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Modelling and analysis of sputter deposited ZrN coating by CFD

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Abstract. The objective of the present work is to investigate the effect of various sputtering parameters such as velocity, mass flow rate on velocity profiles, pressure profiles, density profiles and concentration distribution of the process gases (argon and nitrogen) of zirconium nitride films deposited on glass and silica substrate by RF magnetron sputtering. A three dimensional Computational Fluid Dynamics (CFD) study has been carried out using Fluent-ANSYS commercial code to visualize the mixing behavior of process gases inside the deposition chamber. The results show that the location of gas inlet port has a greater influence on gas distribution inside the chamber where reactive gas will form coating. By having this information, one can able to modify the reactor geometry and gas flow openings along with its positions for better gas flow over the substrate which in turns gives an indirect indication of coating from the composition point of view.

KEY WORDS: CFD; Concentration; Sputtering; ANSYS

1. Introduction

In the last few decades, thin films based on transition metal nitrides have been widely used in different technological areas [1–3], because of their promising properties together with their shiny and golden appearance, which makes them highly attractive for applications such as decorative coatings in several commercial and industrial sectors[4,5]. A variety of nanoscale multilayered coatings have been studied extensively because of their rising properties such as hard coatings in surface engineering for wear protection and friction reduction of mechanical components in the industry[6]. Much of the work on micro and nanolayered films has focused on nitride-based materials of great interest as superhard coating[7]. Zirconium nitride is one of the most intensively studied among all transition metal nitride systems[8,9], whereas properties of zirconium nitride depend significantly on the Ar/N_2 ratio[10,11,12].

Haider (2005) investigated the effect of inert gas flow rate to predict velocity behavior, pressure behavior, density behavior and nitrogen gas concentration distribution across the sputtering chamber [13]. As thin film characteristics are highly depend on process parameters, so by varying deposition parameters (i.e. flowrate, velocity, inert gas ratio), various coatings with required values of mechanical properties can be achieved. Hence, it would be better if CFD simulation is preferred to check the required deposition parameters. A three dimensional Computational Fluid Dynamics (CFD) study was carried out using Fluent-ANSYS analysis package.

Fragiel et al.(2008) deposited zirconium nitride by reactive unbalanced magnetron sputtering at different nitrogen partial pressures on AISI 316L stainless steel substrate. They analyzed as N_2 partial pressure increases, the hardness and young's modulus of the coating decreases [14]. Roman et al.(2011) deposited ZrN thin films on different substrates by DC reactive magnetron sputtering. They varied deposition time, Ar/N_2 partial pressure ratio and substrate temperature on microstructure, composition and corrosion behavior of zirconium nitride thin films deposited under different conditions. The crystalline structure and corrosion resistance of ZrN films were studied by Rutherford backscattering spectrometry(RBS) and scanning electron microscopy(SEM)[15]. It is also evident that the microstructure and properties of ZrN film vary with different deposition techniques and processing parameters [16].

Singh et al.(2013) synthesized ZrN thin films on silicon substrate by using a pulsed DC magnetron sputtering technique. They studied the influence of nitrogen flow rate on coating and observed nanomechanical properties, hardness and elastic modulus, and showed good resistance to plastic deformation at reduced flow rates of nitrogen. Literature reviews of ZrN indicate that the major amount of research work is focused on experimentation and tribological characterization of ZrN coating.

The aim of this research work is to examine the effect of velocity distribution and gas pressure distribution for various gases (argon & nitrogen) used for forming zirconium nitride coatings in sputtering chamber. Density profiles has also been observed across the deposition chamber in order to check whether the mixture of the gases are sufficiently mixed or not. The distribution of gas concentration inside sputtering chamber has also been observed.

2. Analysis Details

In the analysis, zirconium target has been deposited on silica and glass substrate by RF magnetron sputtering. The density taken for argon and nitrogen gases were 1.623 kg/m^3 and 1.138 kg/m^3 respectively.

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The following table gives the input parameters of steady-state chamber pressure, flow rate of argon and nitrogen at inlet and its corresponding velocities. The velocities of process gases has been calculated by dividing the flow rate with the inlet cross-section of circular pipe.

V = Q/A

where Q = Flow rate of process gases

A = Inlet cross section area

Table 2.1 Chamber pressure and velocities at different flow rates of N_2 and constant flow rate of Ar

Pressure (Pa)	**Ar flow rate (sccm)**	**N_2 flow rate (sccm)**	**Ar velocity (mm/s)**	**N_2 velocity (mm/s)**
1.5	20	04	99.21	28.30
1.5	20	08	99.21	56.59
1.5	20	12	99.21	84.89
1.5	20	16	99.21	113.18
1.5	20	20	99.21	141.47

To satisfy with the non-slip condition at the wall, Velocity components at all the outer walls of a chamber (model) has been set to zero (Vx = 0, Vy = 0 and Vz = 0). The reference pressure and relative outlet pressure has been taken as 1.5 Pa and 0.0 Pa respectively.

