

Defect Formation and Surface Evolution of Thin Film Materials

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Abstract

Modern thin film industries require precise tailoring of thin films properties to have excellent performance for specific applications intended. Thin film mechanical behavior and stress presents a technological challenge for material scientists, physics, and engineers. Atomic-scale understanding of the microstructure of thin films is a crucial aspect for the control and manipulation of the film properties for a wide range of industrial applications. Thin film growth of thin films influences the crystallographic orientation of grains, grain shape and distribution thereby affecting their reliability and performance of the material. This article reviews the present understanding of the mechanism(s) determining the microstructural evolution of thin films, defect formation, and the related failure modes. General trends in microstructural evolution, grain morphology, and texture formation mechanisms are briefly discussed in terms of their respective kinetic processes. The temperature dependency of the film microstructure evolution is described using the structure zone models.

Keywords

Thin film, microstructural evolution, kinetic processes, structure zone models

1. Introduction

Modern technologies in industries producing dedicated thin film devise require precise control and manipulation of the thin films properties depending on the intended area of application. A thin film refers to a layer or multilayer of materials created by atomic or molecular particle condensation and having a thickness ranging from 10nanometers to 100micrometers(Adachi & Wasa, 2012). The use of thin film technology to harness the nature of atoms and molecules to achieve enhanced materials properties has significant commercial application and potential. In gas turbines engines, chemical and thermal inert thin surface films are used to increase engine efficiency and stability at elevated temperatures. Structural materials incorporate the tribological and mechanical properties of hard thin films to enhance properties and extend the lifetime of the materials they protect. Other applications of thin films include electronic, magnetic and micro chemical device and systems (Petrov, Barna, Hultman, & Greene, 2003). The controlled synthesis(deposition) of thin films is a fundamental step in many applications since the properties, performance and reliability of the coatings are influenced by the microstructural characteristics of the films (Thompson, 2000). Common techniques for thin film synthesis are illustrated in figure 1(Adachi & Wasa, 2012).

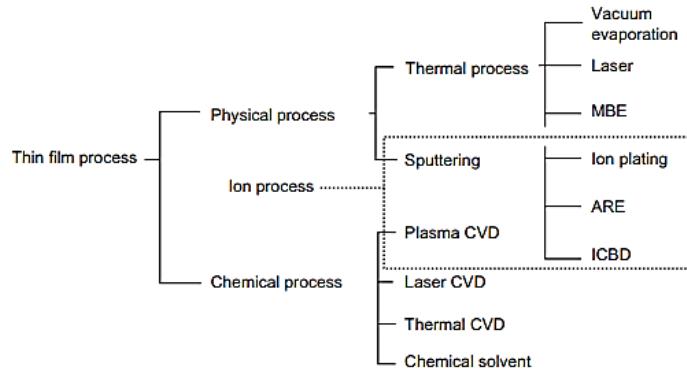


Figure 1.Typical deposition methods of thin film materials.

For every application, the properties of the film have to be carefully controlled and manipulated through processes at the atomic scale to define their structure(Thompson, 2000). Although often complicated, the kinetic processes and mechanisms through which film structures evolve can be used to comprehend the trends in film properties and performance.

2. Surface Evolution

The evolution of the film during various processes is dependent on the specific processing conditions: choice of material, deposition rate, ion bombardments and operating temperatures among others(Almtoft, 2006). Furthermore, the effect of deposition parameters determining the physical and chemical properties of the film are not independent of each other, but rather coupled through the process taking place during film formation. Generally, the melting temperature T_m of the material plays a significant role than the deposition temperature T , when studying the evolution of the microstructure. Thin film deposition occurs through the following three main processes: (a) nucleation, (b) coalescence and (c) continuous growth

2.1. Nucleation

Nucleation is basically the creation of a particle or bubble out of nothing. This process occurs mainly due to diffusion and adsorption of adatoms. During diffusion, arriving adatoms can either meet another adatom forming a stable nucleus and hence a new island or it will meet an existing island and stick to it(Thompson, 2000). During deposition an influx of atoms from the target material arrive at the substrate, lose their momentum and kinetic energy by adsorbing on the surface of a substrate, they are now referred to as adatoms(Thompson, 2000). When this adatoms clusters and continues to grow instead of dissolving, they form tiny islands, we say nucleation has occurred. The adsorption and clustering of adatoms during nucleation is influenced by the incoming flux of atoms, the trapping probability, and the sticking coefficient. Apparent consensus among many detailed kinds of literature indicates that the nucleation rate is given by:

$$I = I_0 R^n \exp\left(-\frac{\Delta G_n}{kT}\right) \text{ Equation 1(Thompson, 2000)}$$

