Film Structure

- surface diffusion
- bulk diffusion
- desorption
- shadowing

Nucleation and growth processes

Structure-Zone Model

Structure-Zone Model

works for several deposition techniques, like PVD and CVD, and for various materials (metals, isolators, semiconductors)

Important parameters:
- Normalized temperature Ts/Tm
- Energy transfer, atoms at high energy

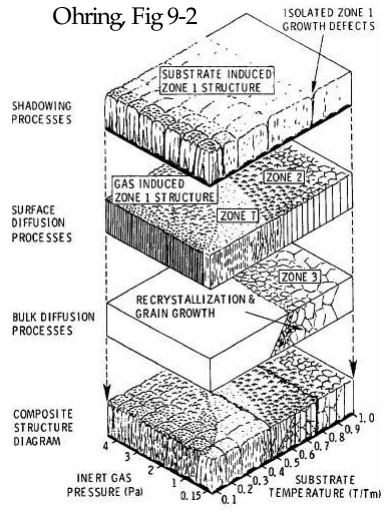
Structural zones as a result of different physical processes

Table 9-1
Zone Structures in Thick Evaporated and Sputtered Coatings

Zone	T_S/T_M	Structural characteristics	Film properties
1(E)	<0.3	Tapered crystals, dome tops, voided boundaries.	High dislocation density, hard.
1(S)	<0.1 at 0.15 Pa to <0.5 at 4 Pa	Voided boundaries, fibrous grains. Zone 1 is promoted by substrate roughness and oblique deposition.	Hard.
T(S)	0.1–0.4 at 0.15 Pa, 0.4–0.5 at 4 Pa	Fibrous grains, dense grain boundary arrays.	High dislocation density, hard. High strength, low ductility.
2(E)	0.3–0.5	Columnar grains, dense grain boundaries.	Hard, low ductility.
2(S)	0.4–0.7		
3(E)	0.5–1.0	Large equiaxed grains, bright surface.	Low dislocation density, soft recrystallized grains.
3(S)	0.6–1.0		

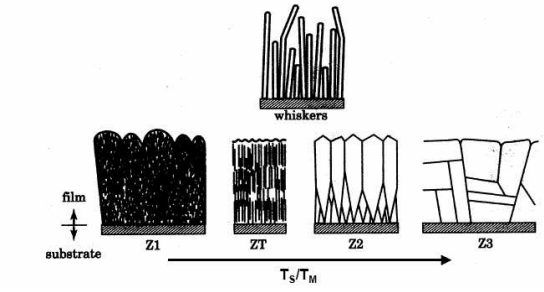
Note: (E) refers to evaporated, (S) refers to sputtered.

Ohring, Fig 9-2

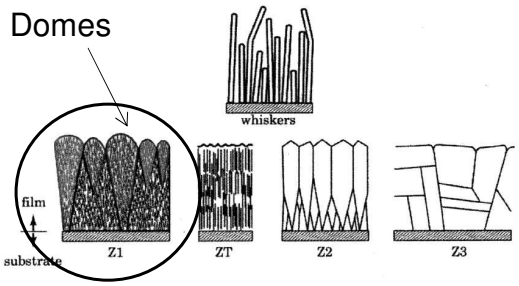


The Basic Structural Zones

- There are no zones in epitaxial thin films
- Transitions between zones are not sharp
- Structural mode can change across the thickness
- Zones are sometimes difficult to identify



Domes



PVD: Ts/Tm<0.3

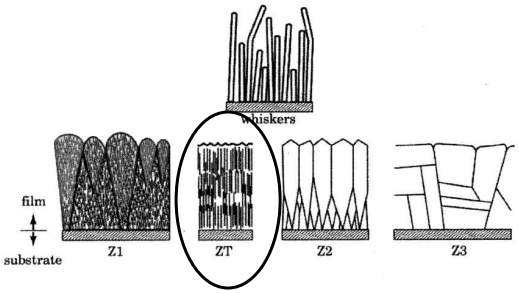
Sputtering:
Ts/Tm<0.1 (0.15 Pa)
Ts/Tm<0.5 (4 Pa)

High-dislocation density, hard

Z1 occurs at Ts/Tm so low that surface diffusion is negligible consists of columns ~10-20 nm in diameter, separated by voids of few nm in diameter. The columns have many defects or even are amorphous.

An array of cones superimposed on this structure will appear in thicker films. The cones terminate in domes at the surface. The thicker the film the larger the domes.

