

GEOMETRIC CONSIDERATIONS IN MAGNETRON SPUTTERING

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The recent development of high performance magnetron type discharge sources has greatly enhanced the range of coating applications where sputtering is a viable deposition process. Magnetron sources can provide high current densities and sputtering rates, even at low pressures. They have much reduced substrate heating rates and can be scaled to large sizes. Magnetron sputter coating apparatuses can have a variety of geometric and plasma configurations. The target geometry affects the emission directions of both the sputtered atoms and the energetic ions which are neutralized and reflected at the cathode. This fact, coupled with the long mean free particle paths which are prevalent at low pressures, can make the coating properties very dependent on the apparatus geometry. This paper reviews the physics of magnetron operation and discusses the influences of apparatus geometry on the use of magnetrons for rf sputtering and reactive sputtering, as well as on the microstructure and internal stresses in sputtered metallic coatings.

Magnetron Sputtering, Coating Technology.

1. Introduction

The past few years have seen a large increase in the use of sputter deposition for applications ranging from microelectronics to architectural glass plates. The reason can be traced largely to the development of

high performance magnetron type sputtering sources.¹ Magnetron discharge sources can provide high current densities, and therefore high sputtering rates, even at low pressures. The magnetic plasma confinement greatly reduces substrate heating, as compared to conventional sources, and permits even heat-sensitive substrate such as plastics to be coated at high rates. Cylindrical and planar magnetrons can be scaled to large sizes. This makes them attractive, for example, for solar energy related applications where large areas must be coated.

Magnetron sputtering sources can have a variety of geometric and plasma configurations. Target geometry affects the emission directions of both the sputtered atoms and the ions which are neutralized and reflected at the cathode surface. When considering the effects of these emission directions we must remember that the structure of vacuum deposited coatings is dependent on the arrival directions of the depositing atoms as well as on bombardment by energetic particles such as the reflected ions. The long mean free particle paths which are prevalent at low magnetron operating pressures permit near line-of-sight passage of atoms from the target to the substrates, thereby making the coating properties very dependent on the apparatus geometry. In the case of reactive sputtering, the coating properties are dependent on the surface chemistry at both the cathode and the surrounding chamber walls. Deposition conditions to produce given film properties can therefore vary from one apparatus to another in very subtle ways, and investigators working with one type of apparatus configuration must be very careful in making generalizations and in scaling to larger apparatus sizes.

This paper reviews magnetron sputtering technology with particular emphasis on some of these geometric effects and their consequences, both on film properties such as coating structure and internal stress, and on the use of magnetrons for rf sputtering and reactive sputtering.

2. Magnetron Discharge Geometries

Magnetron discharge sources can be defined as diode devices in which magnetic fields are used in concert with the cathode surface to form electron traps which are so confined that the EXB electron drift currents can close on themselves.^{2,3} Figure 1 shows some of the more common types of magnetron sources: A is the anode, B is the magnetic field direction, and C is the cathode. Magnetic field strengths sufficient to

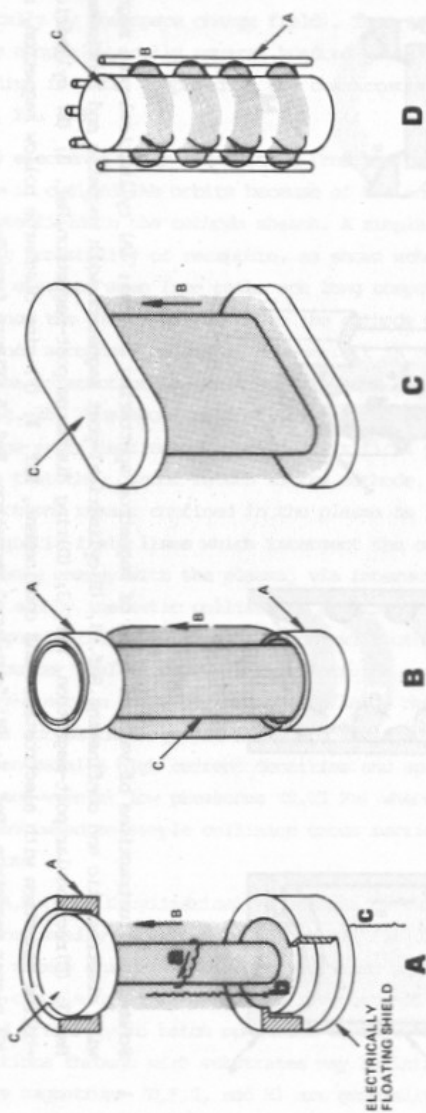


Fig. 1. Cont.

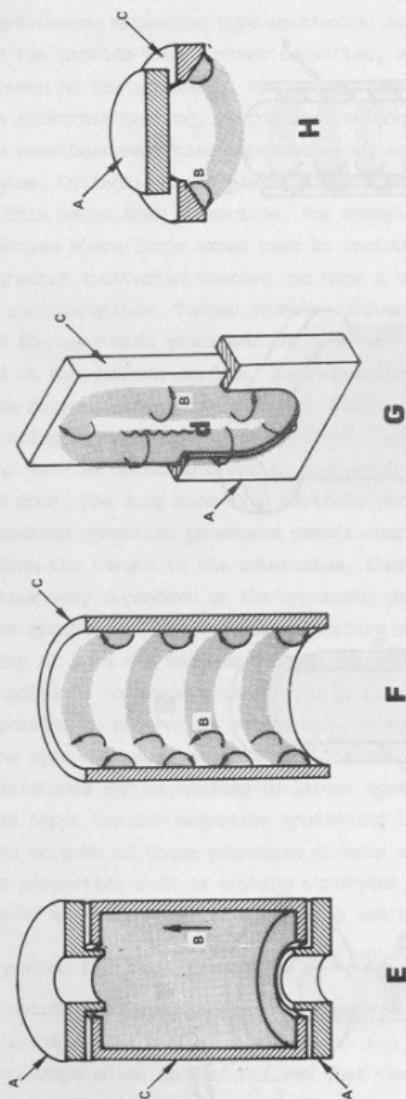


Fig. 1 Schematic illustrations of various types of magnetron sputtering sources: (A) cylindrical-post magnetron with electrostatic end confinement, Ref. 3; (B) cylindrical-post magnetron with magnetic end confinement, Ref. 3; (C) rectangular post-magnetron, Ref. 3; (D) ring discharge post-magnetron, Ref. 3; (E) cylindrical-hollow magnetron with electrostatic end confinement, Ref. 3; (F) ring discharge hollow magnetron, Ref. 3; (G) planar magnetron, Ref. 4; (H) "gun-type" magnetron, Ref. 5. Figure from Ref. 1.

confine the electrons but not the ions are used (the ions are confined electrostatically by the space charge field). Thus the field strength B is made large enough (typically several hundred gauss) so that the electron gyro radius is small compared to the characteristic plasma thickness d ; i.e., $B \propto 1/d$.