Where I_0 is the flux independent constant, K is Boltzman's constant, T is the substrate temperature, n is the critical cluster size and the energy of a cluster of size n is denoted ΔG_n . The nucleation rate is highly dependent on increasing temperature. The inverse proportionality from the equation 1 suggest that nucleation rate decreases when the temperature increases and behaves linearly proportional with deposition rate(Almtoft, 2006; Thompson, 2000). It has been reported that to achieve nanocrystalline films, a higher nucleation rate is preferred since it result in fine grained structures(Almtoft, 2006). Identification of the diffusion species during nucleation is also fundamental to comprehend the atomic process taking place(Greene, 2010)

2.2. Coalescence and Thickening

Coalescence occurs when the growing islands eventually meet causing the previously separated grains to interact by merging structures (Barna P. B. & Adamik M., 1995). The process of coalescence can be visualized as liquid droplets joining one another to form one. For complete coalescence whereby a single crystal develops, according to the theory of sintering, all the following processes have to take place: neck formation, filling of necks by surface self-diffusion, grain boundaries formation and finally recrystallization(Barna P. B. & Adamik M., 1995). Surface atom diffusion and grain boundary motion are the driving force for this process. After coalescence is completed, a continuous film is formed by continuous deposition resulting in thickening. New adatoms approaching the film surface can either nucleate new grains on top of existing ones or join the already formed grain. Sometimes due to impurities, the coalescence process is modified resulting in film defects such as high porosity. The energy of the individual islands formed depend on the grain size and orientation, therefore, structure evolution during coalescence can determine the microstructure of the films (Almtoft, 2006).

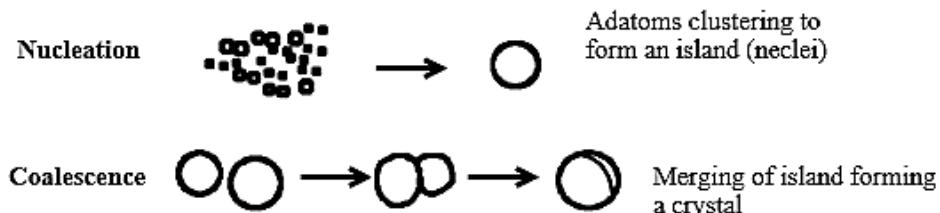


Figure 2. Schematic representation of the nucleation and coalescence mechanisms(Sastry, Dontula, & Hosten, 2003).

2.3. Grain Growth

Coarsening during coalescence is the most active phenomenon leading to the selection of preferred crystal orientation(Petrov et al., 2003). Unlike coalescence, grain growth occurs due to the movement of grain boundaries. During grain growth, two distinguished types of mechanisms take place depending on the energy state. We have grain boundary migration whereby the grains with a certain orientation grows laterally at the expense of other different orientations, this is called restructuration growth texture(Petrov et al., 2003). The grain boundary mobility during this growth is very significant. The other mechanism taking place during grain growth is by competitive growth where now the growing grains grow over the others. This competition is due to crystallographic faces of different surface energies hence the mobile adatoms favoring the lowest crystal planes.

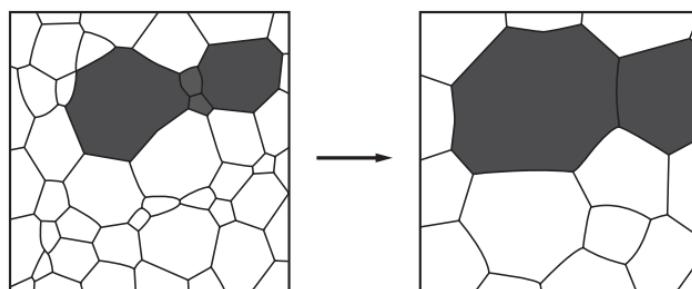


Figure 3.Schematic representation of grain growth in a continuous film(Thompson, 2000)

Table 1. Overview of thin film evolution

Phenomena	Evolution mechanisms	Location
Nucleation	<ul style="list-style-type: none"> • Adsorption • Adatoms migration • Clustering 	Substrate
Crystal growth	<ul style="list-style-type: none"> • Self-surface diffusion of adatoms • Monolayer crystal growth 	Crystal faces
Growth	<ul style="list-style-type: none"> • Coalescence • Thickening • Grain boundary migration 	Substrate Continuous film

In the few past decades, material scientists and engineers have been striving to achieve film microstructure tailoring during lower processing temperatures to meet industrial demands. The temperature specifications led to the development and enhancement of structure zone models(SZMs) to categorize structural evolution of thin films with respect to deposition parameters(Greene, 2010). SZM mainly consist of three zones to characterize the microstructure of pure elements during the surface evolution depending on the driving forces using the ratio T_s/T_m , where T_s is the deposition temperature and T_m is the material melting point. In Zone I films are grown at very low temperatures where adatom diffusion is almost non-existent, Zone T is surface diffusion driven and Zone II represent film growth at higher deposition temperatures where both surface and bulk diffusion occurs(Lieberman & Lichtenberg, 2005). Zone III is characterized by very high deposition temperatures. The effect of temperature using SZM is illustrated in figure 4.

