Optical Thin Films II: New Developments

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Optical Thin Films II: New Developments

R. Ian Seddon
Chair/Editor

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OPTICAL THIN FILMS II: NEW DEVELOPMENTS

Volume 678

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Conference 678, *Optical Thin Films II: New Developments,* was part of a five-conference program on Optical Elements held at SPIE's 30th Annual International Technical Symposium on Optical and Optoelectronic Applied Sciences and Engineering. The other conferences were

Conference 675, *Stray Radiation V*
Conference 676, *Ultraprecision Machining and Automated Fabrication of Optics*
Conference 679, *Current Developments in Optical Engineering and Diffraction Phenomena*
Conference 680, *Surface Characterization and Testing*

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INTRODUCTION

This conference was the first United States general SPIE meeting on optical thin films since 1982. The format was similar to the 1982 meeting with a half-day session of invited papers keyed to the contributed papers in the three following sessions. As in 1982, there was excellent international representation in both the invited and the contributed papers.

It is appropriate to compare the two meetings and explore the extent of which changes in topics and content reflect changes in the field of optical thin films over the past four years. In 1982 the three topics for contributed papers were processes and properties, high volume applications, and instrumentation. For this conference it was decided that instrumentation was adequately covered in parallel sessions and that since the pace of development in high volume processing has been relatively slow, it was more appropriate to broaden this session to cover new applications in general.

The most exciting difference between the 1982 and 1986 sessions was in the areas of film structure and film processes. In 1982 there was one session primarily devoted to the very new field of ion-assisted processes. At the time this was considered a major meeting on this topic, and it evoked considerable interest. However, the papers were primarily reports of experimental work, and there was little evidence that the basic mechanisms were understood. By 1986 this field easily justified two sessions—one on structure and properties and one on new processes. The session on structure and properties demonstrated clearly the tremendous increase in understanding of the nature of thin films that has taken placc in the last four years. The session on processes showed that we are not only developing an arsenal of techniques for adding energy to growing films, but also starting to understand the mechanisms involved in tailoring the properties of the resulting films.

R. Ian Seddon
Optical Coating Laboratory, Inc.

OPTICAL THIN FILMS II: NEW DEVELOPMENTS

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Session 1

Invited Papers

Chair

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Structure and related properties of thin film optical coatings

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Abstract

In this review paper, we provide a survey of nucleation and growth models for thin films. Centered on a simplistic computer simulation of random ballistic agglomeration of molecules represented as two dimensional hard-disks, which is valid for the limit case of very low surface mobility or of no surface mobility at all, we explain various properties of thin film optical coatings, notably their sometimes unstable behaviour.

Introduction

The deposition of thin films in general and of optical coatings in particular involves three fundamental steps, 1) creating individual species of the finally desired coating materials, 2) transporting them from their source to the surface to be coated (the substrate), and 3) rearranging them on the substrate surface in some way to form a thin film with specific physical, in particular optical properties. Although these three steps of additive film formation can be found with every deposition process, we will limit ourselves in the following paper to the most widely used methods of the industry, which are categorized as physical vapor deposition (PVD). In these cases, the individual coating material species are primarily created by evaporation in a most general sense, including thermal (resistive boat and electron beam) evaporation and various kinds of sputtering (DC- or RF-diode sputtering, magnetron sputtering, ion beam sputtering). Ion-assisted and plasma assisted deposition methods are also frequently counted into this category. For the sake of clarity, we will further restrict our considerations to thermally evaporated coatings which represent the largest subgroup of PVD coatings. However, the discussion of fundamental interactions of thin film formation and resulting properties for this subgroup may provide a principal understanding of the peculiarities of thin film coatings which will allow appreciation of improvements brought about by more complex deposition techniques such as sputtering in its various forms, ion-assisted PVD processes, and ion-plating.

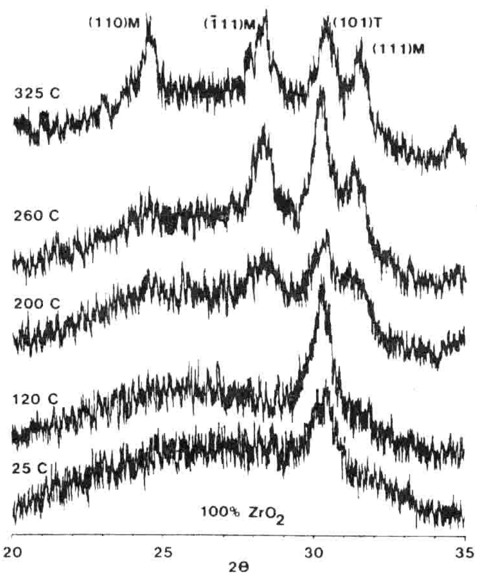
Condensation and nucleation of thin films

In thin[1] film physics, condensation and nucleation have been studied extensively for man years.[2,3] Unfortunately for optical engineering, these mechanisms have almost always bee studied in ultrahigh vacuum (UHV) conditions with model systems of metal deposits (usuall noble metals) on cleaved single crystal surfaces. The reason for this, of course, is th ability to better characterize the individual condensation and nucleation events on a atomic or molecular scale. Results obtained with such model systems may be considered c limited value for real systems, i.e. for dielectric thin film coatings deposited on optica elements, but are essential for the fundamental understanding of thin film formatio processes.[4]

One of the fundamental results of the above mentioned model studies is the strong dependence of the mobility of atoms and molecules after their arrival on the substrate surface (called the surface mobility of adspecies) on the melting temperature of the respective solid material, and on the temperature of the substrate surface. As a direct consequence, the surface mobility of the usually refractory metal oxides used for thin film optical coatings can be assumed very small or negligible, although very little experimental dat exists for this class of materials. This limited surface mobility justifies the simplistic hard-disk model employed in computer simulations reviewed in this paper.

