View metadata, citation and similar papers at core.ac.uk

brought to you by CORE

provided by Open Archive Toulouse Archive Ouverte

Open Archive Toulouse Archive Ouverte

OATAO is an open access repository that collects the work of Toulouse researchers and makes it freely available over the web where possible

This is an author's version published in: http://oatao.univ-toulouse.fr/21802

To cite this version:

Gakis, Giorgos and Vergnes, Hugues and Scheid, Emmanuel and Boudouvis, Andreas G. and Vahlas, Constantin and Caussat, Brigitte *Computational mechanistic investigation of the initial growth of Alumina ALD: Effect of substrate pretreatment on nucleation period reduction.* (2018) In: Rafald 2018, 6 November 2018 - 8 November 2018 (Lyon, France).

Any correspondence concerning this service should be sent
to the repository administrator: tech-oatao@listes-diff.inp-toulouse.fr

ORAL

Computational mechanistic investigation of the initial growth of Alumina ALD: Effect of substrate pretreatment on nucleation period reduction

G.P. Gakis[1, 2*], H. Vergnes[2], E. Scheid[3], C. Vahlas[4], B. Caussat[2], A.G. Boudouvis[1]

[1*] *National Technical University of Athens, School of Chemical Engineering, Athens, Greece.*

[2] *Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INPT, UPS, Toulouse, France.*

[3] *LAAS, Université de Toulouse, CNRS, Toulouse, France.*

[4] *CIRIMAT, Université de Toulouse, CNRS, INPT, UPS, Toulouse, France.*

gakisg@chemeng.ntua.gr

Optoelectronic, microelectronic, energy conversion or even medical devices becoming ever smaller and structured into complex three dimensional shapes, the need for nanometric conformal thin films has never been greater [1]. The Atomic Layer Deposition (ALD) process [2] has emerged as the appropriate process to produce such films. Due to the self- limiting nature of the deposition reactions involving two precursors alternatively fed, the process is characterized by its high film thickness control, uniformity and composition purity.

However, for the deposition of ultra thin films (<10 nm), the substrate initial surface plays a crucial role. The deposition during the first ALD cycles is either enhanced or inhibited[3], depending on the substrate nature. This nucleation period limits the minimum ALD cycles used to obtain a continuous film. Furthermore, even when the ALD regime is attained, the competition between surface mechanisms, such as desorption and surface reactions, play a crucial role on the ALD growth. All these phenomena need to be understood, while the substrate pretreatment should be optimized to minimize the nucleation period.

In this work, the surface mechanisms including reaction, adsorption and desorption steps during the ALD of Al_2O_3 from TMA and H_2O on Si substrates are investigated. The analysis is performed using a surface chemistry model, coupled to a CFD model for a commercial reactor treating 20 cm Si wafers. [4] This model is used to feed a geometric model that simulates island growth on a surface. The model predictions are validated by comparing its results with experimental measurements and literature data. It is shown that for ALD exposures in the range of ms, no reactions between a perfect Si substrate and reactants take place due to the low activation energy of the desorption step. The effect of initial long duration TMA exposures before deposition is investigated, showing that they clearly lead to an increase of nucleation sites on the surface by allowing TMA adsorption and reaction to occur, thus producing methyl groups transformed in active hydroxyl bonds by the subsequent H_2O exposure. This significantly reduces the nucleation period, hence decreasing the number of ALD cycles needed to obtain a conformal continuous film.

[1] R.W. Johnson, A. Hultqvist, S.F. Bent, Mater. Today. 17 (5) (2014), 236-246

[2] S.M. George, Chem. Rev. 110 *(*2010), 111–131

[3] Puurunen, R.L., J. Appl. Phys. 97 (2005), 121301

[4] G.P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, B. Caussat, A.G. Boudouvis, *Chem. Eng. Res. Des*. 132, (2018), 795-811.