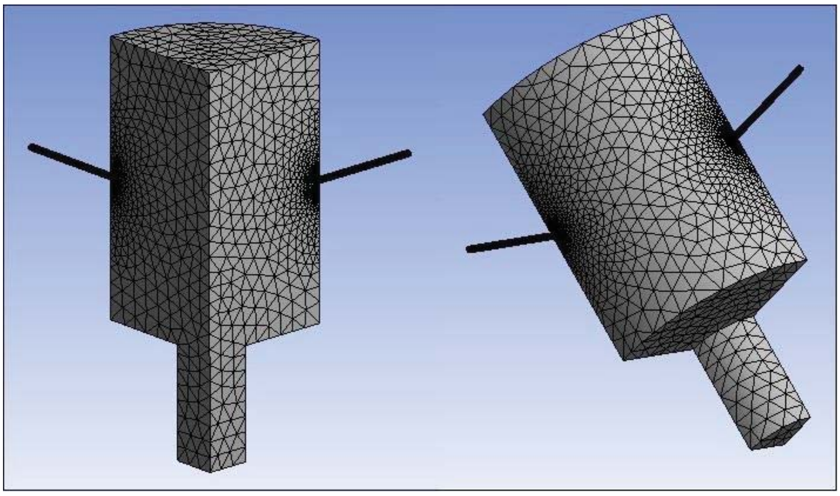

Figure 2.1: *Tetrahedron method meshing*

The tetrahedral method of meshing has been used for getting an accurate results throughout the domain. By doing so, visualization can be carried out very easily. The number of nodes examined for this model is up to an acceptable level of mesh (19677 nodes).

3. Results and Discussion

CFD analysis has been carried out for velocity distribution, gas pressure distribution, gas mixture density and nitrogen gas concentration. A certain observations has been made during deposition process.

Figure 3.1(a) shows the simulated velocity vector plot inside the inlet, within the chamber and outlet whereas figure 3.1(b) shows pressure distribution of gases inside the chamber.

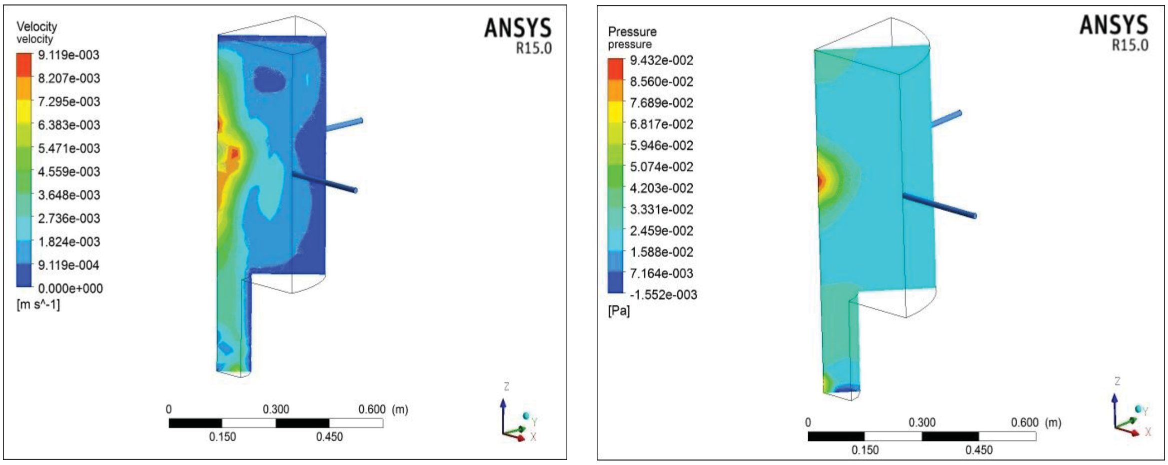

Figure 3.1: *(a)velocity vector and (b)pressure distribution of gases*

Velocity vectors give the information of fluid as well as gas flow behavior through arbitrary geometries. In the inlets and outlets, higher gas velocities has been found due to smaller circular cross section of inlet pipe. But in substrate region, the velocities found to be quite low because of much larger diameter of chamber in substrate region. In the inlet pipe, higher velocity in the middle of the pipe has been observed due to parabolic distribution of fluid through circular pipe.

As the pressure is proportional to inlet velocity, so maximum pressure has also been observed at the inlet. The chamber diameter is much larger than inlet diameter; so this results in uniform decline of nitrogen pressure in the region very nearer to the inlet and after that it decreases slowly inside the chamber. A similar decline of pressure behaviour was observed in a Monte Carlo simulation of gas transport in TiN magnetron sputtering[17].