Another key result of fundamental condensation and nucleation studies is the preferential nucleation of adspecies on defect sites of the substrate surface, such as crystallographic dislocations, cleavage steps, and kinks. This effect, for example, has been intentionally used in electron microscopy with the "decoration" method where the equivalent mass of a submonolayer of gold is deposited on cleaved crystal surfaces in order to study dislocation steps. The physical reason for this preferential nucleation is the variation of binding energies at different kinds of nucleation sites. An adspecies faces roughly two times the binding energy for the undisturbed plain surface when encountering a step, and about three times in the case of a kink. This preferential nucleation favors the further growth of already existing clusters over the settling of adspecies on unoccupied places of the undisturbed and still uncoated substrate surface, since, if they have some surface mobility, the probability of their capture at the edge of an already existing cluster is higher than the probability of finding rest on an unoccupied plain surface site. Adspecies will settle where they arrive in a random manner only at zero surface mobility and result in a highly disordered microstructure which is quasi-amorphous. From this consideration, one can expect films of higher order, i.e. more pronounced crystallinity, for elevated substrate temperatures during deposition, whereas films deposited at lower temperatures should be more amorphous. Indeed this result has been found for instance for ZrO_2 films deposited by electron beam evaporation in an UHV equipment at about 10^{-8} mbar (Fig. 1)[5,6] on substrates kept at temperatures ranging from 25°C to 325°C.

As a third result, it has been found that the surface mobility of metal adatoms (e.g. gold and platinum) is greatly reduced when they are co-deposited with carbon, for example, consequently decreasing the size of nucleating clusters. This effect has been made use of for many years for shadowing of replica films for transmisson electron microscopy and for the conductive coating of dielectric samples for scanning electron microscopy. Notably, a similar decrease in grain size and a corresponding transition from polycrystalline to quasi-amorphous structure has been found for the electron-beam co-deposition of ZrO_2 and SiO_2 (Fig. 2) or MgO at near-UHV conditions[5] and for mixed Al_2O_3/SiO_2 layers co-sputtered from metal targets.[6] The deposition processes in standard high vacuum systems are carried out at a residual pressure of about 10^{-6} to 10^{-5} mbar for thermal evaporation and at about 10^{-4} to 10^{-3} mbar for sputtering. It has to be kept in mind that at these pressure ranges a codeposition of the residual gas from the vacuum chamber takes place, since the rate of impinging molecules from the background gas is about the same as the typical deposition rate itself. Indeed, an influence of the residual gas pressure on the microstructure of thermally evaporated ZnS layers became evident from cross-sectional electron micrographs presented in 1975 at the 3rd International Thin Film Conference in Budapest by two different research groups. Whereas ZnS films deposited in standard production-type high vacuum processes (10^{-5} mbar) displayed the typical columnar microstructure[7] as also known for many other materials; ZnS films deposited in improved high vacuum conditions (10^{-7} mbar) were found to be structureless[8] when examined in the transmission electron microscope by the same cross-section replication technique.[9,10] If reactive evaporation is used by intentionally maintaining an O_2 partial pressure of high 10^{-5} to low 10^{-4} mbar, the desired oxidation of coating material on the substrate surface can be expected along with an influence on the microstructure of the thin film. Such an influence has indeed been observed for Ta_2O_5/SiO_2 multilayer coatings with an increase of the nodular defects density with increasing O_2 partial pressure.[11]



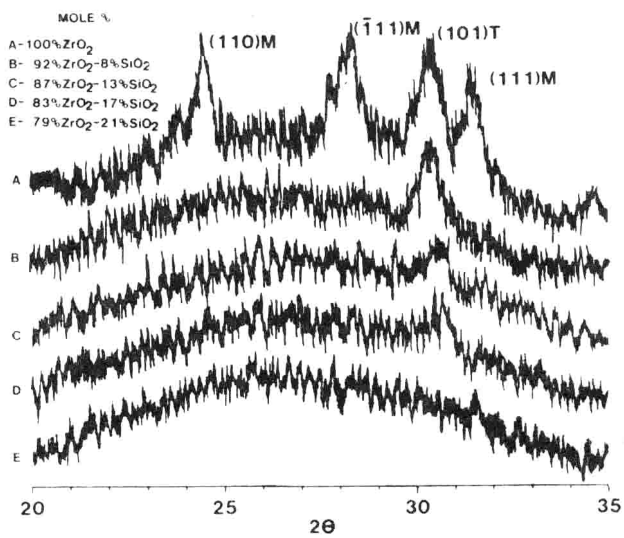


Fig. 1 (left) Influence of the substrate temperature during e-beam vapor deposition of ZrO_2 on the crystallinity of the resulting films as seen by X-ray diffraction analysis.[5] The M-peaks indicate a monoclinic phase, the T-peaks a tetragonal or cubic phase.

