TEMPERATURE DEPENDENCE OF THE OPTICAL CONSTANTS OF TANTALUM NITRIDE FORMED BY ATOMIC LAYER DEPOSITION ON 300 mm WAFERS

BY

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DEDICATION

I would like to dedicate this thesis to my father, Aaron, my mother, Peyma, and my sisters, Annapaula and Karime, who have supported and encouraged me in all the projects I worked on during this journey, both academically and extracurricularly.

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ABSTRACT

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Dr. Stefan Zollner, Chair

The work presented in this thesis describes the dielectric function of atomic layer deposition (ALD) tantalum nitride (TaN) from 0.03 eV to 6.5 eV, where we analyzed its optical constants to determine their temperature dependence from 80 K to 600 K. Tantalum nitride (TaN) layers with 12 nm and 23 nm thicknesses were formed on top of 300 mm silicon dioxide (SiO_2) on Si wafers by atomic layer deposition, and their TaN layer thicknesses and surface roughness were confirmed by x-ray reflectance (XRR). The ellipsometric angles Ψ and Δ were acquired at room temperature at incidence angles from 50° to 80° and photon energies from 0.5 eV to

6.5 eV on a vertical J.A. Woollam ellipsometer (VASE) and from 0.03 eV to 0.70 eV with a J.A. Woollam infrared ellipsometer (IR-VASE Mark II).

Having the ellipsometric spectra for photon energies from 0.03 eV to 6.5 eV at room temperature, we developed an ellipsometry model for the optical constants of the oxide and the TaN layers. After fitting this model, we obtained the optical constants for the TaN layer when measured at room temperature (300 K). The measured thickness of the TaN layer is 23 nm, with two absorption peaks at 3.7 eV and 4.8 eV, and a measured band gap of 1.8 eV. The band gap was obtained by extrapolating the ε_2 component of the dielectric function in a Tauc plot.

The second part of this research was focused on performing a temperature series of measurements at 80 K, 190 K, 400 K, 500 K, and 600 K with an incidence angle of 70° to investigate the temperature dependence of the optical constants and oscillators for the TaN layer. Since the model for the data at room temperature is fitted, the experimentally obtained thicknesses for the SiO_2 and TaN layers were fixed for the analysis of the temperature series.

A Lakeshore Janis ST-400 ultrahigh vacuum cryostat was attached to the VASE ellipsometer to obtain the ellipsometric data for the whole range of temperatures and the photon energies of 0.5 eV to 6.5 eV. For the lower temperatures of 80 K and 190 K, we used a 35-liter tank of liquid nitrogen as the cooling source that feeds the cryostat.

Evident from the temperature series performed, the change in temperature on the thin film slightly changed the pseudo dielectric and dielectric functions of the ALD TaN layer, making the band gap between 1.5 to 1.8 eV for the entire temperature range of 80 K to 600 K, with higher temperatures giving a lower band gap. This also demonstrated a relation of change with temperature that follows an expected behavior of an inverse correlation between thickness and refractive index.

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