

Aspects for the design of sputtering systems

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The factors causing problems in sputter deposition of thin films are analysed and possible design solutions are offered. ZnO sputtered films are used as a probe for studying problems. The physical parameters of the discharge that have influence on the sputtering processes are described and related to the sputtering parameters. A comparison of discharges used in Diode, Magnetron, and Triode arrangements with respect to their system performances results in the conclusion that Magnetrons are superior to Diodes and that Triodes are better than Magnetrons, in spite of the fact that Triodes' discharges are of the supported kind and their deposited layers are difficult to reproduce.

Introduction

Thin ZnO layers had been deposited for a long time before sputtering methods had become a standard deposition technique in the industry^{1,2}. Development of the sputtering methods was pushed by the industrial need for good metal, dielectric, and piezoelectric thin films. ZnO was one of the first sputtered compounds that was extensively studied. This material has a clear X-ray diffraction pattern, tends to form polycrystalline layers with preferred orientations, and is a good example for presenting general arguments for choosing sputter deposition systems. ZnO thin films are sputtered directly from ZnO targets² or reactively sputtered from Zn targets³. In direct sputtering the compound molecule and its fragmented mixture are transferred from the compound target to the substrate, and in reactive sputtering gases are involved in the transfer mechanism. The reactants react at different places: on the surface, on their way to the substrates and on the substrates⁴, depending on the deposition conditions. Three basic sputter deposition configurations are in use: Diodes, Triodes and Magnetrons, with dc and/or rf supplies^{5,6}. Both power sources are usually used for sputtering metals and semiconductor targets, whereas rf is the power source preferred for sputtering insulators. DC triode sputtering systems with ZnO targets are in use⁷ for preparation of SAW transducers and optical wave guides. This deposition system is probably possible because Triodes operate with a supported discharge.

In the following section the design concepts from a physical point of view and their relationship to the sputtering parameters of the three sputtering systems will be discussed. The flakes, geometry of the electrodes and the vacuum chamber will be analysed and comparison between the sputtering systems is given. The concept of ionization density for analysing dc discharges in Diodes and Magnetrons is introduced and finally the use of rf power is compared with that of dc power.

Flakes, electrodes and the vacuum chamber

During the sputtering process flakes are formed and contaminate

the substrates^{8,9}. They appear on the substrates and targets of Diodes, Triodes and Magnetrons from both direct sputtering and from reactive sputtering of oxidized targets. Their maximum dimensions vary from a few millimeters for a hot pressed ZnO target to a few micrometers when reactive sputtering from a Zn target. The particle size increases with increase in deposition time and from run to run. Removal of the particles of the previous run before starting the next deposition helps to keep the dimensions of the flakes down. Their minimum dimension is probably in the molecular size. We have observed how ZnO powder that was collected from a Zn target of a Planar Magnetron at the end of a few deposition runs passed seemingly unperturbed through a package of soft paper. These kind of particles are formed on targets of all configurations: horizontal with target both up and down, and vertical. In the latter they fall down on the chamber floor and do not contaminate the substrates. In the down position they are left on the target which indicates that the vertical configuration is the recommended structure for sputtering ZnO and Zn targets. Contamination phenomena appear sometimes also in the processes of CVD, plasma deposition and plasma etching. However, the vertical configuration in these cases is not a general solution because particles are formed everywhere under these conditions. The origin of the flakes and their growth mechanism is not yet well understood and more study of these topics has to be done. Another aspect of the subject is where the best place is to locate the high vacuum valve (HVV) in the vacuum chamber. According to the traditional design the valve was located at the centre of the chamber floor. Flakes and powder enter into the vacuum pumps through the high vacuum valve. Designing the pumping port in the side wall reduces contamination to a minimum^{10,11}.

A second error in the traditional design is the use of O-Rings to separate cooling water from vacuum in the electrode assembly. During sputtering heating damages the outside face of the O-ring and the combination of electric field and contamination in the cooling water damages its inside face and causes water vapour leaks. The leaks disappear when the discharge is extinguished.

