Investigating Al-CVD using DMEAA: Experiments and modeling of the kinetics and the surface roughness

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Al growth from the gas phase results in thin films with advantageous properties such as low electrical resistivity and quasicrystalline phases with strong technological potential. Chemical Vapor Deposition (CVD) is often used for this purpose, because it ensures film growth with tunable microstructure and deposition rates and provides highly conformal coverage of complex surfaces. The a priori choice of the DMEAA precursor is dictated mainly by low deposition temperatures and its oxygen and carbon free ligands allowing co-deposition with oxophilic elements such as Fe and Cu. The deposition rate as a function of the substrate temperature is experimentally determined in order to construct the Arrhenius plot of the process, with depositions performed at 10 torr, in a vertical, warm wall MOCVD reactor, in the temperature range 140 ºC - 240 ºC. Investigation of the surface morphology of the films includes SEM characterization of the films and roughness measurements by means of optical interferometry.

Aiming at understanding the mechanisms of Al film growth and propose a kinetic scenario for the process, a predictive, macroscopic 3D model of the CVD reactor is built, based on the mass, momentum, energy and species transport equations. According to previous works[1], two reactions, a volumetric and a surface one, are responsible for the deposition of Al. The activation energy of the surface reaction, calculated from the experimental measurements, is incorporated in the computations through an Arrhenius-type formula for the kinetics of the surface reaction. The equations set, augmented with realistic boundary conditions, is discretized and solved with the computational fluid dynamics software Ansys/Fluent[2].

The growth of roughness on the film during Al deposition on an Al(111) surface, is analyzed with microscopic simulations based on the kinetic Monte Carlo (kMC) method. The developed kMC algorithm considers a simple cubic lattice, allows for first nearest-neighbor interactions only, employs the solid-on-solid approximation and accounts for three events, namely adsorption, desorption and migration of the adatoms on the surface[3].

The experimental measurements and the computed theoretical predictions of Al deposition rates and roughness growth are compared along the wafer's radius and for various substrate temperatures, i.e. at the different growth regimes. The comparison is satisfactory and calls for additional microscopic computations for strengthening the validation of the mathematical model and the adopted kinetics.

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