Fig. 2 (right) Influence of the addition of SiO_2 to ZrO_2 thin films by means of simultaneous evaporation from two separate e-beam sources on the resulting film on a substrate held at 325°C. The X-ray diffractograms A to E reveal the crystallinity of single layer ZrO_2 thin films with 0, 8, 13, 17, and 21 Mole % SiO_2, respectively.[5]

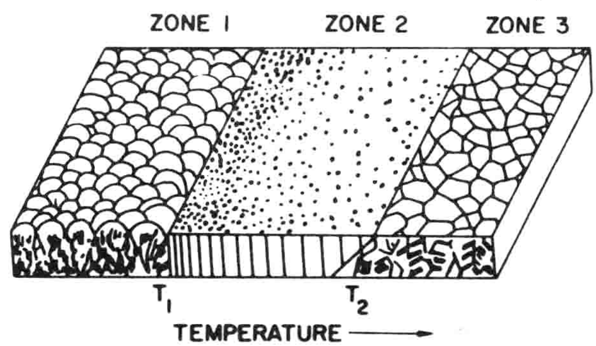
Another result of fundamental condensation and nucleation studies is the proven influence of the condition of the surface to be coated on the number and size of initial stage clusters, which in turn determine the further growth and resulting microstructure of the thin film. This remarkable influence of cleanliness on an atomic scale versus adsorbed foreign material such as water vapor or backstreamed vapor from oil diffusion pumps has been demonstrated, for example, with silver deposits on freshly evaporated SiO films which were partially "contaminated" by exposure to water vapor or diffusion pump oil vapor prior to the deposition of the silver.[12] The result was a higher number and a smaller average size of isolated clusters for the contaminated SiO surfaces as compared with a network-like discontinuous silver film on a fresh SiO surface, in both cases for an equivalent mass thickness of 5 nm.

Already nucleated deposits (atoms, molecules, clusters) can gain an increased surface mobility when the substrate temperature is raised. When Au or Cu is deposited in such small amounts that discontinous films basically consisting of an array of isolated clusters are formed, a post-deposition heat treatment of some hundred degrees Celsius will reduce the number and increase the size of these clusters or islands considerably.[13] A similar thermally induced change can be assumed for the microstructure of dielectric thin films, although on a less pronounced scale because of lower mobility. Even with low mobility, though, long-term changes of the microstructure can occur at room temperature which are commonly known as aging effects.

Thin film growth models

Structure models

Since nucleation is governed by the free energy of cluster formation and by the surface mobility of adspecies which are both functions of the temperature at which nucleation occurs, it is not surprising that the best known model for thin film growth, the structure zone model by Movchan and Demchishin[14], relates the observable structure of electron beam evaporated films to the substrate temperature T_s. More precisely, it is the reduced sub-



	ZONE 1	ZONE 2	ZONE 3
METALS	$<0.3\,T'_m$	$0.3-0.45\,T'_m$	$>0.45\,T'_m$
OXIDES	$<0.26\,T'_m$	$0.26-0.45\,T'_m$	$>0.45\,T'_m$

	T_1 [K]	T_2 [K]	T_m [K]
ZrO_2	648	1273	2973
Al_2O_3	623	1173	2323

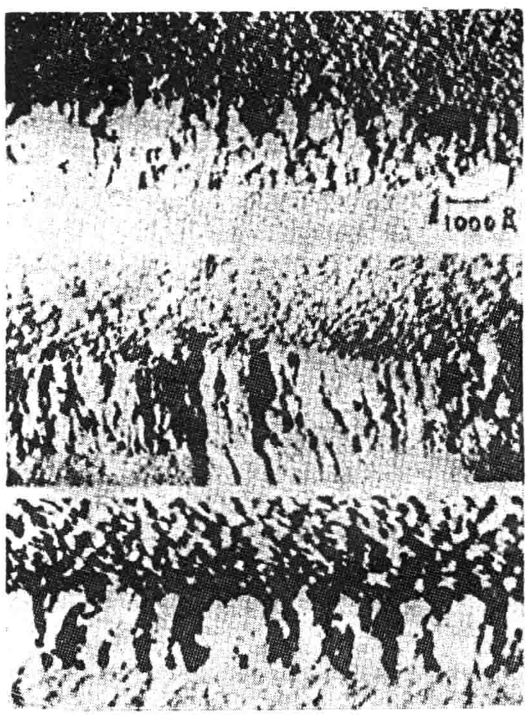


Fig. 3 (left) Structure zone model according to Movchan and Demchishin.[14]

Fig. 4 (right) TiO_2 single films of nominally equal thickness, vapor deposited by reactive evaporation on substrates held at different temperatures T_s: (a) ambient ($T_s = 30^\circ C$), (b) $T_s = 150^\circ C$, (c) $T_s = 400^\circ C$. The microstructure can be seen to follow the structure zone model (zone 1 and 2).

strate temperature T_s/T_m which determines the film structure, with T_m as the melting temperature of the respective solid material (Fig. 3). This model was later expanded by Thornton[15] to include the influence of gas pressure which causes resputtering effects for magnetron sputtered films. More recently, Messier, Giri, and Roy,[16] and Messier and Yehoda[17] offered a further revision of the structure zone model to take into account ion-bombardment induced mobility as well as thermal induced mobility. Also, they introduced the consideration of evolutionary growth development which in short accounts for film thickness effects. In this volume, Messier summarizes these revisions in a comprehensive manner.[18] Fig. 4 shows electron micrographs of the changing microstructure of TiO_2 films of nominally equal thickness for three different substrate temperatures T_s.

