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# On the difference between optically and electrically determined resistivity of ultra-thin titanium nitride films

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ABSTRACT

This work reports on the determination and comparison of the resistivity of ultra-thin atomic layer deposited titanium nitride films in the thickness range 0.65–20 nm using spectroscopic ellipsometry and electrical test structures. We found that for films thicker than 4 nm, the resistivity values obtained by the two techniques are in good agreement. However, below 4 nm, the comparison shows an increasing difference with decreasing film thickness. A difference with a factor of 3 was found at 1.8 nm and increased up to hundreds at 0.65 nm. We attribute this significant difference to the electron scattering effects at grain boundaries and interfaces which can not be fully taken into account by spectroscopic ellipsometry measurements.

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## 1. Introduction

During last several decades, titanium nitride (TiN) has gained much interest because of its low resistivity and compatibility with complementary metal-oxide-semiconductor (CMOS) processes. Thin TiN films made by atomic layer deposition (ALD) are commonly used as diffusion barriers and gate material for CMOS devices [1,2]. The ALD of TiN can be realized via either a thermally activated process, which is carried out at elevated temperatures, e.g. 350–450 °C, or plasma-assisted ALD, where TiN can be deposited at lower temperatures [3–5].

The resistivity of TiN thin films can be measured either by electrical four point probe (FPP) method, or by spectroscopic ellipsometry (SE) [6,7]. However, the optical and electrical characterizations are based on different physical models. SE measures the resistivity of a film on the basis of the determination of its conduction electron concentration and electron scattering effect which is caused by the interaction between electrons and electric field of the incident light. In contrast, direct electrical measurements are based on the current flow under an applied electric field meaning the physical carrier transport. This dc transport can be strongly influenced by the scattering of electrons at local constrictions, e.g. at grain boundaries and interfaces, which can tremendously increase as the film thickness is reduced. However, this influence is hardly taken into account by SE. Therefore, for ultra-thin films, the scattering effects are expected to increase the resistivity measured electrically relatively to that obtained by optical SE.

The purpose of this study is to compare resistivity obtained by electrical and optical means, on ultra-thin TiN films in the thickness range 0.65–20 nm. The optical measurements were carried out during the deposition of the films. We used the Drude–Lorentz model [6] to parameterize the optical functions of TiN from which the resistivity was determined. The optically measured resistivity was compared to the value for the same film thickness obtained by electrical measurements which were performed using both the circular transfer length method (CTLM) [8] and the linear test structures specially designed to measure the resistivity of ultra-thin films.

## 2. Experimental

### 2.1. Deposition of TiN and a-Si passivation layers, and in situ SE

TiN films were grown via thermal ALD at 350 °C on Si wafers covered with 100 nm thermal oxide. The ALD and the growth of TiN were reported in our previous work [9]. Directly after the deposition of TiN, an amorphous silicon (a-Si) layer was deposited to prevent TiN oxidation in the same reactor at 325 °C by low pressure chemical vapor deposition (LPCVD) using trisilane ($Si_3H_8$) as the source gas. The in situ SE monitoring was performed by using a Woollam M2000 spectroscopic ellipsometer operating in the wavelength range between 254 and 1688 nm, in combination with COMPLETEEASE modeling software. The ellipsometer was mounted

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on the reactor with an angle of incidence of 70° with respect to the substrate normal. The SE measurements were taken every 2.5 s during the deposition.

### 2.2. Fabrication of test structures

The fabrication of the CTLM structures was presented in a previous study [10]. The linear structures were realized by a two-mask process flow. The first mask was applied to fabricate the electrodes using a metal lift off process after sputtering the metal (Pt). The second mask was used to pattern the conducting TiN and the a-Si passivation layer following a photolithography-etching process. The a-Si and the TiN layers were etched in $H_2O$:$HNO_3$:HF and $H_2O$:$NH_4OH$:$H_2O_2$ solutions, respectively, at room temperature.

### 2.3. Material characterization and electrical measurements

The film thickness was measured by SE and verified by high-resolution transmission/scanning electron microscopy (HR-TEM/SEM) and X-ray fluorescence (XRF) spectroscopy. The electrical measurements were carried out using both the Karl-Suss PM8 and Cascade Microtech IV/CV Measurement low leakage manual probe stations. Coating a primer layer on the surface prior to the measurements ensured a negligible surface leakage current.

