Titanium Nitride: Sputter Modeling

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A model for sputter based deposition of TiN films was developed by simulations. The rate of change of partial sputtering yield with coverage was considered. The deposition pressure and time were varied to get films of different thickness.

Keywords: Sputtering, simulations, TiN

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The surface behaves different from bulk. It possesses different atomic structure and crystal structure. The electronic, transport as well as physical and chemical properties are quite different from bulk [1]. We need to study surface and try to improve its properties as it has tremendous technological importance. There are various methods to modify a surface: heat treatment, plasma surface modification and thin film deposition to name a few. Among all the surfaces, Ti surface is a significant one especially in areas where high strength components are requires like aerospace. In this communication focus has been given on TiN surfaces. TiN are materials with high chemical and thermal stability as well as good mechanical properties. They are used extensively in semiconductors as well as for protective and decorative purposes [2, 3].

A modeling has been shown for the growth mechanism of TiN films during reactive sputter deposition. This model has been developed for the epitaxial growth which is based on the atoms getting sputtered out from the target surface and ultimately being deposited on the substrate to form the film [4]. The rate of sputtering i.e. the amount of target materials sputtered per unit time is given by eqn 1, where M is molar weight of the target [kg/mol]; r is the density of the material [kg/m^3]; NA is the 6.02×10^{26} 1/kmol; (Avogadro number); e is the 1.6×10^{-19} As (electron charge); S is the sputtering yield (atom/ion) and jp: primary ion current density [A/m^2]. This rate divided by atomic diameter gives us the rate of sputtering in terms of atomic layers (AL) per second [5]

$$zt = M/(rNAe)\ S\ jp \qquad (1)$$

There is a preferential sputtering of Nitrogen if a TiN target is used. Also the partial sputtering yields as well as the sticking coefficients of Ti and N are different. The sputtering yield of Ti was taken from 0.1 to 1.0 as per ref [2]. The radius of Ti is 147 pm and that of N is 56 pm. Therefore the radius of TiN was taken as 200 pm as a rough estimate.

The adatoms sputtered from the target are multiplied with exp (-d/L) to get rough estimate of the deposited atomic layers per second. L (cm) is the mean free path of the sputtered atom which is related to the sputtering pressure P (Torr) and the molecular diameter Da of the reactive gas (252 pm for O_2) $L = 2.303\times10^{-20}T/\ (PDa^2)$ where T is the deposition temperature and d (cm) is the distance traversed by the adatom for deposition which was taken as 30 cm considering the target the substrate distance [4, 5].

A ratio was given in ref [2] as the ratio of the partial yields of Ti and N as given below in eqn 2. The ratio q depends on the composition of the target and energy of the incident ion.

$$q = \frac{s_N}{s_{Ti}} \qquad (2)$$

The atomic flux of N/Ti plays a key role in the growth of TiN films [6]. The change in composition during the sputtering process was not considered which has been tried to inculcate here. So instead of q we introduce here the rate of change of q w.r.t coverage (= $dq/d\theta$). The rate decreases from the initial value due to preferential sputtering of N and the target is deficient of N. Based on our previous publication, we can assign an equation

$\theta = (1 - e^{-x})$ to the coverage and $S = e^{-x}$ to the sticking coefficient. The parameter "x" is stoichiometry of the compound being formed [7]. The variation of partial yield and derivative of partial yield with coverage is shown in fig 1

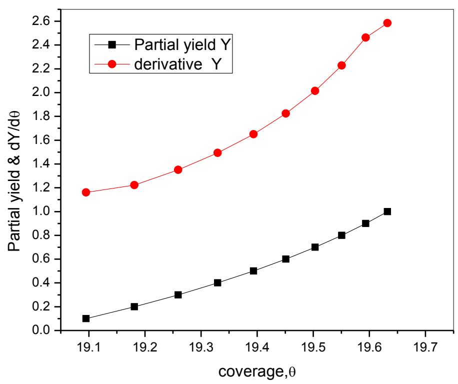

Fig 1: Variation of partial yield and derivative of partial yield with coverage

The variation of deposition pressure caused difference in deposition thickness of the TiN films as shown in fig 2. Increase in vacuum caused a decrease in deposition which is quite different phenomenon.

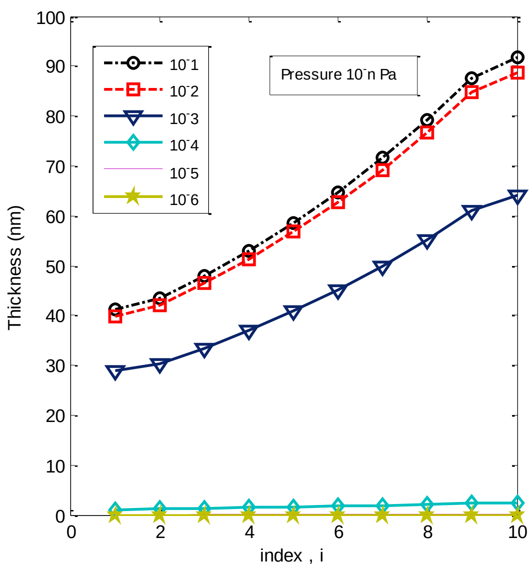

Fig 2: Simulated TiN of various thicknesses deposited at different pressures

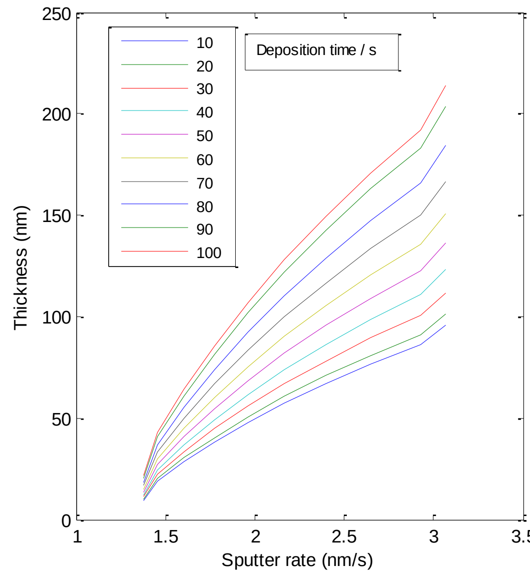

Fig 3: TiN film thickness variation with sputter rate at different deposition time.

From fig 3 a deposition of upto 200 nm was observed on changing the deposition time to 100s.

Conclusions

A model was developed for sputtering of TiN film. An increase in the rate of partial yield with coverage was observed. The variation of deposition pressure and deposition time was obtained.

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