Sputtering only

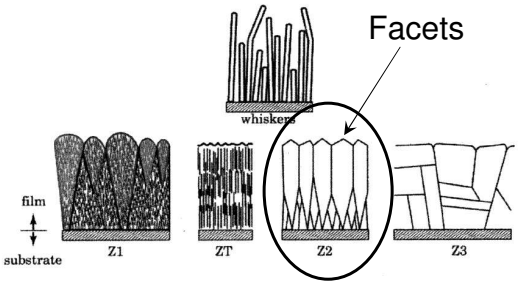


0.1 < Ts/Tm< 0.4 (0.1 Pa)
0.4 < Ts/Tm < 0.5 (4 Pa)

ZT is essentially the same as Z1, i.e. occurs when the surface diffusion is negligible, but the voids and domes are absent.

Fibrous grains, dense grain boundaries

High dislocation density, high strength, low ductility, hard

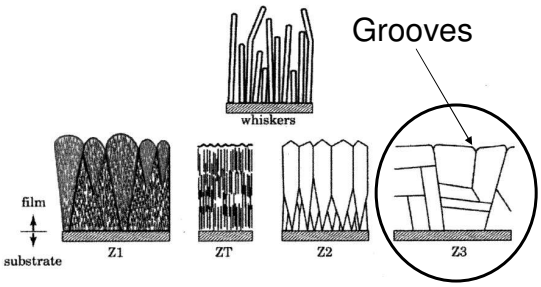


PVD: 0.3 < Ts/Tm < 0.5

Sputtering:
0.4 < Ts/Tm < 0.7

Z2 takes place at Ts/Tm > 0.3. The surface diffusion becomes essential. Z2 consists of columns with tight grain boundaries between them. Characteristic diameter increases with Ts/Tm. Better crystal structure of the grains. Facets on the surface. Can also occur in amorphous films. Transition temperature Z1→Z2 increases with deposition rate.

Hard, low ductility



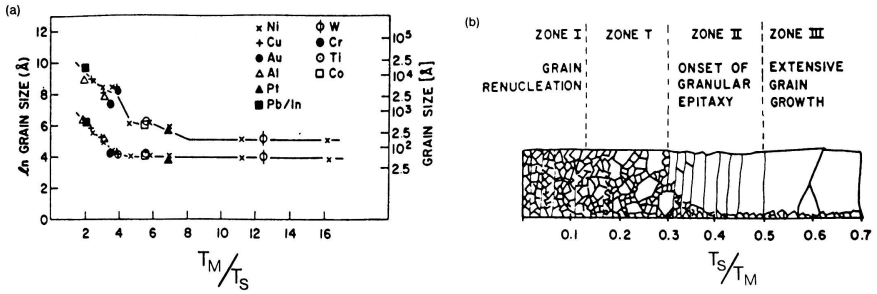
PVD: Ts/Tm > 0.5

Sputtering:
0.6 < Ts/Tm < 1

Z3 takes place at Ts/Tm > 0.5. The surface and bulk diffusion are strong. Z3 consists of larger equiaxed crystallites. Surface is smooth but with grooves between grains. Grain size is about the film thickness.

Low dislocation density, soft

ZSM for PVD thin films

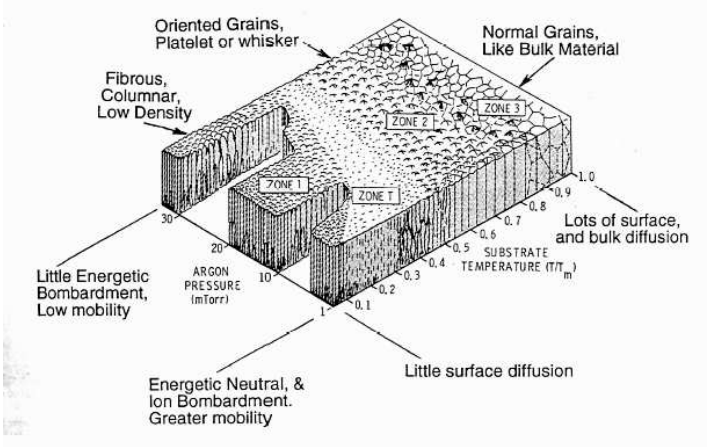


The behavior is similar for a number of metals

Grain Structure: conclusions

- Film growth is a non-equilibrium process
- Grain size is determined by mobility of atoms on surface
- The mobility depends on
  1. Substrate temperature
  2. Surface and bulk diffusion (Tm)
  3. Energy supplied by ion bombardment
  4. Adsorption strength