Secondary electrons which are emitted from the cathode by ion bombardment move in cycloidlike orbits because of the influence of the strong electric field in the cathode sheath. A simple calculation indicates a strong probability of recapture, as shown schematically in Fig. 2a, since the electron mean free paths are long compared to the orbit length and since the electrons return to the cathode with insufficient energy to induce secondary emission. However, it is believed that the electron-plasma interaction is enhanced by plasma oscillations, as indicated in Fig. 2b. Thus about half of the emitted electrons are believed to exchange sufficient energy during their first passage through the plasma so that they cannot return to the cathode. These "escaped" secondary electrons remain confined in the plasma as long as they are trapped on magnetic field lines which intersect the cathode. They continue to exchange energy with the plasma, via interaction with plasma oscillations² and by inelastic collisions, and in so doing advance across the magnetic field and finally, along with other low energy electrons, encounter field lines that intersect the anode(s). The average secondary electron therefore produces a large number of ions before it advances across the magnetic field and is lost from the system. This ionization permits high current densities and sputtering rates to be maintained even at low pressures (0.13 Pa) where the electron mean free paths based on simple collision cross sections can of the order of 100 cm.

The type A,B,C and E cylindrical magnetrons use uniform magnetic fields that are usually generated by solenoidal field coils mounted external to the vacuum chamber.⁶ This configuration permits the use of thick targets capable of storing a large inventory of coating material, but is limited primarily to batch operation because the field coils limit the directions through which substrates may be introduced. Ring type discharge magnetrons (D,F,G, and H) are generally configured to use permanent magnets mounted behind the target. Target thicknesses are

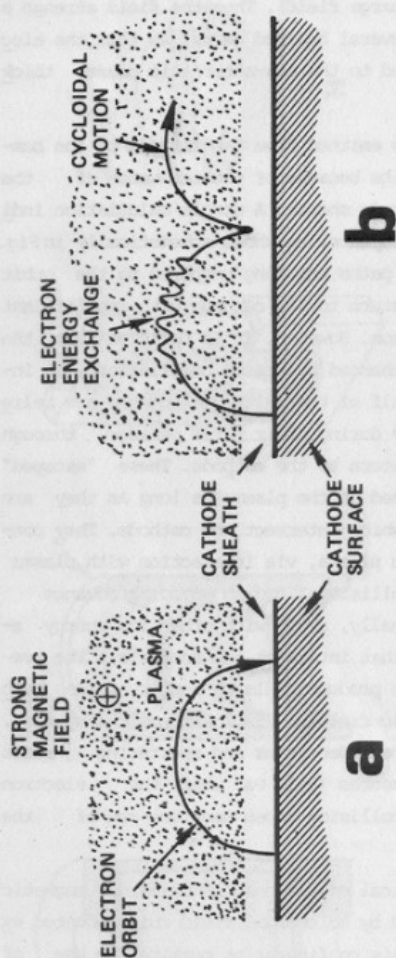


Fig. 2. Schematic illustration of the trajectory of secondary electrons emitted from the surface of a magnetron cathode in the presence of perpendicular magnetic and electric fields: (a) case of static fields; (b) case of plasma oscillations which produce temporal variations in electric field strength.

therefore limited. However, there is no restriction on substrate movement. Planar magnetrons (type G) are particularly effective for in-line processing. Hollow cathode magnetrons (E and F) are effective for coating wire, strip, or complex shapes, since the sputtered flux is uniform at all points within the hollow cathode, where end effects can be neglected.⁷ Cylindrical and planar magnetrons can be scaled to long lengths. Thus type A magnetrons over 2m long are used to metallize plastic automobile parts⁸ and type G magnetrons 2-4m long are used to coat architectural glass plates. When magnetic materials are to be sputtered, provisions must be made for magnetically saturating the target³.

3. Magnetron Discharge Performance

The discharge current-voltage (I-V) characteristic provides a signature which reveals a great deal about the discharge process.^{2,3} Figure 3 shows dc I-V characteristics for several of the magnetrons shown in Fig. 1, along with comparative data for a conventional planar diode. All the magnetron types are seen to have nearly identical I-V characteristics, of the form $I \propto V^n$, with n values in the range between 5 and 7. Operation at a low voltage, nearly independent of the current (a large value of n), is indicative of efficient ion generation by the secondary electrons in the plasma discharge.¹⁻³ Thus the dc driven magnetron discharges are very efficient.

Experiments have been conducted¹⁰ in which a cylindrical post magnetron was operated at current densities ranging from 10 mA/cm^2 to about 250 mA/cm^2 . The $I \propto V^n$ relationship was obeyed throughout this range, indicating that no new physical processes that are detrimental to the cathode operation became important as the device was driven to high current densities. Figure 4 summarizes the performance that was achieved at $J = 200 \text{ mA/cm}^2$. Note that the cathode erosion rate was about 1 mil/min. The sputtered flux spread radially to yield a deposition rate of about 40,000 Å/min at a radius of 56mm. It is interesting to note that under these operating conditions the density of sputtered Cu atoms leaving the target was of the same order of magnitude as the Ar working gas. In fact, Hosokawa et al.¹¹ have achieved sustained self-sputtering under similar conditions using type A and D magnetrons with Cu targets.

