Relation between nucleation mechanism and mechanical properties of ALD/MLD grown Cu thin films with interfacial gradients on soft materials.

NuMeCu

Atomic & Molecular Layer Deposition (ALD & MLD) have recently emerged as top techniques for obtaining ultrathin films with the precision at the atomic level. The ALD cycle is composed of two subsequent pulses of precursor gases interacting with the substrate, separated by the pulse of a purge gas. By properly selecting chemistry for precursor gases almost any film material on a given type of substrate with highly uniform 3D conformality can be fabricated. This is the unique advantage of ALD and MLD with respect to more standard deposition techniques such as PVD or CVD. Although ALD and MLD are generally more expensive, they have been already commercially implemented in application fields using microelectronics, solar cell devices, high k-transistors, and anti-reflective glass coatings. Whereas most of the deposited materials include metal oxides, the deposition of uniform thin metal films still remains a challenge. It is especially the case when using soft materials as film substrates as in foldable electronic devices but also in the emerging field of **soft biorobotics**. Future devices for health monitoring and implants, sensors integrated into textiles, and flexible displays will need to work in environments with harsh conditions and be durable to stretching, twisting or folding. Copper as one of the best electrical conductors is among the most demanded material for ultrathin film deposition on soft substrates, which requires the deposition to be carried out at low temperatures.

Recent studies reported successful Cu ALD of thin films using reducing agents of hydroquinone, $Zn(Et)_2$, and hydrogen plasma at temperatures below 150 Celsius degrees, which are adequate for organic substrates. Although the underlying principle of the self-limiting surface reactions in ALD & MLD is rather simple, the dissociative chemisorption of gas molecules on the substrate and deposit surface evolves into complex phenomena of interface bond formation, nucleation, and further film growth. They strongly affect the adhesion of the metal Cu film and its mechanical properties with respect to fracture toughness.

To unravel the exact mechanisms of Cu film nucleation and growth, we propose the complementary study of the interface formation by means of ***in-situ experiments*** with synchrotron radiation, transmission electron microscopy (TEM) studies of the interface, and ***atomic-scale simulations*** (DFT). Soft X-ray absorption spectroscopy using the total electron yield and X-ray photoelectron spectroscopy are surface sensitive techniques that give insight into the deposition process, providing details of the early stages of growth – the nucleation and enable to identify the type of created bonds. The DFT calculations allow for in-depth look into the reaction paths at the atomic level. This part of investigation will help to better understand mechanisms behind the evolution of the microstructure during the thin film growth: the operation of different precursor gases during deposition and chemical reactions that are in control. On the macroscopic level a detailed experimental study on the ***mechanical properties*** will be performed to correlate the previously collected information about the interface and film structure with the film's adhesion, strength, fracture toughness, and hardness. The output of the mechanical experiments will feed back into the design of interfacial gradients between the polymer and metal film by using the inherent atomic precision of ALD & MLD for optimized adhesion and strength of metallic films on polymers.

Overall, the project tackles the subject of metal deposition on soft materials from several perspectives of materials science, chemistry and physics: (i) the synthesis of thin films and interface gradients with monolayer precision techniques of ALD and MLD, (ii) the characterization by in-situ synchrotron chemical analysis of interfacial bond formation and ex-situ TEM observations, (iii) atomistic modelling, and (iv) the correlation of internal film structure to the mechanical robustness. With this comprehensive materials science approach inherent to successful materials development, we want to ensure the optimization of copper film on soft materials being critical for production of reliable devices in future flexible electronics.