Table 1. Recent and old design for ZnO sputtering chambers

Traditional design	Problems	Recent design
Pyrex chamber	Dangerous and impossible to use walls	Stainless steel chamber
No temperature control of the chamber walls	Water is condensed on the walls	Temperature control of the chamber walls
Horizontal configuration	Contamination by flakes	Vertical configuration
Target area	Hard to scale up	Easy to scale ⁹
O-ring seals between water and vacuum	Leaks of water while operating	Elimination of water-vacuum interface
High vacuum valve under the baseplate	Maintenance problems	Valve in the side wall
Cable hoist	Can oscillate during raising	Rigid hoist

In recent designs O-rings never seal plasma-water interfaces. Their separation is obtained by two interfaces: water to atmospheric pressure and atmospheric pressure to plasma. A comparison between recent and old designs for sputtering chambers is given in Table 1. In the recent design two multi-target systems for sputtering inward¹² and outward¹⁰ are developed. In the former, problems of cross deposition prevent simultaneous sputtering from different targets, but target installation is relatively simple, while in the latter the opposite is true: target installation is complicated and problems of cross deposition are eliminated.

The discharge parameters

An ideal sputtering system is one in which the parameters effecting the discharge are independent, can be varied over a wide range, and are under operator control. The dc Diode is an example of a *non-ideal* system. The cathodic current is voltage and pressure dependent; increase in the cathodic voltage shifts the system from the normal glow to the arc region and to maintain the discharge in the normal glow the gas pressure has to be changed. The gas pressure itself has a strong influence on film growth¹³ whereas negligible dependence is desired. A comparison between the dc sputtering discharges, Diodes and Magnetron, is given in Table 2.

The film properties (structure, optical, electrical, mechanical, etc.) depend on the physical parameters at the substrate during sputtering, such as substrate nature, temperature, kinetic energies for all particles in the substrate environment and densities. These variables are monitored by the discharge parameters and thus modification in the film properties can be designed. The relationship between the physical and discharge parameters are still in question. Why, for example, deposition rate of Table 2 is low for Diodes and high for Magnetrons, and why Magnetrons work at high current densities and Diodes at high voltages? In a recent publication¹⁴ a model for the voltage-current-pressure characteristics for diode sputtering discharges was described. In Diodes the target secondary electrons are accelerated in the cathodic dark space and ionize the gas. A very small fraction (<0.1%^{14,22}) of the total number of the gas molecules in the discharge are usually in the form of ions. Less than 1%¹⁴ of the electrons cause ionization. The other electrons are collected by the

Table 2. A comparison between parameters of dc sputtering discharges with 6 in. round targets

Discharge parameters	DC Diode sputtering	DC Magnetron sputtering	DC Triode sputtering
Cathode voltage	2-5 KV	200-600 V	0-1500 V
Electric current	50-500 mA	1-10 Amp	1-20 Amp
Argon pressure	> 50 mtorr	> 5 mtorr	> 0.5 mtorr
Deposition rate	Low	Low to high	Low to very high
Reactivity in Ar-O ₂ plasma	Low	High	Very high
Substrate location	Inside the discharge	Inside or outside the discharge	Anywhere

anode and raise its temperature. (Mechanisms of recombination in the gas phase are negligible.) The process of ionization happens mainly near the interface between the negative glow and the dark space.

In Figures 1 and 2, α and γ , Townsend's first and second coefficients, versus the electron energy and the ion energy are described respectively^{15,16}. The operating ranges for dc Magnetrons' and Diodes' discharges are marked on the graphs. In the former the curves for most gases in use have maximum around 100 eV and in the latter a monotonic increase in γ is described. In Figure 3(a) the general I-V characteristic for dc Diode discharges is described¹⁵. In Figure 3(b) the distribution zones for the normal glow is given, and the anode locations for the general case and for sputtering discharge are marked. In Figure 3(c) the electric field and its potential are drawn versus the distance from the cathode. For self-supported discharges a relationship between α , γ , and the cathode dark space length L was developed¹⁴. This formula is an extended Townsend's condition for the normal glow and was proved independent of the breakdown condition. The maximum efficiency for the sputtering discharge depends on the numerical values for α , γ and L , which give a maximum deposition rate for a given power. This condition is independent of the sputtering

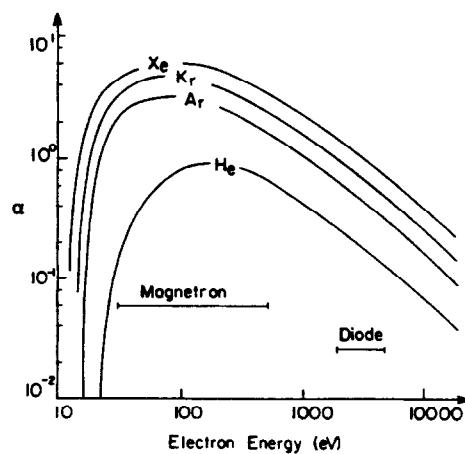


Figure 1. α , the first Townsend's coefficient for ionization by electrons, versus the electron energy. The working ranges for Diodes and Magnetrons are marked¹⁵.