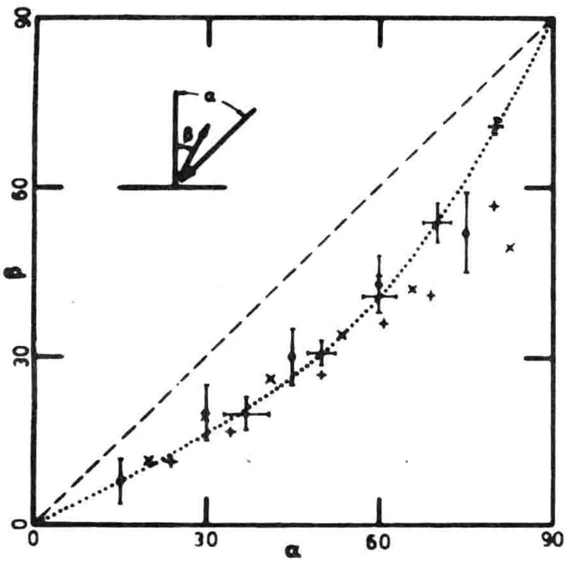
Selected computer models of thin film structure

Among the first and probably now the most often cited researchers to investigate thin film microstructure by means of a numerical simulation model were Dirks and Leamy.[19] Their hard-disk model was literally a model in which they simulated the random ballistic aggregation of molecules arriving at a surface by cardboard disks. The disks were allowed to slide down an inclined plane on trajectories normal or oblique to the horizontal plane. The position of the trajectories was selected sequentially by a random number generator.

Dirks and Leamy found that the "tangent rule" (Fig. 5) derived earlier by Nieuwenhuizen and Haanstra[20] from a number of experimental observations for various coating materials is well obeyed by this very simple simulation model. The tangent rule

$$\tan \alpha = 2 \cdot \tan \beta \qquad (1)$$

is an empirical formula which relates the angle of vapor incidence, α, to the angle, β, in the plane of vapor incidence and the surface normal, at which the observable thin film microstructure (filaments, needles, columns) inclines. The tangent rule can be also deduced from geometric arguments with the hard disk model, assuming parallel obliquely inclined trajectories and a sticking coefficient of unity, which causes the disks to rest where they arrive. Consequently, a disk captured by a previously "deposited" disk will shadow the trajectories going through its diameter from further deposits, as shown in Fig. 6 with a real computer simulation where the materialistic hard disks are replaced by circles drawn by a computer-controlled plotter. As for the simulations of Dirks and Leamy, the trajectories of the incident particles are assumed to be stationary, i.e. at a fixed angle to the normal of the substrate surface.



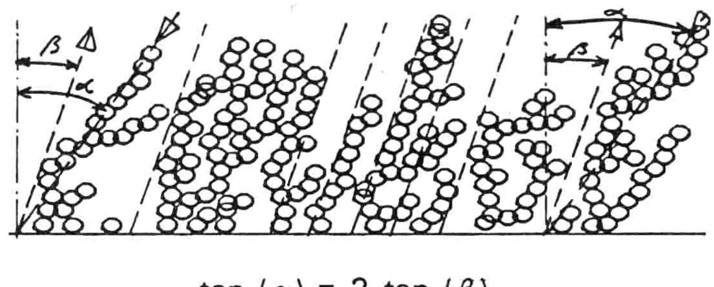


Fig. 5 (left) Graphic representation of the tangent rule tan α = 2·tan β (dotted line).[19,20] Bars, x and + represent actual measurements compiled from various publications.

Fig. 6 (right) Computer model of film growth at oblique angle of particle incidence α. The resulting film structure is inclined at an angle β, following the tangent rule where already deposited particles shadow the path of newly arriving particles. Where no shadowing occurs, the structure inclines into the direction of the particle incidence. Particles are simulated by two-dimensional hard disks, represented by the circles, and are assumed to stick immediately where they arrive without further relaxation.[21]

A modification of this model allowing relaxation of arriving disks into the nearest pockets or saddle points yields denser packed columns but also larger voids in between them, particularly for increased angles of vapor incidence. Much more realistic results with higher packing density of the simulated films are obtained with a further modification accounting for periodically varying angles of particle incidence in a range which for example represents the geometrical condition of an excentrically mounted vapor source on the baseplate and the substrate mounted on a rotating dome above it, and accounting for some statistical rate fluctuations with a Gaussian distribution.

Guenther and Leonhard[21] were among the first to explore the effect of both substrate surface asperities and coating spatters on the resulting thin film microstructure with such a modified model, still assuming zero surface mobility. A typical result of their simulation is shown in Fig. 7 for a substrate surface asperity assumed to be 3 and 6 molecules (disks) high and long, respectively. Although this particular simulation represents just a dozen molecular layers and therefore can be questioned from a vigorous physical point of view, it shows clearly the three major features of nodular growth as observed experimentally by electron microscopy. These features are:

(1) a replication of the disturbing asperity in its height,

(2) a significant increase in the lateral dimension of the defect,

(3) the formation of pronounced voids at the borders of the distortion, making it appear as an independent identity.

Basically the same features can be found with the further elaborated model and simulations over many more molecular layers as described below.