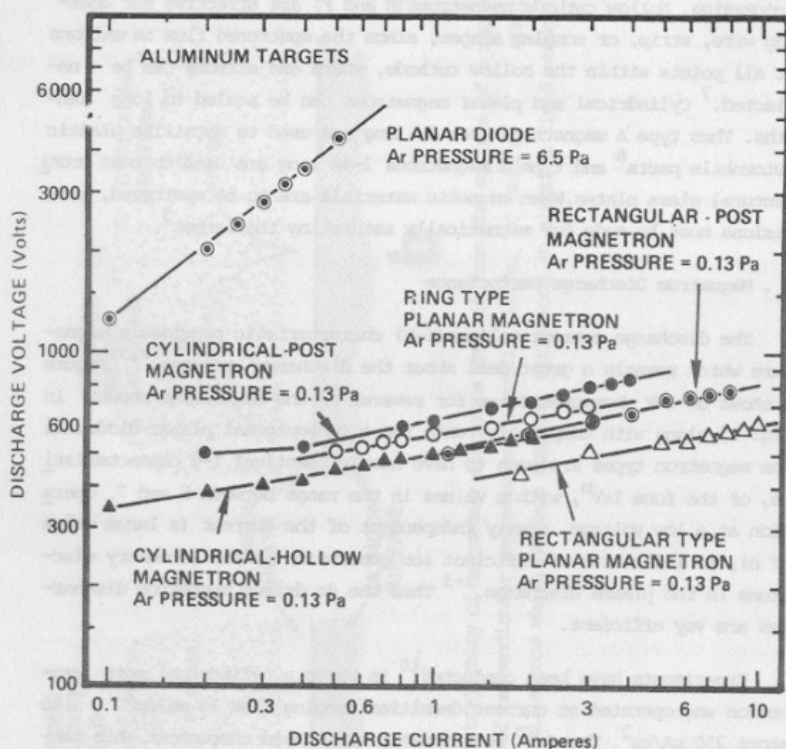


Fig. 3. Current-voltage (I-V) characteristics for dc operation of several of the magnetron sources shown in Figure 1. Comparative data for conventional planar diode is also shown. Figure from Ref. 1.

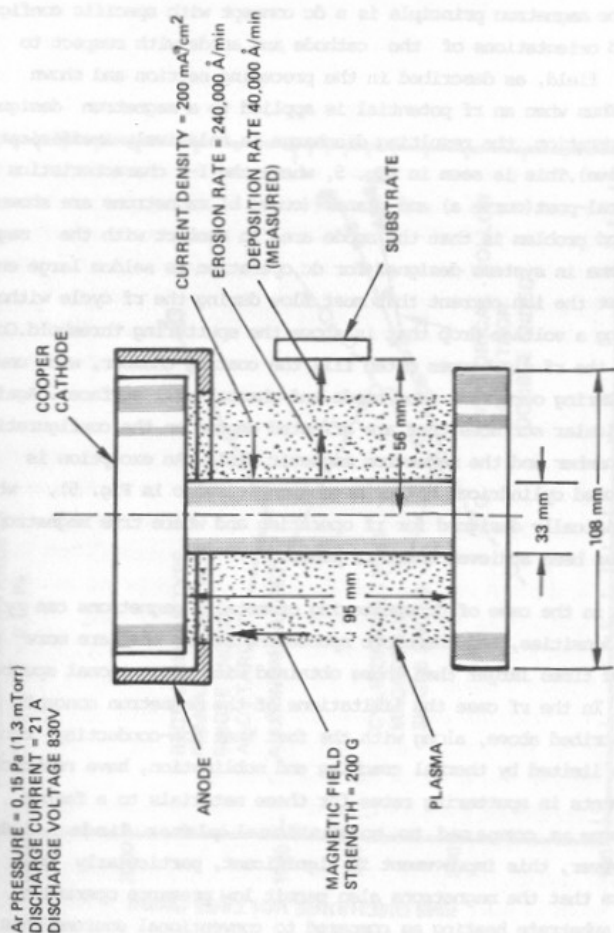


Fig. 4. Summary of cylindrical-post magnetron operation in high rate sputtering experiment. Figure from Ref. 10.

Unfortunately, the magnetron approach is not so effective for the case of rf sputtering non-conductors.¹ There are several reasons for this. First, the magnetron principle is a dc concept with specific configurations and orientations of the cathode and anode with respect to the magnetic field, as described in the preceding section and shown in Fig. 1. Thus when an rf potential is applied to a magnetron designed for dc operation, the resulting discharge is relatively inefficient (has low n-value). This is seen in Fig. 5, where the I-V characteristics for cylindrical-post (curve a) and planar (curve b) magnetrons are shown. The second problem is that the anode area in contact with the magnetron plasma in systems designed for dc operation is seldom large enough to collect the ion current that must flow during the rf cycle without developing a voltage drop that is above the sputtering threshold. Consequently, the rf discharges often fill the coating chamber, with unwanted sputtering occurring from anode and chamber wall surfaces. Again the particular surfaces that are affected depend on the configuration of the chamber and the magnetron magnetic field. An exception is the double-ended cylindrical hollow magnetron (curve c in Fig. 5), which was specifically designed for rf operation and where true magnetron behavior has been achieved under rf power.¹²

Thus in the case of dc sputtering of metals, magnetrons can yield current densities, and therefore sputtering rates, that are more than a hundred times larger than those obtained with conventional sputtering sources. In the rf case the limitations of the magnetron concept that were described above, along with the fact that non-conducting targets are also limited by thermal cracking and sublimation, have restricted improvements in sputtering rates for these materials to a factor of about three as compared to conventional planar diode sources. However, this improvement is significant, particularly when one considers that the magnetrons also permit low pressure operation and reduced substrate heating as compared to conventional sources. Thus rf driven magnetrons, particularly of the types shown in Figs. 1-G and 1-H, are becoming widely used.

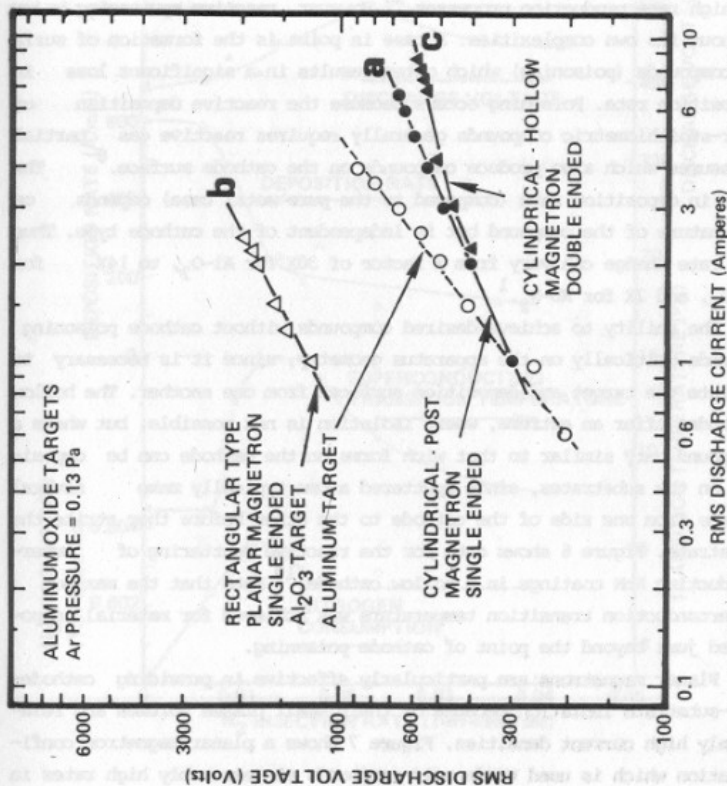


Fig. 5. Current-voltage (I-V) characteristics for rf operation of several of the magnetron sources shown in Figure 1. Figure from Ref. 1.