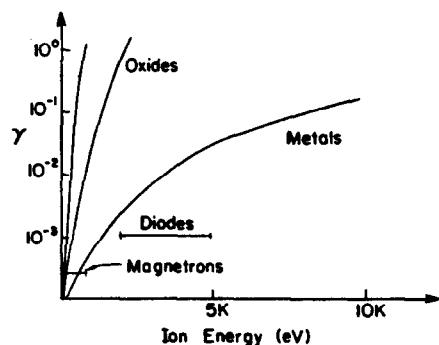


Figure 2. γ , the second Townsend's coefficient for electron emission due to ion bombardment, versus the ion energy. The working ranges for Diodes and Magnetrons are marked¹⁶.

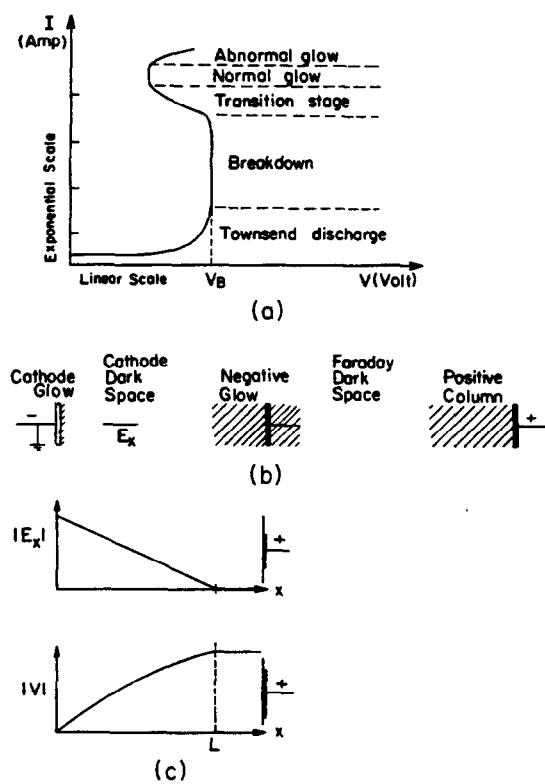


Figure 3. (a) I-V characteristics for dc Diode discharges in gases¹⁵. (b) A description of the normal glow zones. The two different locations for the anodes, one for the general dc discharge and the other for the dc sputtering discharge¹⁵. (c) The electric field E and the potential V for dc sputtering discharge versus the distance from the cathodes¹⁵.

system; Diodes and Magnetrons with dc or rf power, unless the discharge is self-supported. The Magnetron cathodes were described in detail elsewhere¹⁷. Permanent magnets are installed on the backside of the cathode to form confinement field configuration of E_xB at the front of the cathode. The secondary electrons are trapped by the discharge and describe loops of electrical current (the Plasma Ring) in the front of the target. Escaping outside the discharge becomes almost impossible before losing their energy to the gas. They return to the target unless losing energy during the first orbit. It has been suggested¹⁸ that a field configuration could be designed in a way that the entire electron orbit will never return to the cathode. This is probably the case in some high efficiency Magnetrons like the S-Gun and planar

cathodes. However, in Cylindrical systems¹⁷ the E_xB configuration is uniform and too perfect to be very efficient. The escaping electrons lose energy by collisions with the gas. The slow electrons diffuse outside the discharge and are collected by the anode and the chamber walls. The anodes on the one hand are to be designed for collecting the slow electrons and on the other hand not to interfere with the process of film growth on the substrates.

