Atomic Scale Processing Focus Topic
Room Ballroom A - Session AP-TuP
Atomic Scale Processing Poster Session

AP-TuP-1 A Computational and Experimental Investigation of Platinum Vapor Deposition Reactions on Oxygen and Nitrogen Functionalized Carbon, *I. Campbell, N. Nayir,* Penn State University*; S. Kuespert, N. Ortlieb, A. Fischer,* University of Freiburg, Germany*; A. Van Duin,* ***Suzanne Mohney***, Penn State University

Nitrogen-doped carbons are useful as supports for catalysts due to their low cost, low density, and enhanced metal-support interaction. We used density functional theory (DFT) to evaluate the effects of N-doping and oxidation of graphene on the adsorption and dissociation of trimethyl (methylcyclopentadienyl) platinum ($MeCpPtMe_3$), which is commonly used for synthesizing platinum nanoparticles and films by chemical vapor or atomic layer deposition. We confirmed that oxygen incorporation in graphene via oxidation of monovacancies is thermodynamically favorable with and without N doping and discovered that N doping elongates substrate-oxygen bonds, indicating increased reactivity of the oxygen atoms bound to the substrate. According to nudged elastic band calculations, the transfer of a Me ligand from $MeCpPtMe_3$ to oxidized substrates with and without N-doping displays positive enthalpies of reaction and activation energies, making Me transfer a rate determining step. However, nitrogen doping thermodynamically and kinetically drives the Me dissociation reactions by lowering the enthalpies and activation energies of the reactions. We also showed that the dissociation of $MeCpPtMe_3$ and subsequent adsorption of Me and $MeCpPtMe_2$ on identical oxidized monovacancies is endothermic but is made exothermic by pyridinic N dopants. Thus, the adsorption and dissociation of $MeCpPtMe_3$ is expected to occur more readily on N-doped substrates than undoped ones. We also experimentally demonstrated that elevated N and O content in mesoporous carbon supports causes $MeCpPtMe_3$ to deposit more platinum but only at increased temperature (300 °C).

AP-TuP-2 Subtractive Printing of Atomic Layer Deposition using Electrohydrodynamic Jet Printing, ***Tae Cho***, *N. Farjam, K. Barton, N. Dasgupta,* University of Michigan, Ann Arbor

Traditional lithography requires multiple processing steps in a resource-intensive cleanroom environment. To overcome the limitations of traditional lithographic patterning and alignment, there has been tremendous interest in developing new methods for additive manufacturing. E-jet printing is an additive manufacturing technique which allows for fast and versatile printing with high resolution. Previously, e-jet printing was used to directly deposit functional materials on the surface with solution inks. Compared to this, ALD can deposit high-quality materials with unparalleled control of film thickness and uniformity at relatively low temperatures.

Our previous work has shown that by directly printing inhibitor polymers on the surface, we can locally activate/passivate atomic layer deposition (ALD) growth for area-selective ALD (AS-ALD) [1,2]. This technique allows customizable patterns with different geometries and high resolution without the need for premade alignment masks. However, AS-ALD may suffer from defect growth and/or vapor-phase-infiltration through the inhibitor polymers which can cause undesired growth on the surface. In this study, we demonstrate the use of subtractive electrohydrodynamic jet (e-jet) printing with acid-based ink to directly pattern the metal oxides deposited with ALD.

To pattern 50 nm thick ALD ZnO that was deposited on the silicon substrate, 0.1M hydrochloric acid mixed with glycerol was used as the ink for e-jet printing. When the ink was printed, glycerol residue was left behind on the surface after ink evaporation. After soaking the sample in water, the glycerol residue was washed away with ZnO; ZnO was removed on the printed regions, exposing the underlying silicon surface. Atomic force microscopy, scanning electron microscopy, and energy dispersive spectroscopy were performed to analyze the surface topology/chemistry after patterning the ZnO layer. With e-jet, linewidth and etched depth can be precisely controlled with printing speed and the number of printed layers. This new technique can provide flexible and customizable patterning of metal oxides without the need for AS-ALD or lithography.

[1] T.H. Cho, N. Farjam, C. R. Allemang, C. P. Pannier, E. Kazyak, C. Huber, M. Rose, O. Trejo, R. L. Peterson, K. Barton, N. P. Dasgupta, *ACS Nano* **14**, 17262 (2020)

[2] N. Farjam, T.H. Cho, N. P. Dasgupta, K. Barton, *Appl. Phys. Lett.***117**, 133702 (2020)

[3] T. H. Cho, N. Farjam, K. Barton, N. P. Dasgupta, *In preparation* (2022)

AP-TuP-4 Design of Gas Flow Field for a Sustainable ALD Process Chamber, ***Kyung-Hoon Yoo***, Korea Institute of Industrial Technology (KITECH), Republic of Korea*; G. Song,* KUMYOUNG ENG Inc., Republic of Korea*; C. Kim,* TNG Co., Republic of Korea*; J. Hwang, H. Lee,* Korea Institute of Industrial Technology, Republic of Korea*; K. Lee,* SAMSUNG DISPLAY, Republic of Korea

In order to develop a sustainable ALD process cluster tool, it is necessary to establish a manufacturing technology for a high-productivity high-efficiency ALD process chamber that reduces the intrinsic excessive consumption of energy and materials.[1] In the present study, as the part of countermeasure to the excessive consumption, a micro-gap ALD process chamber is considered for the optimized design. The changes in the flow field of nitrogen in the process space of the process chamber with the gap sizes of 1 mm and 10 mm respectively are observed at 200 °C, utilizing computational fluid CFD numerical analysis. For the present nitrogen flow field with a background pressure of 1 Torr and a temperature of 200 °C, the Knudsen number Kn<0.1 and Reynolds number Re<<2300 are evaluated, and consequently the continuity and momentum equations of a steady-state compressible laminar flow field are considered.[2]

Acknowledgment

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References

[1] C.Y. Yuan and D.A. Dornfeld, 2010, *J. of Manufacturing Science and Engineering*, 132, 030918 (2010).

[2] M. R. Shaeri, T.-C. Jen, C. Y. Yuan and M. Behnia, *International Journal of Heat and Mass Transfer*, 89, 468 (2015).

AP-TuP-5 Atomic Structure Characterization of PEALE Semiconductors by Using HRSTEM, ***Chien-Nan Hsiao***, *C. Chen,* National Applied Research Laboratories, Taiwan*; W. Chen,* National applied research Laboratories, Taiwan*; F. Chen,* National Applied Research Laboratories, Taiwan

An in-situ plasma enhanced atomic layer etching system has been design and fabricated. N_2O , BCl_3 and Ar plasma were used as the precursor for advanced semiconductor at various temperature. The optical detector was used to in-situ monitor the plasma spectrum during the step by step etching process. The AlGaN/GaN hetrostructure and MoS2 2D materials etching per cycle of ALE were investigated using an aberration-corrected scanning transmission electron microscope with energy distribution spectrometer. It is found that the layer by layer etching feature shows the process is a controlled self-limited reaction. The saturation curve of atomic etching rate and precursor pulsed time has been established. The etching per cycle of AlGaN is around 0.33 nm.In addition, the influence of various aberration coefficients such as defocus, astigmatism, coma, spherical aberration and star aberration on the shape of the probe and more importantly on the electron intensity distribution within the probe was calculated. The accuracy required for compensation of the various aberration coefficients to achieve sub-angstrom resolution (0.078 nm) with the electron optics system was evaluated by the calculation of phase shift. The (100) lattice spacing of MoS2 2D materials is around 0.274nm.

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