4. Reactive Sputtering

Magnetron dc reactive sputtering is attractive for depositing compounds because of the relative simplicity of the required target and power supplies compared to the rf case and because of the problems with rf magnetron sputtering that were described above. In fact, it is generally conceded that reactive sputtering will be required for large area or high rate production processes.¹³ However, reactive sputtering is not without its own complexities. A case in point is the formation of surface compounds (poisoning) which often results in a significant loss in deposition rate. Poisoning occurs because the reactive deposition of near-stoichiometric compounds generally requires reactive gas partial pressures which also produce compounds on the cathode surface.⁶ The loss in deposition rate (compared to the pure metal case) depends on the nature of the compound but is independent of the cathode type. Thus the rate change can vary from a factor of 30X for Al-O₂, to 14X for Ti-O₂, and 2X for Nb-N₂.¹

The ability to achieve desired compounds without cathode poisoning depends critically on the apparatus geometry, since it is necessary to isolate the target and deposition surfaces from one another. The hollow cathodes offer an extreme, where isolation is not possible, but where a compound very similar to that which forms on the cathode can be deposited on the substrates, since sputtered atoms typically make several passes from one side of the cathode to the other before they strike the substrate. Figure 6 shows data for the reactive sputtering of superconducting NbN coatings in a hollow cathode.¹⁰ Note that the maximum superconduction transition temperature was achieved for material deposited just beyond the point of cathode poisoning.

Planar magnetrons are particularly effective in providing cathode-to-substrate isolation because of their small plasma volumes and relatively high current densities. Figure 7 shows a planar magnetron configuration which is used to deposit compounds at reasonably high rates in the absence of poisoning. The slotted shield, along with the gettering of reactive species which enter into the cathode region, is used to permit a reactive gas concentration gradient to be maintained between the substrate and the cathode. A large cathode-to-substrate spacing is very helpful. Indeed, the combination of high cathode power densities and a large cathode-to-substrate spacing has been found to be particu-

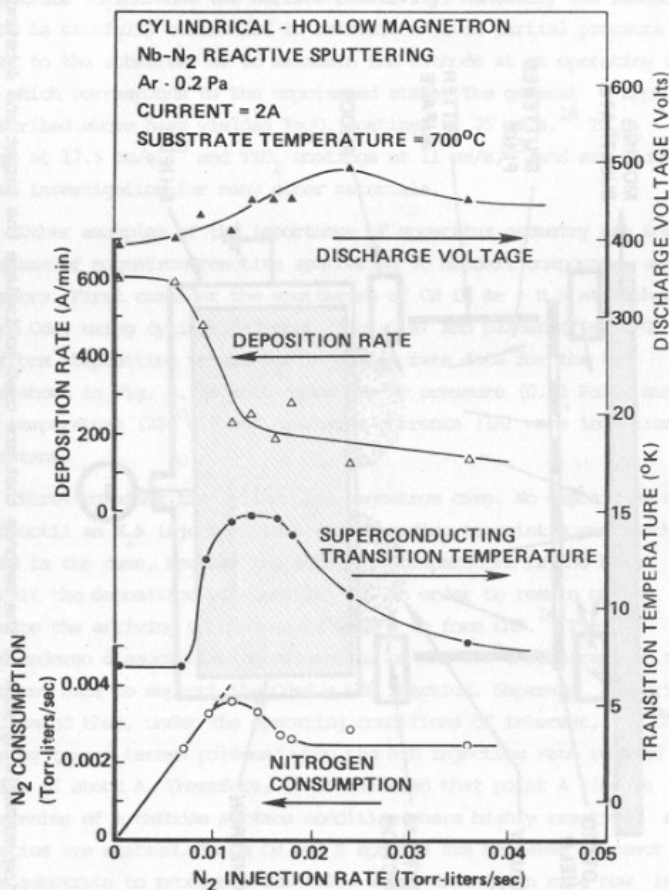


Fig. 6. Experimental data showing change in deposition and coating parameters due to cathode poisoning during Nb-N₂ reactive sputtering in hollow cathode. Figure from Ref. 10.

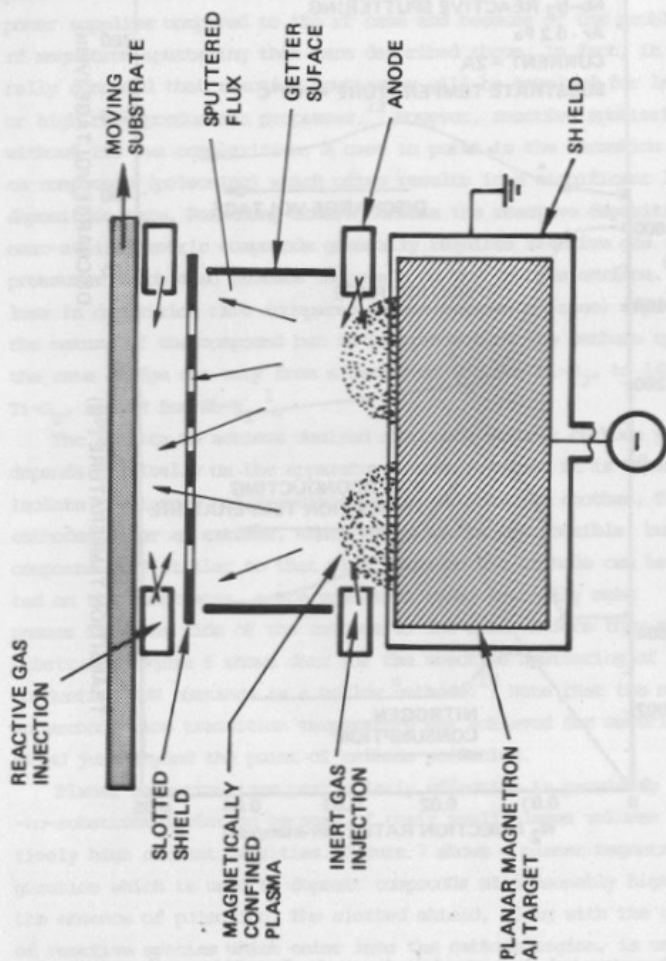


Fig. 7. Schematic drawing summarizing some of the methods that are used to isolate the target and substrate chemistry in reactive sputtering.

larly effective.¹³ A plasma discharge may also be placed adjacent to the substrate to increase the surface reactivity. Generally the reactive gas flow is carefully controlled to maintain a given partial pressure adjacent to the substrate or to maintain the cathode at an operating voltage which corresponds to the unpoisoned state. The general approaches described above have yielded In_2O_3 coatings at 25 nm/s,¹⁴ Ta_2O_5 coatings at 17.5 nm/s,¹⁵ and TiO_2 coatings at 11 nm/s,¹⁵ and are under active investigation for many other materials.

