

# Inherent Area-Selective Deposition of Low-resistivity Molybdenum Carbide Films by Thermal Atomic Layer Deposition

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With the ongoing downscaling of logic and memory devices, one of the main challenges has emerged such as edge placement error issues resulting from top-down patterning. To overcome the limitations of lithography, a recent focus in bottom-up patterning is based on area-selective atomic layer deposition (AS-ALD) [1,2]. Numerous studies have investigated AS-ALD that employed precursor inhibitors such as SAMs or SMIs to prevent precursor adsorption in non-growth areas. However, there is an increasing need for research into inherent AS-ALD strategies, which exploit the intrinsic properties of substrates with the chemical adsorption of the precursor to enable selective adsorption at targeted surface sites. Molybdenum carbide (MoC<sub>x</sub>) has attracted as promising materials for metallization [3,4], particularly as bottomless diffusion barriers, liners, capping layers, and interconnects, due to their high melting points, low resistivity, excellent thermal stability, and low reactivity with Cu and its area selective deposition methods have been requiring.

In this work, we developed conductive MoC<sub>x</sub> films via thermal ALD without the use of halogen-based precursors, at the deposition temperatures of 200–300 °C. This process enabled area-selective growth of MoC<sub>x</sub> films on metallic substrates (TiN, Ru, Cu) over oxide substrates (SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>) by utilizing the intrinsic chemical adsorption of the precursor. We investigated the crystallinity, chemical bonding states, impurity, and resistivity of the MoC<sub>x</sub> films (Fig. 1), and evaluated the selectivity between substrates through analysis of Mo areal density and film thickness. Moreover, the selective growth of MoC<sub>x</sub> films on metallic substrates was demonstrated on metal/dielectric patterns using auger electron spectroscopy (AES) mapping and energy-dispersive X-ray spectroscopy (EDS) analysis, indicating the feasibility of implementing this process in practical device applications (Fig. 2). To elucidate substrate-dependent surface chemistry in MoC<sub>x</sub> AS-ALD, density functional theory (DFT) calculations were conducted, revealing the relative adsorption energies of Mo precursor between metal and dielectric substrates (Fig. 3). In conclusion, a newly developed inherent AS-ALD of MoC<sub>x</sub> films presents a promising alternative to top-down processes, offering a simplified workflow and potential conducting materials for advanced metallization.

## References

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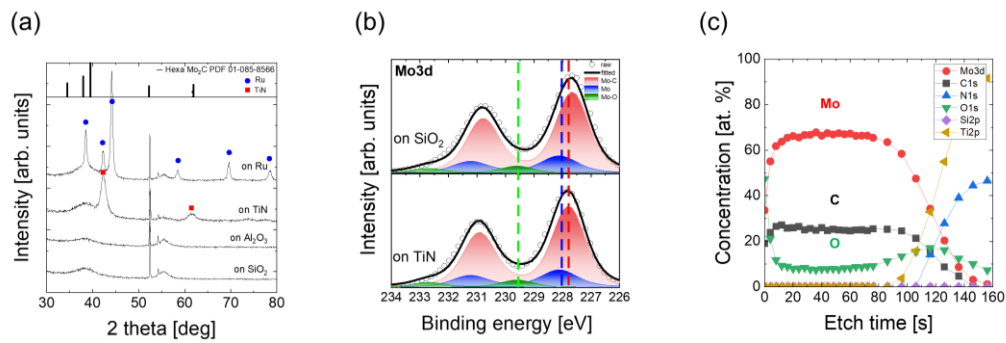


Figure 1 (a) GIXRD patterns of MoC<sub>x</sub> films depending on metal and dielectric substrate, (b) XP spectra of Mo 3d for MoC<sub>x</sub> films on SiO<sub>2</sub> and TiN substrate, (c) The XPS depth profiling for atomic concentration of MoC<sub>x</sub> films

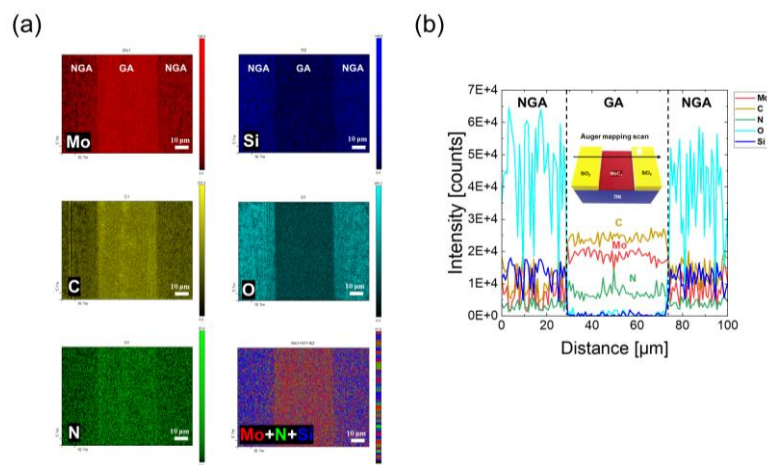


Figure 2 (a) Auger elemental mapping images and (b) auger line scan in a lateral direction of MoC<sub>x</sub> films on SiO<sub>2</sub>/TiN patterned substrates

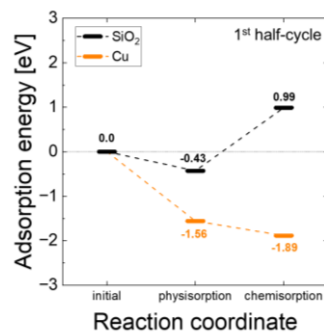


Figure 3 The adsorption energy of Mo precursor depending on the substrates for 1<sup>st</sup> half-cycle