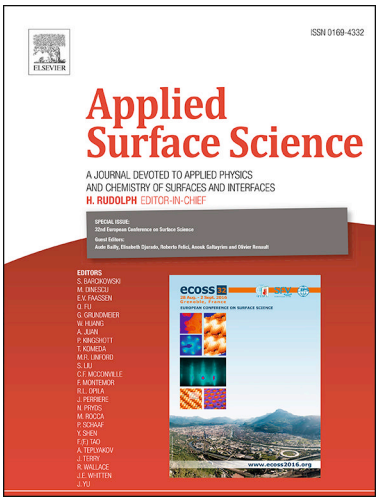
Accepted Manuscript



Full Length Article

A comprehensive study of the TiN/Si interface by X-ray photoelectron spectroscopy

V.G. Antunes, C.A. Figueroa, F. Alvarez

PII: S0169-4332(18)30953-X
DOI: https://doi.org/10.1016/j.apsusc.2018.04.005
Reference: APSUSC 39004

To appear in: *Applied Surface Science*

Received Date: 16 November 2017
Revised Date: 11 February 2018
Accepted Date: 1 April 2018

Please cite this article as: V.G. Antunes, C.A. Figueroa, F. Alvarez, A comprehensive study of the TiN/Si interface by X-ray photoelectron spectroscopy, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.04.005

A comprehensive study of the TiN/Si interface by X-ray photoelectron spectroscopy

V. G. Antunes[1], C. A. Figueroa[2] and F. Alvarez[1]

[1]*Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, Campinas, SP, Brazil*
[2]*PGMAT, Universidade de Caxias do Sul, Caxias do Sul, RS, Brazil*

Abstract

In this paper, a comprehensive X-ray photoelectron spectroscopy (XPS) study of the first atomic layers of TiN nanofilms grown by ion beam assisted deposition on crystalline silicon is reported. This deposition technique allows a fine control of the ion species and energy arriving at the substrate. The substrates are prepared by ion beam cleaning involving Xe^+ ion bombardment in different partial pressures of molecular H_2. The expected hydrogen passivation effect by the Si-H formation bond limiting the Si-O bonds was quantitatively evaluated and correlated with some retention of H and O at the substrate surface. The effects of molecular H_2 and residual H_2O atmosphere present during the process on the chemical bonding on both the naked Si substrate and afterward on the interface are reported. A detailed XPS analysis performed in an attached UHV chamber to the preparation chamber of the TiN/Si interface shows that the bombarding cleaning procedure plays an important role in the bond formation at the interface since minute amounts the oxygen jeopardize the bulk properties.

Keywords: Interface TiN/Si; XPS; Oxygen contamination; Ion Beam Assisted Deposition (IBAD)

Corresponding author e-mail: vi.antunes@gmail.com

1 Introduction

Titanium nitride (TiN) thin films show interesting properties such as hardness, chemical inertness, and an attractive golden color being used in nano-microelectronic, cutting tools, protective coatings, optics and decoration. Particularly, this material has relevance in mechanics and optical purposes [1,2]. Besides those applications, TiN is broadly used as diffusion barriers of catalytic metals in carbon nano-tubes growth and self-organized metallic particles deposition [3–7]. Most of the application of the thin TiN film requires avoiding impurities incorporation at the interface to guarantee good adhesion compact and homogeneous films. This is so because a minute quantity of impurities can seriously jeopardize the bulk properties [8,9]. ~~This is particularly important in commercial deposition machines where the surreptitious minute of oxygen can be incorporated via the presence of residual H_2O.~~ Therefore, one of the goals of this paper is highlight experimental conditions leading to answer a question about the optimal H_2 used to reduce oxygen and tolerable residual chamber water, i.e., vacuum quality to guarantee a proper interface and thus good film properties deposited on crystalline Si <100>.

The goal of the paper is to present a detailed study of the bonds being prompted in the interface in the presence of both the residual oxygen and hydrogen. As it is well known, hydrogen is commonly used to control its incorporation of oxygen because its