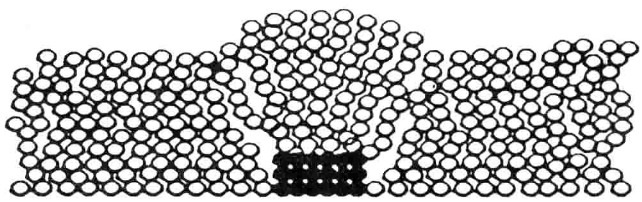


Fig. 7 Computer model of nodule growth at a substrate surface asperity represented by 3x7 particles in this two-dimensional hard-disk simulation. Periodically varying oblique angle of incidence was assumed, simulating the rotation of the substrate above an excentrically mounted vapor source.[21]

The modified hard disk model[22,23] includes the migration process which occurs during actual condensation when an adatom or admolecule moves some distance over the surface after impact because of transverse momentum conservation and thermal diffusion. This migration which depends criticaly on substrate temperature, kinetic energy of incident particles, residual gas content, surface topography, and the activation energies of the adspecies is taken into account by allowing an incident disk to migrate across the surface by jumping from site to site until an eligible site is reached. A probability-density distribution is established for the likelihood of a newly ariving disk undertaking 1, 2, or n jumps after impact and before coming to rest. R_1, R_2 .... R_n are the probabilities for 1, 2, ... n sequential jumps, satisfying

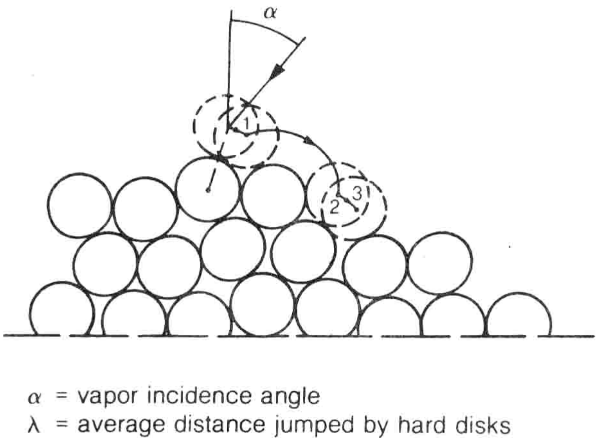
$$\sum_{j=1}^{n} R_j = 1 \qquad (2).$$

The migration parameter λ combines this probability density with the average distances covered by the jumping disks for 1, 2, ... n jumps:

$$\lambda \doteq 0.6 \cdot R_1 + 1.6 \cdot R_2 + \ldots + a_n \cdot R_n \qquad (3),$$

where the coefficients a_n are the average distances traveled by the disks (Fig. 8). These distances are derived from a separate set of simulations. In simulating different adatom mobility conditions, a suitable value for the migration parameter λ is chosen, and restrictions are imposed on the probability distribution in order to obtain a set of values for the R_n.

Experimental observations of some thin film structures indicated a need for the model to include the effect of a Lennard-Jones interaction potential in describing the forces among the lattice constituents. A simplified representation of this potential is chosen for reasons of computational speed. It constitutes a compromise between the simplest hard-disk interaction - i.e. one in which the attractive force is constant up to twice a disk radius and in which the disks have to touch before the force acts - and the computationally unwieldy, full Lennard-Jones interaction. Typically a constant force is used which is truncated in range by an adjustable extension factor that is heuristically set between 1 and 1.75. Disks[24] passing within this extended capture length are attracted to the fixed disks (Fig. 9).



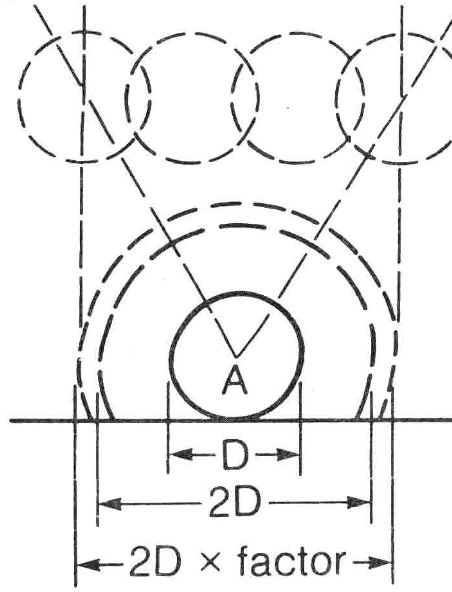
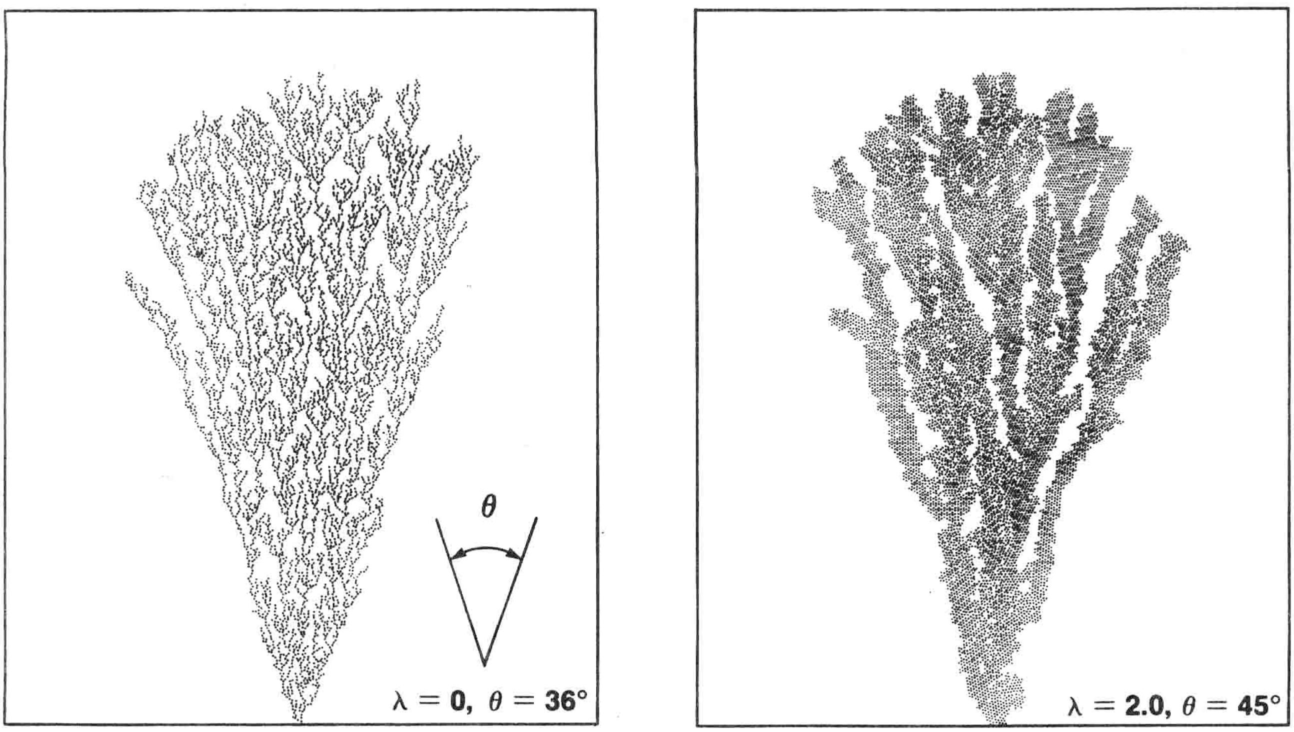