## 3. Principles of the optical and electrical measurements of TiN resistivity

### 3.1. Optical SE measurements of TiN resistivity

Spectroscopic ellipsometry is a non-destructive optical characterization technique in which the sample to be analyzed is illuminated with a beam of polarized light. Ellipsometry characterizes the light reflected from (or transmitted through) the sample upon measuring the change in polarization state in terms of ellipsometric parameters psi ($\Psi$) and delta ($\Delta$) [11]. To extract the film thickness and dielectric functions, an optical model must be built and the dielectric functions have to be parameterized. For TiN, the dielectric functions are parameterized by applying the Drude–Lorentz model consisting of a Drude term and two Lorentz oscillators described as [6]:

$$\varepsilon = \varepsilon_\infty - \frac{\omega_{pu}^2}{\omega^2 - i\Gamma_D\omega} + \sum_{j=1}^{2} \frac{f_j\omega_{0j}^2}{\omega_{0j}^2 - \omega^2 + i\gamma_j\omega} \quad (1)$$

The Drude term describes the intraband absorption by free conduction electrons in a material and is characterized by the damping factor $\Gamma_D$ and the plasma frequency $\omega_{pu}$. The damping factor $\Gamma_D$ is due to the scattering of electrons and determined as the inverse of the mean time between collisions, $\tau_D$ [12,13]. The relation between resistivity $\rho$, $\omega_{pu}$ and $\tau_D$ is given by:

$$\rho = \left(\frac{1}{\varepsilon_0\tau_D}\right)\frac{1}{\omega_{pu}^2} \quad (2)$$

where $\varepsilon_0$ is the permittivity of free space. In SE measurements, the plasma frequency $\omega_{pu}$ and $\tau_D$ are measured [14]. From Eq. (2), the resistivity is calculated.

### 3.2. Electrical measurements of TiN resistivity

The determination of resistivity by CTLM structures was described in [8,10]. The layout of the linear structures is schematically shown in Fig. 1. In this structure, by applying a voltage $V$ between the two metal electrodes, the current $I$ running through

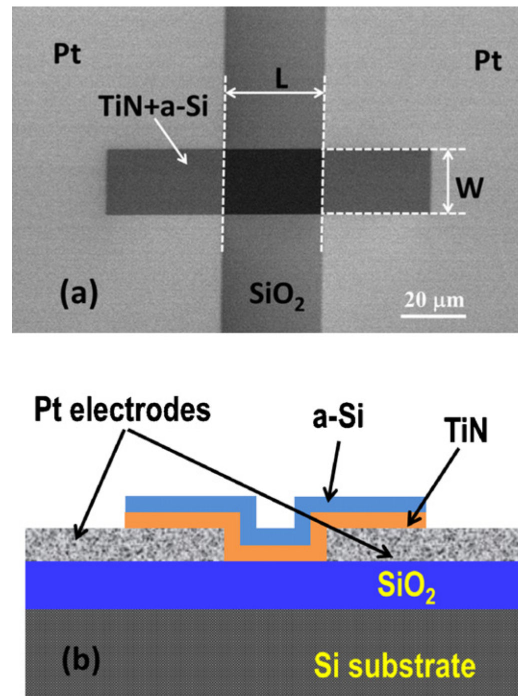


**Fig. 1.** (a) SEM image (top-view) and (b) schematically drawn cross-sectional view of a linear structure for electrical resistivity determination of ultra-thin TiN films.

the titanium nitride is measured. The total resistance between the electrodes is calculated as:

$$R = \frac{V}{I} = \rho\frac{L}{tW} + 2R_c = R_{sh}\frac{1}{W}L + 2R_c \quad (3)$$

where $\rho$ is the resistivity of the film, $t$ is the film thickness. $L$ and $W$ are the length and the width of TiN sheet between the electrodes, respectively. By $2R_c$ the doubled contact resistance is expressed. The term $R_{sh} = \rho/t$ represents the sheet resistance of the layer. For a given $W$, by changing the gap spacing $L$ between the two electrodes, the measured resistance $R$ as a linear function of $L$ can be plotted. The sheet resistance $R_{sh}$, and therefore the resistivity $\rho$ of the film are obtained from the slope of the linear curve. The intercept with the vertical axis gives $2R_c$.

## 4. Results and discussion

*Optical measurements of resistivity.* Fig. 2(a) shows the fitting between the measured and simulated ($\Psi$, $\Delta$) spectra for a 10-nm thick TiN layer. The corresponding real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the complex dielectric function, which are extracted from the fitting, are shown in Fig. 2(b). The individual contributions of the Drude term ($D$) and the Lorentz oscillators ($L_1$, $L_2$) to the dielectric function are shown in Fig. 3. It is found that the Lorentz oscillators are located at 0.7 and 5.4 eV. According to the TiN band structure reported by Ern and Switendick [15], these two oscillators represent the $\Gamma_{25'}$-$\Gamma_{12}$ and $L_3$–$L_{3'}$ interband transitions in the Brillouin zone, respectively.

The resistivity of TiN is determined by the Drude term, which is characterized by $\Gamma_D$ and $\omega_{pu}$. In an ideal metal, the plasma frequency is defined as the point where the real part of the dielectric function is zero ($\varepsilon_1 = 0$). However, in real metals, the existence of interband transitions at energies lower than $\omega_{pu}$ shifts the point where $\varepsilon_1 = 0$ to lower energy, which is called screened plasma frequency $\omega_{ps}$ [6]. Therefore, the $\omega_{pu}$ in Eq. (1) corresponds to the point where the contribution of the Drude term to $\varepsilon_1$ is zero, as denoted in Fig. 3(a). SE measurements on a 10 nm TiN resulted

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