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Elucidating the Mechanisms for Atomic Layer Growth through In Situ Studies

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ABSTRACT Atomic Layer Deposition (ALD) provides exquisite control over film thickness and composition and yields excellent conformality over large areas and within nanostructures. These desirable attributes derive from self-limiting surface chemistry, and can disappear if the self-limitation is removed. Understanding the surface chemical reactions, i.e. the ALD mechanism, can provide insight into the limits of self-limitation allowing better control, successful scale up, and the invention of new processes. In situ measurements are very effective for elucidating ALD growth mechanisms. In this presentation, I will describe investigations into the growth mechanisms of ALD nanocomposite films comprised of conducting (e.g. W, Mo and Re) and insulating (e.g. Al_2O_3, ZrO_2 and TiO_2) components using in situ measurements. These ALD nanocomposites have applications in particle detection, energy storage, and solar power. We have performed extensive in situ studies using quartz crystal microbalance (QCM), quadrupole mass spectrometry (QMS), Fourier transform infrared (FTIR) absorption spectroscopy, and current-voltage measurements. These measurements reveal unusual ALD chemistry occurring upon transitioning between the ALD processes for the two components. This results in unique reaction products that affect the properties of the films in beneficial ways. The knowledge gained from our in situ studies of the ALD nanocomposite films has helped us to overcome problems encountered when we scaled up the ALD processes to large area substrates. Beyond fundamental understanding, in situ measurements are extremely effective in ALD process development and process monitoring. I will end my talk by describing our recent work combining in situ measurements and machine learning to accelerate ALD process development.

BIO **Jeff Elam** is a Senior Chemist and Group Leader at Argonne National Laboratory where he directs a program in atomic layer deposition (ALD) technology with the goal of developing new applications for ALD in fields such as solar power, energy storage, water remediation, and large-area detectors. Jeff earned his B.A. in Chemistry from Cornell University and his Ph.D. in Physical Chemistry from the University of Chicago. As a Postdoctoral Researcher at the University of Colorado, Jeff developed ALD thin film growth methods. Dr. Elam has authored over 250 papers and is an inventor on over 100 patents and inventions related to ALD. Jeff won the ALD Innovation Award in 2017, and has received five R&D100 Awards including the Editor's Choice Award for "Oleo Sponge", the top invention in 2017. Dr. Elam is an AVS Fellow, and is involved in chairing and organizing sessions at AVS and ECS.

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