Fig. 8 (left) Principle of modified hard-disk model which allows multiple jumps of an adatom after it impinges on the substrate. In the example shown, the adatom is allowed to jump three times before coming to rest.

Fig. 9 (right) Schematic of the capture length of an adatom simulated by a two-dimensional hard disk. In the original hard-disk model, the capture length is two times the diameter of the adatom. In the modified model, this length is extended by a factor ranging from 1 to 1.75, approximating an interaction potential.



Nucleus: single disk **Extending factor = 1.5**

Fig. 10 Model simulating cluster growths in "free space" (without the influence of a surrounding film), assuming (a) zero adatom mobility and (b) high adatom mobility with extended capture length.

Modeling and experimental verification of nodular defects

The models[25] described above lend insight into the mechanism of the formation of nodular defects. The models can be configured to ignore the effects of the surrounding film. In this case one can refer to the isolated growth structures as clusters (Fig. 10). This shows that nodular growth on a seed nucleus is an intrinsic effect to the process and can occur independantly of other influences of the surrounding film. This growth of a nodule is called self-extension and it is examined by varying the adatom mobility and capture length.

A disk (A) can have a capture length greater than its diameter, as shown in Fig. 9. Disks newly arriving within this capture length will impinge upon (A) such that the cluster starting at disk (A) extends its diameter during growth and forms a cone regardless of the specific seed size or adatom mobility. Typical cone angles for clusters with zero mobility and no extension of capture length vary from 30° to 40° depending on the seed size. An increase in the adatom mobility results in a decrease in the cone angle when the capture length is not extended. However, if the capture length is extended, the cone angle of the nodular cluster increases. This increase means that longer range attractive forces between adatoms produce larger cone angles.

In the computer simulations, clusters forming simultaneously and in close proximity to one another on a smooth substrate will not initiate the self-extending process because of competition among adjacent clusters. Nodules do not form spontaneously from homogeneous nucleations on a smooth substrate surface for the same reason. Only those clusters that start at protrusive seeds have chances to develop the nodule shapes. Approximate values for the mobility of adatoms may be obtained by calculating the packing density for a given model and comparing the result to real films. Likewise approximate ranges for the capture length can be determined by examining the cone angles of nodules grown at normal incidence. A comparision between a modeled nodule and an actual nodule is seen in Fig. 11.

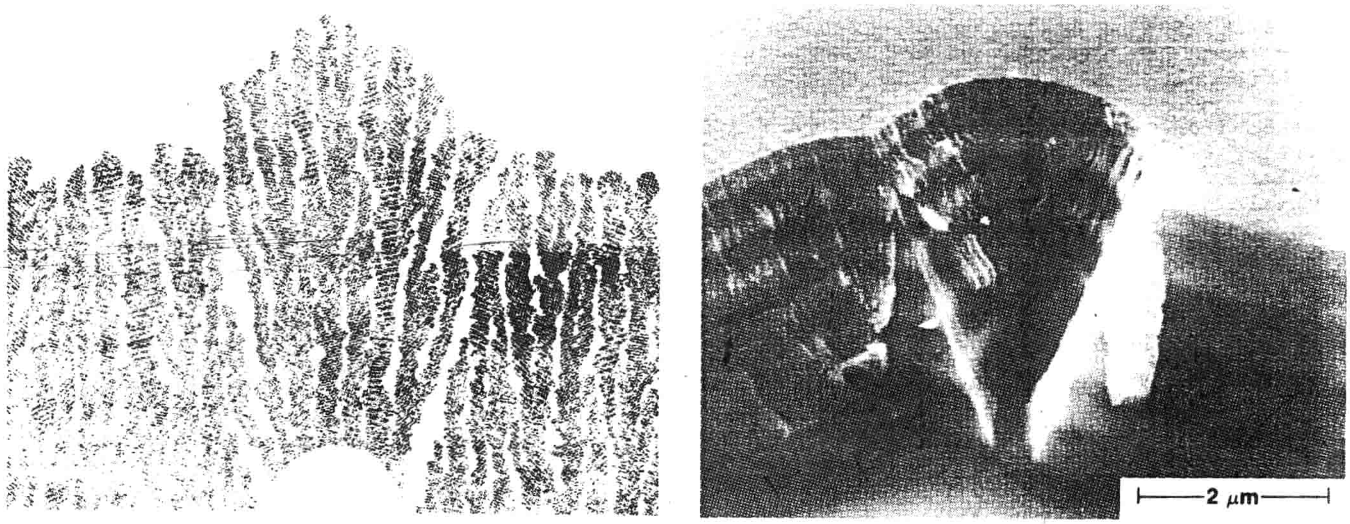


Fig. 11 The characteristic shape of a nodule formed on a fixed substrate with normal vapor incidence is an inverted cone. The model (left) is supported by experiment (right).