Other examples of the importance of apparatus geometry are seen in the use of magnetron reactive sputtering to deposit compound semiconductors. First consider the sputtering of Cd in Ar + H_2S atmosphere to form CdS, using cylindrical-post (Fig. 1-A) and planar (Fig. 1-G) magnetrons. Deposition versus H_2S injection rate data for the two cases are shown in Fig. 8. In both cases the Ar pressure (0.13 Pa), substrate temperature (250°C), and discharge currents (1A) were identical and constant.

First consider the cylindrical magnetron case. No deposition occurred until an H_2S injection rate corresponding to point A was reached. This is the case, because the substrate temperature is too high to permit the deposition of elemental Cd. In order to remain on the substrate the arriving Cd must react with S to form CdS.¹⁶ The H_2S does not undergo dissociative chemisorption on the 250°C substrate at a sufficient rate to support the $\text{Cd} + \text{S} \rightarrow \text{CdS}$ reaction. Separate experiments indicated that, under the operating conditions of interest, the Cd sputtering target became poisoned when the H_2S injection rate reached a value of about A. Therefore, it is believed that point A signals the beginning of a cathode surface condition where highly reactive sulfur species are emitted. These Cd and S species are believed to react on the substrate to produce a CdS film, whose deposition rate now increases with the H_2S injection rate. Thus the sulfur flux is rate-limiting in region B of the figure. At higher H_2S injection rates (region C) the deposition rate is limited by the available Cd flux. The coatings deposited in regions B and C are different. Thus In doping was found to be very effective in reducing the resistivity of coatings deposited in region B, but relatively ineffective for coatings deposited in region C (Cd flux rate-limiting), apparently because of compensation by Cd va-

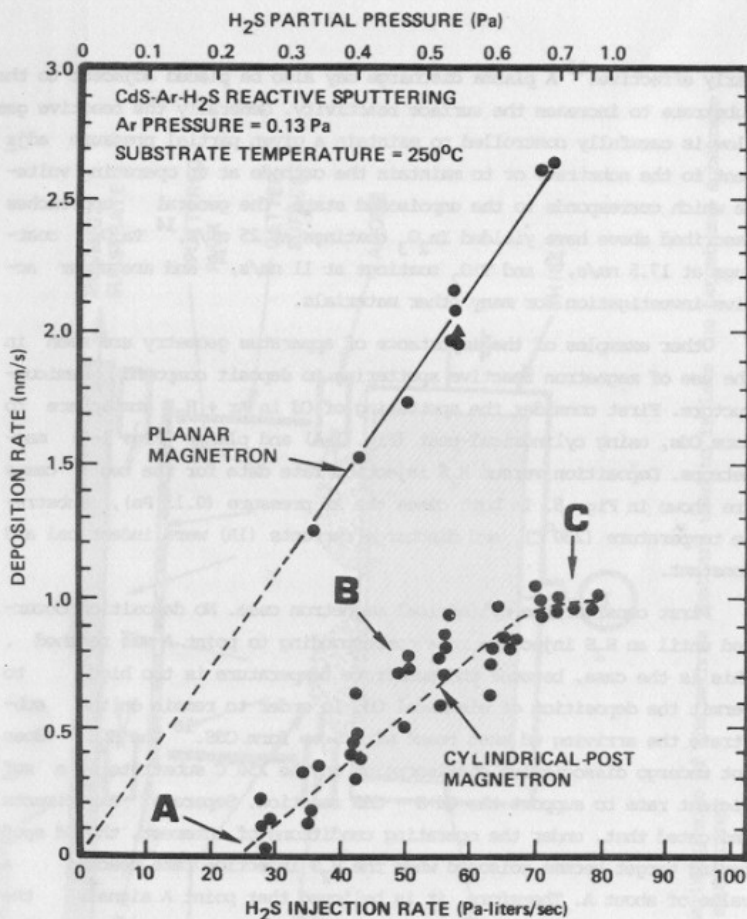


Fig. 8. Deposition rate versus H₂S injection rate for CdS coatings deposited by Cd-Ar-H₂S reactive sputtering using a cylindrical-post and a planar magnetron sputtering source under otherwise constant deposition conditions.

cancies.¹⁷

The planar magnetron data in Fig. 8 differ from the cylindrical magnetron data in two ways. First, the planar magnetron deposition rates are larger by a factor of three. This is a simple consequence of the fact that the sputtered flux from a planar magnetron tends to pass in one direction, rather than radially as in the case of the cylindrical magnetron. Second, the linear region of sulfur-rate-limited deposition for the planar magnetron appears to project through zero with no threshold H_2S injection rate being required. The exact cause of the latter point is not known. However, one of the significant differences between the two cathode geometries is that the current density and surface chemistry are relatively uniform in the cylindrical case, while they are not in the planar case. The nonlinear current density in the planar magnetron case causes some regions of the cathode surface to be poisoned even at very low H_2S injection rates. Sulfur Species emitted from these poisoned regions might be the precursors that permit deposition to occur at all H_2S injection rates.

Figures 9 and 10 illustrate the importance of apparatus surface chemistry in achieving steady state operation.¹⁸ Figure 9 shows the resistivity versus H_2S injection rate for Cu_xS coatings deposited under otherwise constant conditions using a type 1-A cylindrical magnetron. Figure 10 shows the variation in resistivity during equilibration of the system at a constant H_2S injection rate (point X in Fig. 9) for the following different starting conditions: Cases a and a - the cathode and wall surfaces were initially in a fresh Cu state; Case b - the cathode was in the Cu-state and the walls were in a conditioned state achieved by sustained operation (200 min) at condition x; and Case c - the cathode was in the conditioned state and the walls were in the Cu-state. It is seen that the required conditioning times, before consistent coatings are deposited, can be as long as 100 min.

