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**Mass Spectrometry 2017: Knudsen cell applied to the investigation of organometallic precursors vapors. - Ioana Nuta - Orleans's University****Abstract**

Introduction In the field of microelectronics, the continuous decreasing size of integrated circuits (IC) silicon devices requires improvement of the manufactory Chemical Vapour Deposition (CVD) and Atomic Layer Deposition (ALD) processes as well as raw materials used as molecule sources. To achieve low temperature deposition of pure and conformal films, very reactive precursors leading to completely self-limiting surface reactions are needed. Pentakis(dimethylamido) tantalum (PDMAT) is the most common tantalum source for the deposition of TaN layers which are used as barriers to prevent copper diffusion into silicon and dielectric in multilevel metallization semiconductor devices. The barrier material should have a resistivity  $>1000 \mu\Omega \text{ cm}$  to maintain excellent electrical conductivity between the copper and silicon layers. For this purpose TaN phase satisfied these requirements, but most of the attempts to deposit pure TaN phase have often failed [1,2]. Some thin films with a ratio N/Ta within 0.8 to 1 have been obtained from PDMAT with plasma assisted ALD [3] and thermal ALD [4]. However, information about physical and chemical behaviour of this precursor is scarce and namely species that were transported to the deposition chamber are unknown. This information would be necessary to manage the reduction of Ta(V) into Ta(III) oxidation state in the deposition process. Mass spectrometer coupled with a

Knudsen effusion cell has already proved to be a powerful tool for studying the stability of gaseous molecules, thermodynamics of condensed phases and, more generally vaporization processes [5,6]. The goal of this study is to investigate vaporization properties of PDMAT using a specific "Organometallic (OM)-reactor" coupled to a mass spectrometer. 2. Experimental Pentakis(dimethylamido) tantalum (PDMAT),  $\text{Ta}[\text{N}(\text{CH}_3)_2]_5$ , was purchased from Air Products (98% pure). In addition to decomposition products, PDMAT contains few metallic impurities such as Al, 0.52 ppm, Li, 0.25 ppm, Na, 1.03 ppm and Sn, 0.3 ppm. Due to its sensitivity to moisture, cleaning and filling the cell should be made in a glove box under dried argon ( $\leq 1 \text{ ppm H}_2\text{O}$ ). The study of the PDMAT vaporization was carried out using a magnetic mass spectrometer (original Nuclide Corporation 1967) coupled with Knudsen effusion cell. In the field of microelectronics, the continuous decreasing size of integrated circuits (IC) silicon devices requires improvement of the manufactory Chemical Vapour Deposition (CVD) and Atomic Layer Deposition (ALD) processes as well as raw materials used as molecule sources. To achieve low temperature deposition of pure and conformal films, very reactive precursors leading to completely self-limiting surface reactions are needed. Pentakis(dimethylamido) tantalum

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state in the deposition process. Mass spectrometer coupled with a Knudsen effusion cell has already proved to be a powerful tool for studying the stability of gaseous molecules, thermodynamics of condensed phases and, more generally vaporization processes. The goal of this study is to investigate vaporization properties of PDMAT using a specific "Organometallic (OM)-reactor" coupled to a mass spectrometer, relevant thermodynamic parameters are taken from literature, such as activities, partial pressures and interaction coefficients. According to our results, distillation of phosphorus under vacuum occurs at high temperatures. Yet, the residual oxygen present in the vacuum is a hindrance to the distillation, since it evaporates in the form of silicon oxides.

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