Typically, optical thin films are deposited on substrates rotated in their own plane for uniformity reasons. The nodules grown on these rotated substrates differ from those grown by stationary normal incidence deposition. As seen above (Fig. 10), a nodule formed by normal incidence is initially straight sided. As the vapor angle of incidence, α, is increased on a rotating substrate, the initial growth cone angle γ of the nodule increases as well (Fig. 12). For small γ, the following approximation holds:

$$\tan\gamma = [1/(1-\pi)]\cdot\tan\alpha \qquad (4).$$

After initial growth of a nodule the surrounding film restricts continued growth. While the step around a seed disappears and the dome on top of the nodule forms, the increase in nodule diameter slows down. As a result, parabolic sides on a bowl-like bottom evolve, in contrast to the straight sides of the nodules grown under normal incident flux on stationary substrates. Nodules in a coating stationarily deposited by a wide source (for instance sputtering) exhibit similar shapes as nodules in coatings deposited from a point source on rotating substrates due to the spread in the particles angle of incidence typical for such a condition. Fig. 13 shows a simulation and a corresponding nodule grown in a single film with 45° vapor incidence. There is a fairly good agreement seen between the model shape and the shape of the actual nodule in this figure.

$$tg\gamma = \frac{1}{(1 + \Pi)} tg\alpha$$

$\alpha = 50°$, $\lambda = 3.5$
extending factor = 1.5

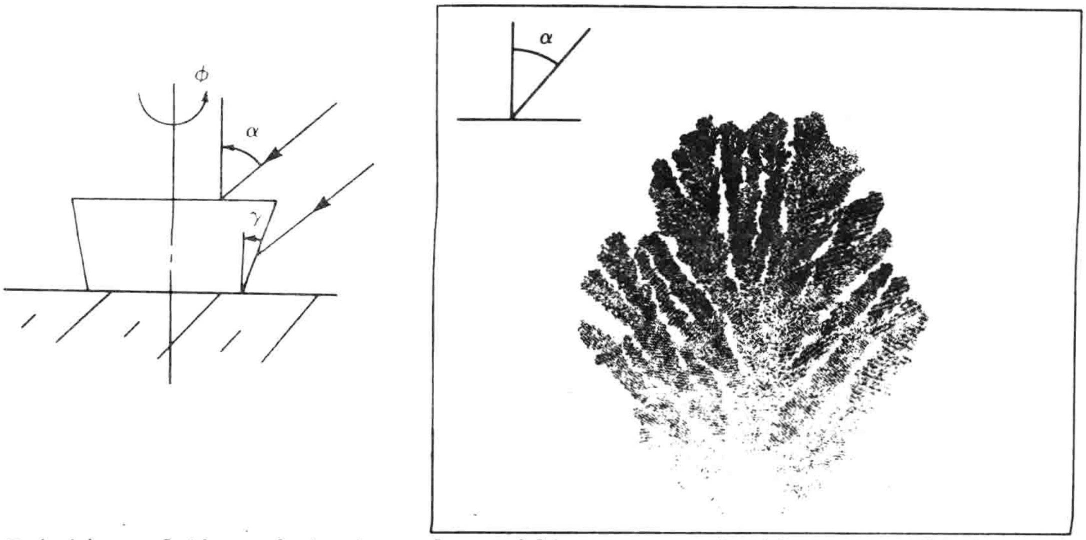


Fig. 12 Rotation of the substrate and an oblique vapor incidence result in an increase in the nodule cone angle.

Higher angles of particle incidence have two effects on nodules. The first is an increase in the initial growth angle γ, which produces larger nodules. The second effect is a decrease in the size of a seed (or defect) required to produce a nodule. A seed which may have been below the nodule-formation threshold at a low angle of vapor incidence has a greater chance of forming a nodule at a high angle, because of, in part, the shadowing effect it produces on the surrounding substrate. This shadowing reduces the effect of the surrounding clusters competing for growth and provides a better opportunity for unhindered growth of the nodule.

