimethylamino)molybdenum(VI) and H_2S precursors. Polycrystalline MoS_2 is conformally deposited on carbon nanotubes, Si-wafers, and glass substrates. Moreover, the morphologies of the deposited MoS_2 films are tuned from smooth film to vertically grown flakes, and to nano-dots, by controlling the reaction parameters/conditions and post sulfurization process. Noticeably, the deposited MoS_2 nanostructures show morphology-dependent optical and electrocatalytic properties, allowing us to choose the required morphology for a targeted application.

[1]T. Jurca, M. J. Moody, A. Henning, J. D. Emery, B. Wang, J. M. Tan, T. L. Lohr, L. J. Lauhon, T. J. Marks, *Angew. Chem. Int. Ed. Engl.***2017**, 56, 4991.

[2]C. Shen, M. H. Raza, P. Amsalem, T. Schultz, N. Koch, N. Pinna, *Nanoscale***2020**, 12, 20404.

[3]C. Marichy, M. Bechelany, N. Pinna, *Adv. Mater.***2012**, 24, 1017.

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