5. Coating Structure and Stress

The microstructure and the stress state in sputter deposited coatings are strongly affected by: [1] the angle of incidence of the arriving coating atoms; [2] bombardment by energetic working gas atoms (i.e., ions which are neutralized and reflected at the target surface); [3] bom

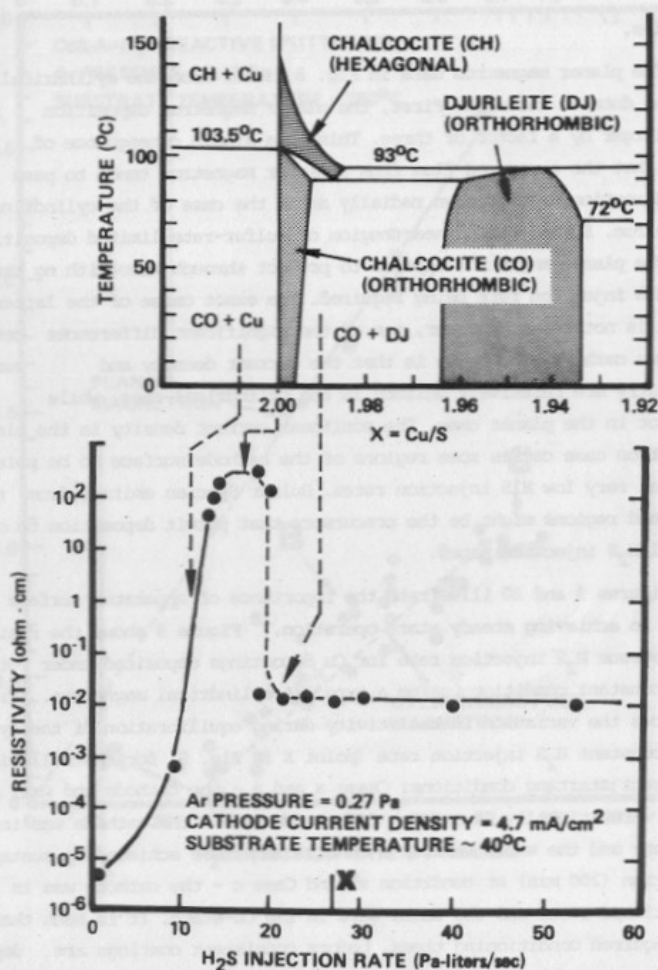


Fig. 9. Resistivity versus H_2S injection rate for Cu_xS coating deposited by Cu-Ar- H_2S reactive sputtering using a cylindrical-post magnetron. Figure from Ref. 18.

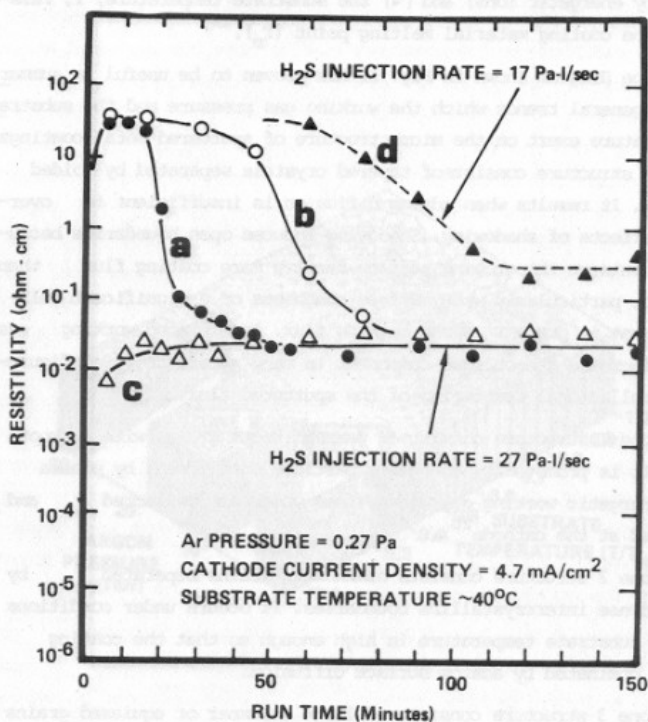


Fig. 10. Resistivity versus run time data showing the conditioning of the cathode and wall surfaces during Cu-Ar- H_2S reactive sputtering using a cylindrical-post magnetron source. See text. Figure from Ref. 18.

bombardment by energetic ions; and [4] the substrate temperature, T , relative to the coating material melting point (T_m).¹⁹

The Zone Diagram shown in Fig. 11 has proven to be useful in summarizing the general trends which the working gas pressure and the substrate temperature exert on the microstructure of sputtered metal coatings. The Zone 1 structure consists of tapered crystals separated by voided boundaries. It results when adatom diffusion is insufficient to overcome the effects of shadowing. Shadowing induces open boundaries because high points on the growing surface receive more coating flux than valleys do, particularly when surface roughness or a significant oblique component is present in the coating flux. An elevated working gas pressure increases the oblique component in many apparatus configurations by collisional scattering of the sputtered flux.

The Zone T structure consists of dense fibrous grains with a smooth surface. It is promoted by energetic particle bombardment by plasma ions or energetic working gas atoms (ions which are reflected and neutralized at the cathode²⁰).

The Zone 2 structure consists of columnar grains separated by distinct dense intercrystalline boundaries. It occurs under conditions where the substrate temperature is high enough so that the coating growth is dominated by adatom surface diffusion.

The Zone 3 structure consists of large columnar or equiaxed grains which result from recrystallization or grain growth due to bulk diffusion.

Many sputtering applications, particularly with refractory metals, involve deposition at low T/T_m where the Zone T and Zone 1 structures are relevant. The magnetic plasma confinement minimizes ion bombardment in the magnetron case. Thus the energetic neutral atoms which are created by ion reflections at the target are particularly important in promoting the Zone T structure. Magnetron operating pressures are frequently low enough so that these energetic particles can reach the substrates with little loss of energy.