$\alpha = 50°$, $\lambda = 3.5$, extending factor = 1.5

45° vapor incidence/single ZnS film

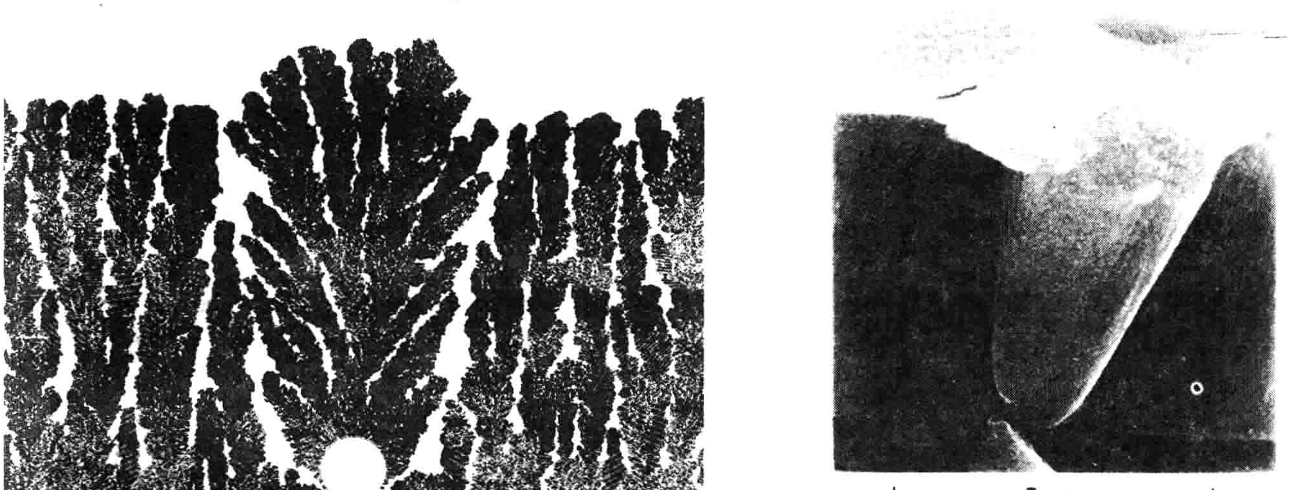


Fig. 13 Nodule simulations and experiments on rotating substrates at 45° vapor incidence.

Properties of thin film optical coatings related to their microstructure

Effects of columns and voids

Structure-related optical properties of thin films have been reviewed in a number of recent articles[25-27] which mostly focus on the form birefringence induced by the elongated shape of the columns, and on the difference in the refractive indices between bulk and thin film material. The refractive index of a material in the form of a thin film is lower when the latter contains voids. In case these voids fill up with contaminants (oil, hydrocarbons, or simply water), their index changes from unity to that of the contaminant (1.33 for water), altering the effective medium index. Knowing the volume fraction of the voids and assuming the bulk indices as the actual ones, it is possible to calculate the effective medium index fairly accurately.[28]

The columns, however, also have other effects on the thin film in addition to optical effects. Notably, the intrinsic mechanical stress depends on the observable microstructure of thin films. Although there is no firm general rule, it has been observed that thin films displaying a columnar microstructure are often under tensile stress, which can be explained qualitatively by the insufficient filling of the available space with the coating material. Or, in other words, the columns which are slightly separated by the voids try to get together. In contrast, compact, structureless looking films such as SiO_2 exhibit compressive strain. The latter is sometimes relieved by buckling the film, creating a periodic pattern which has become known as buckling waves.[26] One would expect that with the decrease in crystallinity of mixed oxide films[5] a similar decrease in the observable microstructure comes along, which eventually finds its effect in the mechanical properties of the films. Indeed this result has been found for co-sputtered Al_2O_3/SiO_2 thin films, which showed a minimum of intrinsic stress at a certain composition.[6]

It is common experience that thin films change both their optical and mechanical properties when they are subjected to a thermal treatment, which is commonly referred to as annealing. Not only does annealing reduce intrinsic mechanical stresses but sometimes it is found to cause the adverse effect of reducing the adhesion of the coating to the substrate. This observation has been explained recently with a computer model for postdeposition annealing of porous thin films,[29] which shows that the loosely connected atomic network caused by self-shadowing during vapor deposition undergoes an aging effect, depending on the film's temperature. The vacancies or voids, quenched-in due to the low atomic mobility during growth, migrate and eventually coalesce or merge with larger preexisting voids. When the film-substrate bonding energy is weaker than the bonding energy between film atoms, the substrate-film interface acts as a sink for vacancy coalescence, which further reduces the adhesion of the film to the substrate.

Effects of the nodules

The growth models and the scanning electron micrographs illustrate some problems associated with nodules. Most obvious is the poor mechanical contact with the surrounding film characterized in the simulation by a distinctive gap between the nodule and the film, which sometimes can also be seen in scanning electron micrographs. More often, however, this poor mechanical contact becomes evident when nodules pop out of the film leaving a pinhole behind in the coating, which not only is disturbing because of the resulting discontinuity of the optical properties of the coating, but also because it provides easy access for contaminants, including humidity, to penetrate deeply into the interior of the coating. This is true also for nodules remaining in the coating because of the gap around them as metioned above.

In thick coatings such as complicated multilayers for the visible, and of course even more likely in coatings for the infrared, the top of a nodule may act as a microlens[30] depending on the size to wavelength ratio. In high energy applications, this may cause radiation being focused into a high electric field within the nodule. Since the gap around the nodule acts also as a thermal barrier, the onset of laser damage may be caused in such a situation.[11] In fact, it has been observed that nodules are the preferred sites for laser damage events in optical coatings.[31]

Discussion

It has been shown that a modified hard disk model of random sequential ballistic aggregation of molecules from a vapor phase on a substrate surface is useful for understanding the growth process and formation of thin film structure. The model has been used to simulate typical evaporative processes. Other deposition technologies or unusual evaporation conditions may also be modeled but would likely require modifications of the simulation process. One example would be studying the influence of elevated residual gas pressure on the spontaneous formation of nodules which has been observed with variations of the O_2 partial pressure for reactive evaporation of Ta_2O_5, as mentioned earlier.[11] Future work could include modeling sputtering or CVD processes to help determine what advantages these processes could show over the evaporation method. An extension of the model towards simulation of ion-assisted thin film deposition has recently been published by Karl-Heinz Müller.[32]

Conclusion

We have discussed various models of thin film structure and shown that they describe the observed microstructure adequately. A variety of properties of thin films which are important for their application as optical coatings can be explained consistently with these microstructure models.