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Table 3.1 Calculated velocity vector and pressure plot at different inert gas velocities of Ar and N_2

Sr. No.	Inert gas velocities (mm/sec)		Output Parameters	
	Ar	N_2	Velocity vector plot (m/sec)	Pressure plot (Pa)
01	99.21	28.30	0.0026-0.0130	0.0071-0.0943
02	99.21	56.59	0.0018-0.0091	0.0100-0.1426
03	99.21	84.89	0.0031-0.0155	0.0230-0.1411
04	99.21	113.18	0.0039-0.0197	0.0119-0.1692
05	99.21	141.47	0.0018-0.0091	0.0153-0.2229

Figure 3.2 (a) and (b) illustrates the gas mixture density and nitrogen concentration inside the chamber, outlet and inlet at 12 sccm of argon and 8 sccm of nitrogen flowrates respectively.

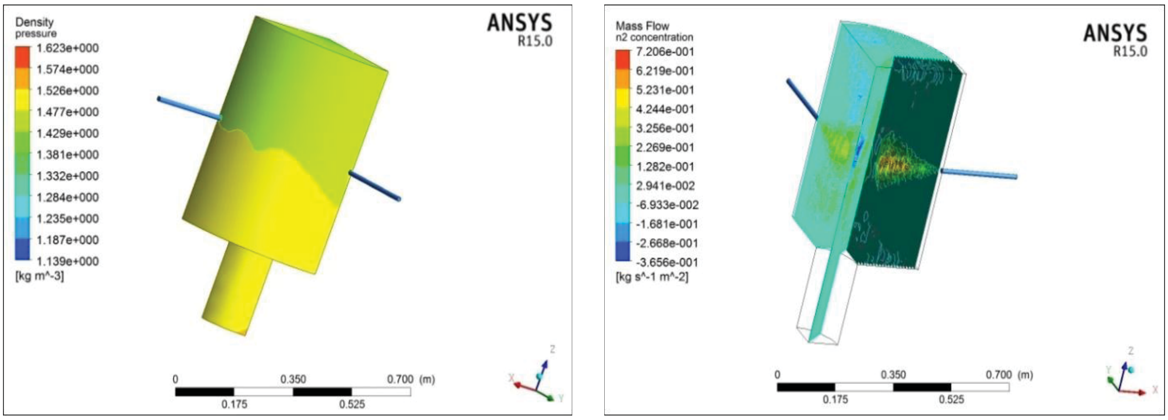

Figure 3.2 *(a)gas mixture density and (b)nitrogen concentration*

Table 3.2 Calculated density plot and nitrogen concentration plot

Sr. No.	Inert gas flow rates (sccm)		Output Parameters	
	Ar	N_2	Density plot (Kg/m^3)	Nitrogen concentration (x100 %)
01	20	04	1.139-1.623	0.12-0.72
02	20	08	1.139-1.622	0.12-0.72
03	20	12	1.139-1.622	0.12-0.71
04	20	16	1.139-1.555	0.12-0.71
05	20	20	1.139-1.541	0.12-0.71

The density of gas mixture was observed as single contour inside the chamber due to small fluctuation of density inside a chamber. Appropriate range of concentration was selected in order to see the fluctuation of density distribution inside the chamber. The density of the gas mixture inside the chamber varies slightly as density of the gas mixture is a linear combination of process gases. The density plot suggests that nitrogen and argon gases were satisfactorily mixed inside the chamber that are in good agreement with the work of J. Haider[13].

The concentration of nitrogen in a whole chamber was also observed as single contour inside the chamber due to small fluctuation of nitrogen gas inside a chamber. The range of concentration, which fell only inside a chamber, was selected in order to see fluctuation inside the chamber. Nitrogen concentration was high nearer to nitrogen inlet and decreased towards substrate region. Nitrogen concentration was found to be low near argon inlet and increased towards center of the chamber. The concentration found in the middle of chamber was almost constant. As a result, uniformly nitrogen distribution at substrate region has been observed.

4. Conclusion

CFD modeling has been carried out to analyze gas flow and its mixing behavior within the chamber by ANSYS-Fluent commercial code for ZrN films deposited by magnetron sputtering technique. Analysis results showed to be an important aspect to predict gas flows and mixing behavior in terms of gas velocity, pressure and gas concentration distribution inside deposition chamber. Simulation has been carried out by taking constant argon flow rate and varying nitrogen flow rate. The purpose of taking argon flow rate constant was to check the difference in distribution behavior of velocity profiles, pressure profiles, density profiles and nitrogen concentration profiles. Velocity and pressure were high at inlet, after that it decreases and observed to be low at chamber region. This was due to expansion of the model from lower to higher. The density of gas mixture observed constant inside the chamber.

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6. References

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