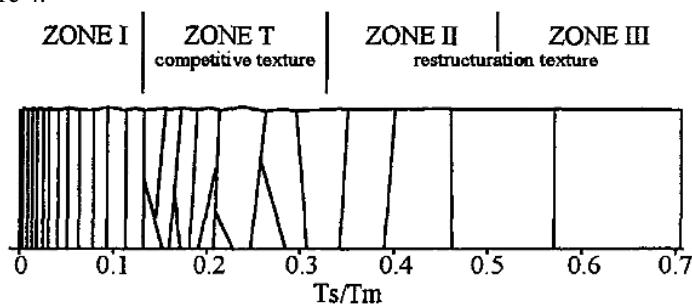


Figure 4. Schematic of the basic structure zone model(Barna P. B. & Adamik M., 1995)

3. Defect Formation

Perfect bonding between film and substrate is always assumed in thin film systems. However, defects, weakly bonded areas and sometimes impurities always exist at the interface. These flaws may be due to the different properties of the film material and the substrate hence causing a mismatch at the bond. Example this mismatch is the thermal coefficient of materials which will result in deformation under temperature variations(Cao, Thouless, & Evans, 1988). The main failure susceptible areas in the thin film system are at the preexisting flaws which would act as stress concentrators thereby influencing plastic deformation.

Due to the effect of ion/atom implantation during deposition, residual stresses will build up. These residual stresses may cause crack growth with the film, in the substrate or at the interface and emerging at the film resulting in delamination or fracture(Cao et al., 1988; Freund & Suresh, 2003; Suo, 2001). Thin film residual stress generation can be due to; epitaxy, precipitation, shrinkage of grain boundary voids, grain boundary relaxation, grain growth, impurities amongst many other mechanisms.

If the film is under compressive stress, cracks form at the interface of the film substrate and cause delamination and buckling, under tensile stresses the crack propagate from the preexisting defects forming intersecting cracks leading to fracture susceptibility(Ibru, Kalaitzidou, Kevin Baldwin, & Antoniou, 2017). Figure 4 depicts the simplified schematics of typical failure modes by the action of both compressive and tensile residual stresses(Huang, 2017)

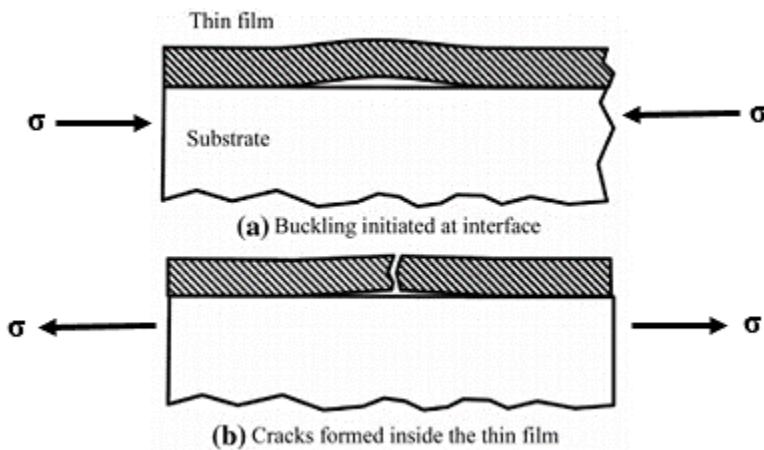


Figure 5. Typical thin film failure modes due to (a) compressive straining and (b) tensile straining

One of the other thin film defects is porosity. Irrespective of the thin film deposition method used, voids or pores will exist in the film due to phase transformation. Also, porosity may be caused by inadequacies of prior deposition such as cleaning, machining, and heat treatments. It has been reported that the material strength and ductility decrease with increasing porosity(Bourcier, Koss, Smelser, & Richmond, 1986; Potecaşu, Marin, & Potecaşu, 2015).

Table 2. Overview of the effect of porosity on material properties.

Property	Effect of Voids
Mechanical	Decreased ductility Creep resistance Decreased adhesion Lowered yield strength
Corrosion	Reduced corrosion resistance due to pores
Wear	Voids in the films lead to increased wear degradation
Electrical	Resistivity increases

4. Conclusion

The surface and microstructural evolution of thin films have been demonstrated. The kinetic energy and the surface diffusion of adatoms plays an important role in the size of grains, grain distribution and hence the crystal orientation of the film. Thin films are subjected to defects or flaws due to the nature of the synthesis (fabrication and deposition). Presence internal stresses and voids in thin films are usually inevitable, such defects tends to lower the mechanical properties of the film making it susceptible to a various form of thin film modes aforementioned. The understanding of surface evolution and defects formation in the thin film is of critical value since the performance of the thin film system is attributed to the influence of particles and propagation at scales as low as atomic level, hence this review.

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Biographies

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