The emission angles of sputtered atoms from a target surface depend on the nature of the target and the ion energy.²¹ The energy and flux of reflected and neutralized ions depends on these same parameters,

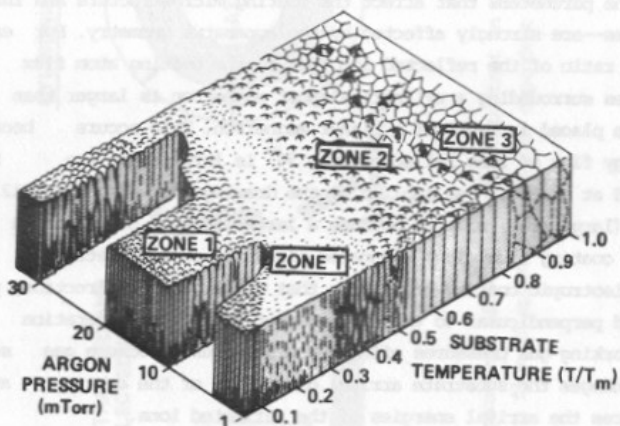


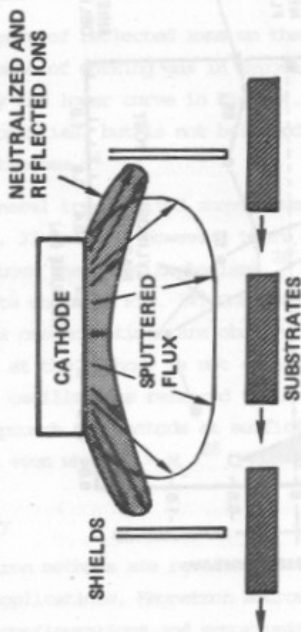
Fig. 11. Zone diagram relating microstructure of sputtered metal coatings to argon working gas pressure and substrate temperature, T , relative to the coating material melting point, T_m . From Ref. 19.

and also on the scattering cross section.^{22,23} Consequently, the two fluxes are not proportional. As noted above, many magnetron systems are operated at sufficiently low pressures so that both the sputtered atoms and the neutralized and reflected ions can reach the substrate without making collisions.³ Consequently, the relative fluxes of reflected ions and sputtered atoms and the angles of incidence of the sputtered atoms—i.e., the parameters that affect the coating microstructure and internal stress—are strongly affected by the apparatus geometry. For example, the ratio of the reflected ion flux to the coating atom flux for substrates surrounding a cylindrical-post magnetron is larger than for substrate placed in front of a planar magnetron. This occurs because the energy flux of ions reflected at $\sim 90^\circ$ is larger than the flux reflected at $\sim 180^\circ$,²⁴ as implied by the drawings shown in Fig. 12. Extended (large area) sources produce a larger oblique component in the arriving coating flux. Thus elongated planar or post magnetrons can yield anisotropic coating properties that differ in the direction parallel and perpendicular to the long axis of the source. Operation at higher working gas pressures affects the structure, because gas scattering changes the substrate arrival directions of the coating atoms and reduces the arrival energies of the reflected ions.

Zone T coatings have been found generally to be in a state of compression.²⁴⁻²⁸ It is believed that the compressive stresses are produced by an atomic peening process.²⁴⁻³² Oblique incidence, resulting from the apparatus geometry effects at low pressures or gas scattering at high pressures, promotes the more open Zone I structures and tensile stresses. Thus shields such as those shown schematically in Fig. 12 are often used to limit the oblique coating flux.

Figure 13 shows internal stress versus pressure data for planar, cylindrical-post, and cylindrical-hollow magnetrons. The anisotropic effect is shown in the planar magnetron data;³¹ i.e., the greater oblique component of coating flux in the direction parallel to the cathode axis promoted a tensile stress. The greater reflected ion flux in the post cathode case resulted in the formation of dense coatings with compressive stresses, even at higher working pressures. In the hollow cathode case the reduced reflected ion component, and the larger oblique component of the coating flux, resulted in only tensile stresses.²⁴ However,

PLANAR CATHODE



CYLINDRICAL CATHODE

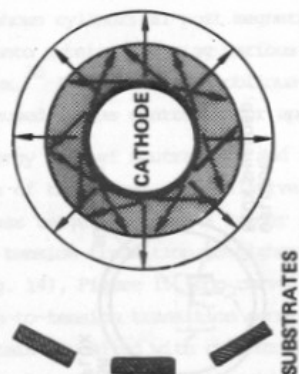


Fig. 12. Schematic illustration showing some of the geometric effects that are important in sputtering. The ratio of the flux of reflected and neutralized ions to flux of sputtered atoms is dependent on the cathode shape and the substrate position. Figure from Ref. 10.

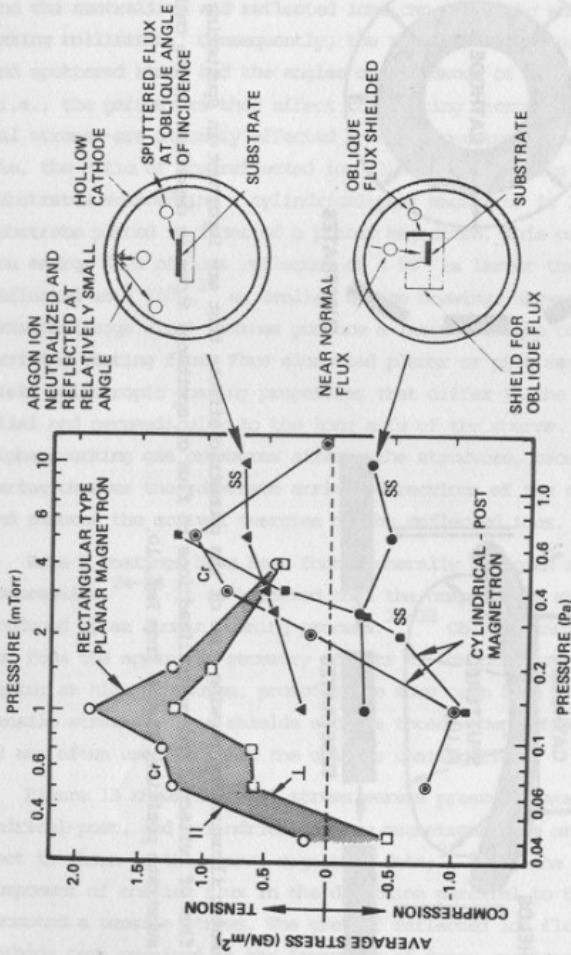


Fig. 13. Internal stress versus argon working gas pressure for planar, cylindrical-post, and cylindrical-hollow cathodes with chromium or stainless steel (SS) targets. Hollow cathode case with shielded substrate also shown. Data from Ref. 24 and 31.

when shields were added to remove the oblique coating flux, the hollow cathode coatings were in compression, even at relatively high pressures. Figure 14 shows cylindrical-post magnetron coatings deposited at low pressures onto substrates having various orientations relative to the coating flux.³⁰ It is seen that oblique incidence promotes tension, whether it is caused by gas scattering or apparatus configuration.