Several ionization mechanisms are present in the sputtering discharge¹⁹, but the collision between electrons and molecules in the gas phase is the most probable process. Ions are formed in the plasma ring, accelerated to the target in nearly straight lines and cause sputtering. The erosion pattern on the target is a vertical projection of the plasma ring where the topography follows the distribution function of the plasma density²⁰. It was thought that the problems of target shielding will disappear in magnetron systems. Several years of experience in deposition of semiconductors and optical waveguides by magnetron sputtering have shown that in these specific cases small amounts of impurities dramatically change the film properties. A small number of electrons escape the discharge near the target material causing sputtering of the backing plate or any supported material. Therefore shielding the target periphery is still important in Magnetron systems. Comparison between performances of Diodes and Magnetrons is described in Table 3. Note that the ionization coefficient, α is system independent, and the electron density distribution function, ρ , is system dependent. In dc diodes ρ has two main peaks versus the electrons energies²¹: the 'thermal' peak at about 5 eV and the 'cathodic voltage' peak at $V_c \approx 2-5$ keV. The thermal peak is populated by the low energy electrons. They do not contribute to the ionization process because of their small energies. The latter peak belongs to those electrons which cross the discharge from the cathode without losing much energy. Their energies are too high for efficient ionization process (see Figure 1).

The ionization density (ID) is given by $ID \propto \int_0^\infty \rho(v) \alpha(v) dv$, where ρ and α were defined before. The overlap range of ρ over α is a measure of this factor and it is described in Figure 4(a) and (b) for Diodes and Magnetrons, respectively. It is small in dc Diodes and very intense in dc Magnetrons. In dc Diodes, as mentioned before, the only contribution for ionization comes from the high energy electrons. However, these electrons make a small contribution to the ionization density. For maintaining the discharge the cathodic voltage V_c and the coefficient for the secondary electrons γ , have to be high. In Magnetrons $\rho(v)$ has just one peak near 100 eV. The ionization density is very high; the current is high too and the cathodic voltage stays at a low level.

In supported discharges like Triodes, the ionization density is kept high by supplying extra electrons at the right energies for efficient ionization from an additional electrode. For this, the parameter ranges in Triodes are considerably wider compared to those of the self-sustained discharges.

The minimum working pressure strongly depends on the ionization density of the system. At low ID the number of electron-ion pairs is kept high by increase in the gas pressure. Because of the possible control on the additional electrode in Triodes, the ID is extended from very low to very high, and therefore the working pressure can be changed from very high to very low, respectively.

Reactivity of the discharge depends among others on the presence of reactive species in the discharge atmosphere²². In any oxygen discharge, for example, the reactant concentration depends on the electron density distribution function²³. A high

Table 3. A comparison between performances of dc Diode and Magnetron sputtering

	dc Diode	dc Magnetron
Ionization density $\propto \int_0^{\infty} \rho(v) \alpha(v) dv$	Very low	Very high
The use of electrons	Minority of electrons are used for ionization and the others are lost to the anode	Most electrons are used for ionization
The cathodic voltage at constant pressure and electric power	Low ID = > Low current density = > High voltage	High ID = > High current density = > Low voltage
Gas pressure	Low ID requires high pressure to maintain the discharge	High ID works in both: low and high pressures
Electrical power P	Sparks limit the voltage below 5 KV	Limited by the cooling efficiency
Shielding	Shielding protects backing plate from sputtering	Confined discharge eliminates shielding
Deposition rate ²⁴ $\propto \int \frac{PS dv}{v(1+y)}$	Limited by the power density	Practically unlimited for metals
Target area	Limited	Unlimited

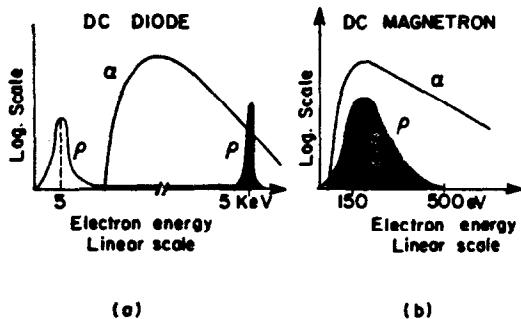


Figure 4. (a) and (b). The ionization coefficient α , and the electron density distribution function ρ , for dc Diode and Magnetron, respectively, versus the electron energy. The integral $\int_0^{\infty} \rho \alpha dv$ for Diodes is much smaller than for Magnetrons.

concentration of 'reactive' electrons (i.e. 100 eV electrons) means high ionization and disassociation rates and a high concentration of atomic oxygen. Therefore, Magnetrons are very reactive and Triodes are even more.

RF sputtering

Because of electrical charge accumulation on the target surface, dc power cannot be transferred to insulating targets. This difficulty can be overcome by using radio frequency sputtering²⁵. At high frequencies (MHz range) ions, unlike electrons, cannot follow the time variation in the applied field. Accordingly, in a steady state, symmetric system both electrodes develop negative dc self-bias, V_{sb} , with respect to the plasma potential. The ions follow the dc bias and move towards both electrodes and cause sputtering.

To convert the sputtering system from two sputtering electrodes to a single sputtering electrode modification in the sheath capacitance is required, that is, in the charge separation across the dark space. Electrodes of greater area will develop smaller bias potential²⁶.

With respect to the dc, the rf discharge is more efficient and extends over a larger volume. That is because in rf, the electron energy oscillates and passes through the maximum in the function of α versus electron energy twice every rf cycle. The extensive discharge volume is a result of rf propagation and reflection in lobes over the electrode space. A comparison between parameters of dc and rf sputtering discharges is given in Table 4. The differences between rf and dc in Diodes are more significant than in Magnetrons due to the motion of electrons in a nearly closed orbit in the ExB field configuration of the dc Magnetron. In this sense the motion of electrons in dc Magnetron is similar to the motion in rf Diodes.

Film properties

Film structure and morphology depend among other things; on substrate temperature and gas pressure. A two dimensional

Table 4. A comparison between dc and rf sputtering systems

	RF	DC
Target materials	Metals, semiconductors oxides	Metals, semiconductors
Pressure range for diodes for magnetrons	$p > 5.0 \text{ mtorr}$ $p > 0.5 \text{ mtorr}$	$p > 50 \text{ mtorr}$ $p > 5 \text{ mtorr}$
At constant power	Low V_{sb} High current	High V_c Low current
Plasma volume	Extended	Concentrated
Plasma reactivity	High	Low
Deposition rate	No difference	
Film properties	No difference	

diagram for sputtered films versus the gas pressure and the substrate temperature was described by Thornton^{27,28} for metal coatings by Magnetron sources. Similar behaviour was obtained for ZnO reactively sputtered by Planar Magnetron¹³.

ZnO layers, like other II-VI compounds, tend to grow with their *c*-axis perpendicular to the substrate²⁰. This crystallographic property is not entirely clear yet, and sputtering parameters such as ion energy, substrate temperature, gas pressure, impurities in the gas atmosphere or in the target material, substrate position with respect to the target, and substrate motion¹³ have considerable influence on this tendency. Most publications on piezoelectric ZnO layers suggest sputtering condition for optimum orientation of substrate temperature between 200 and 400°C. However, well oriented films were recently obtained at room temperature¹³. Considering the fact that crystals grow from water solutions, this is not surprising. The sputtered atoms and molecules carry enough kinetic energies for crystallization in any morphology and crystallographic form on the substrates at room temperature. Therefore the substrate temperature itself is probably not the key parameter for the growth mechanism, but the combination of the sputtering parameters that control the cooling mechanism of the sputtered species that is important. Unlike the methods of crystal growth from the melt, or solution, sputtering is a nonequilibrium method. The fact that preferred orientation along the *c*-axis is obtained, at different sputtering conditions, probably indicates that for the right cooling rate there is more than one combination of the sputtering parameters. Better control over the film properties will be obtained in a sputtering system of independent and wide ranging parameters. Even in this case, designing for new film properties requires an understanding of the intimate relationship between the sputtering parameters and the film properties.

Conclusion

We have reviewed and compared the principle parameters of the three basic sputtering deposition systems: Diodes, Magnetrons and Triodes, and have discussed some physical concepts of their discharges that have direct influence on system performance. We have found that Magnetrons in general are better than Diodes and Triodes have higher potential for future development than Magnetrons. The difficulty with Triodes is its supported discharge which is hard to control for reproducible results. DC Magnetrons

are at present the best methods for metallic targets and the rf Magnetrons are the best for insulators.

In some particular cases, deposition has to be made under special sputtering conditions: for example, bombarding the substrates by electrons. Diode sputtering systems seem to be the right method for this application. However, a combination of Magnetron and electron gun will probably do better.

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