The energy flux of neutralized and reflected ions depends on the atomic mass of the target (M_t) relative to that of the working gas (M_g). The high mass targets produce a larger reflected ion energy flux and extend the tension transition to higher pressures (Fig. 13) or larger angles (Fig. 14). Figure 15 (top curve) shows the pressure at which the compression-to-tension transition occurred, as a function of M_t/M_g , for various metals deposited with cylindrical-post magnetrons. The triangle data points show that the relationship is independent of whether M_g or M_t is varied.

The impact of reflected ions on the growing coating also results in the entrapment of working gas in deposits formed at low T/T_{II} . This effect is shown by the lower curve in Fig. 14. The entrapped gas can affect coating properties, but is not believed to be responsible for the compressive stresses.²⁴

The general trends cited above have been observed by many investigators (Refs. 33 and 34). However, there are still many questions to be answered about the exact mechanisms.²⁸ A case in point is the amorphous silicon data shown in Fig. 14. Compressive stresses and high entrapped working gas concentrations are observed at mass ratios where simple ion reflection at the cathode is not expected.²⁸ It has been speculated that the plasma oscillations referred to in Section 2 may cause some of the ions to approach the cathode at sufficiently oblique angles to undergo reflection even when $M_g > M_t$.²⁸

6. Summary

Magnetron methods are revolutionizing sputtering technology and its range of applications. Magnetron sources provide a wide variety of apparatus configurations and opportunities for scaling to large deposition areas. However, extreme care must be exercised in process development, since scaling, the application of methods such as rf and reactive

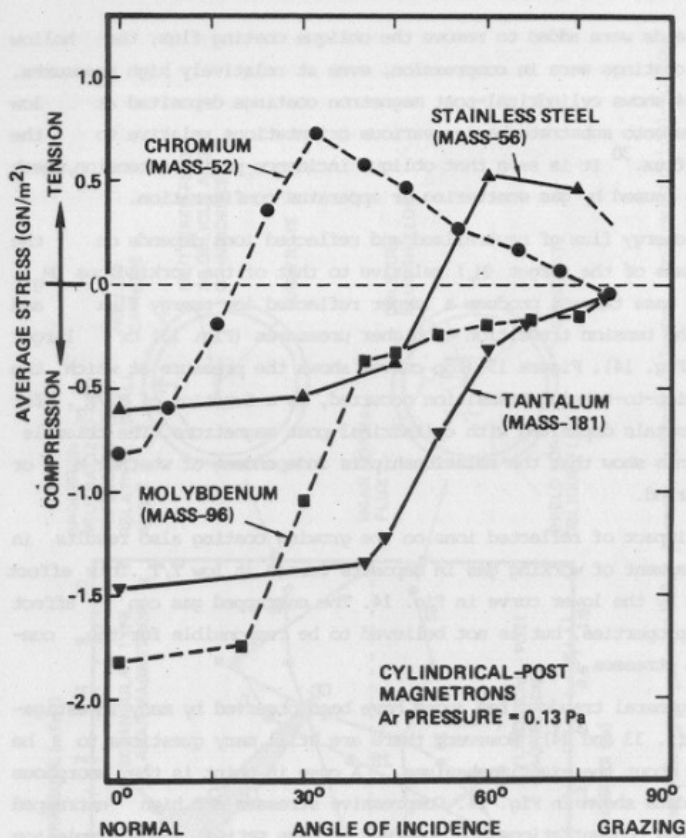


Fig. 14. Internal stress versus orientation substrate normal relative to line from substrate passing through axis of cylindrical magnetron source. Data from Ref. 30.

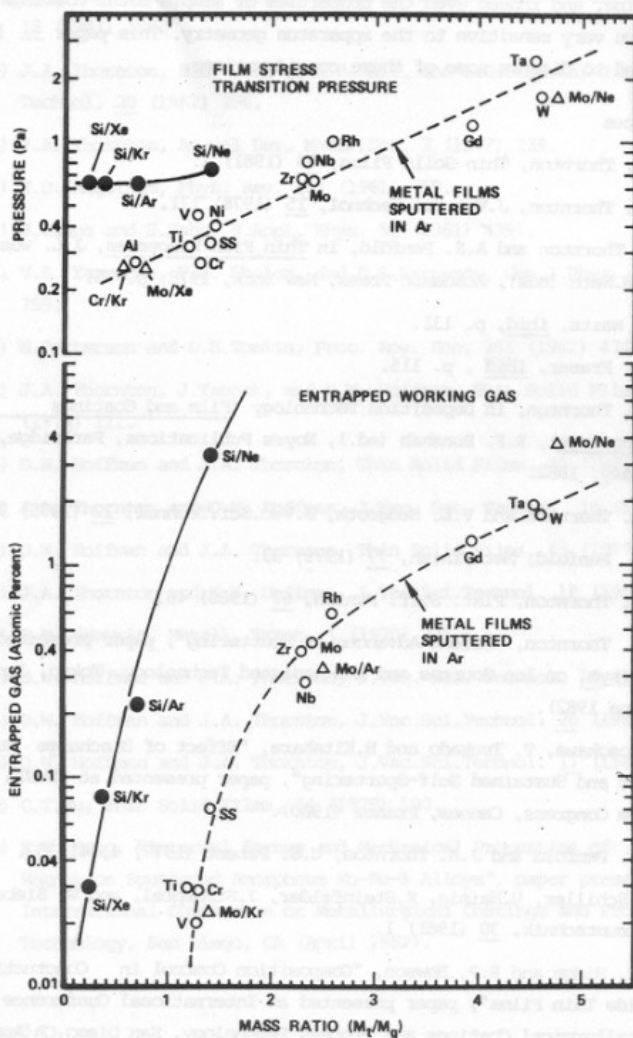


Fig. 15. Internal stress transition pressure and amount of entrapped working gas as a function of the target-to-working-gas mass ratio for sputtering with cylindrical post magnetrons. Data include experiments with various target and working gas combinations. See Ref. 28.

sputtering, and indeed even the properties of simple metal coatings are often very sensitive to the apparatus geometry. This paper has attempted to discuss some of these considerations.

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