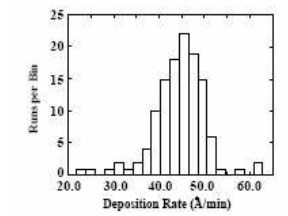
The Famous Diagram



What is good and what is bad

- Z1 in most cases is not good (large resistance, large optical scattering in optical coatings, leakage in insulators, traps in semiconductors)
- Porosity of Z1 is good for
  i) gas detectors
  ii) catalytic applications (fuel cells)
  iii) applications with large T-changes
  iv) light absorption

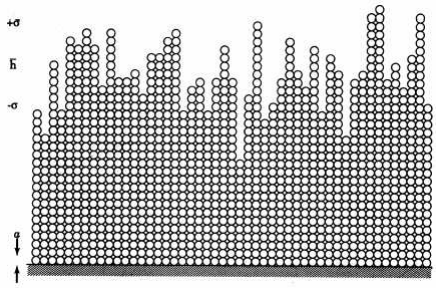
Statistical Roughening

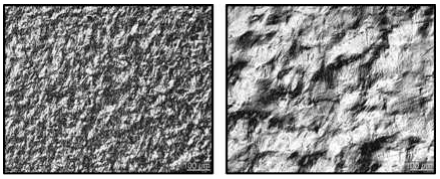


121 deposition rate observations for the Michigan LPCVD nitride for 3 years (1995-1997)

Statistical fluctuations in the deposition rate → variations in thickness

A model: atoms fall and stick to their column only

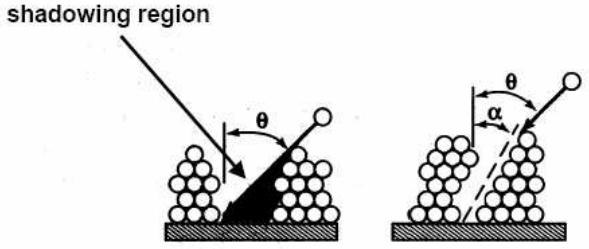




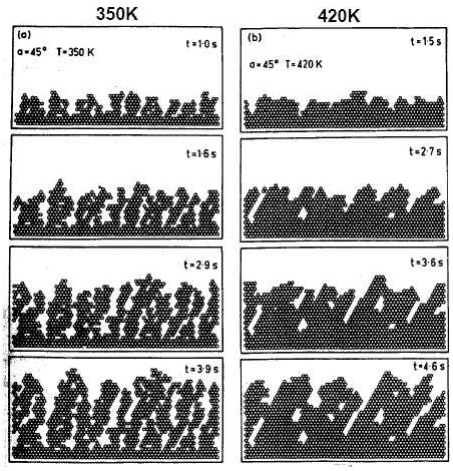
The same average roughness but different morphology

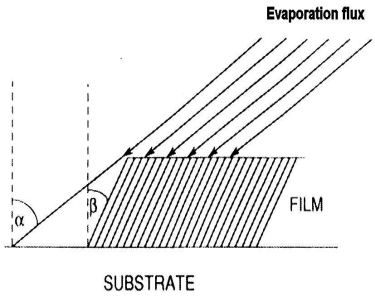
Shadowing

- Makes surface roughness larger than statistical value
- Deposition at an angle (oblique deposition)→shadowing
- Tangent rule: $\tan\alpha = 1/2 \tan\theta$



Shadowing: simulations



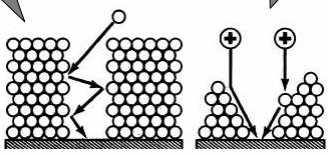


Monte Carlo simulations of microstructure of Ni films during deposition

Shadowing is smaller for high energy of atoms

No shadowing when there is no sticking (high T, CVD)

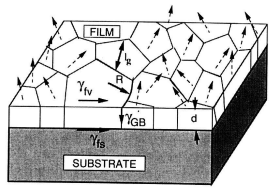
No shadowing when there is forward sputtering PLD, sputtering



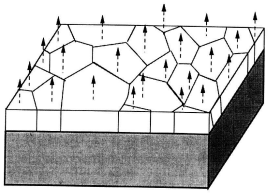
Good: voids and trenches can be filled

Textured Films

(non-random distribution of grain orientations)



RANDOM ORIENTATION



PREFERRED ORIENTATION (TEXTURE)

Film and grain-boundary surface tension depends on crystallographic orientation
+
Strain energy (adhesion) and thermal stress

Minimization of total film energy = selection of grains (certain orientations are preferable) → textures

Affected by
- Substrate nature
- Particle bombardment (IBAD)

Simulation of trench filling by PVD

High Ts promotes diffusion thus helping filling trenches

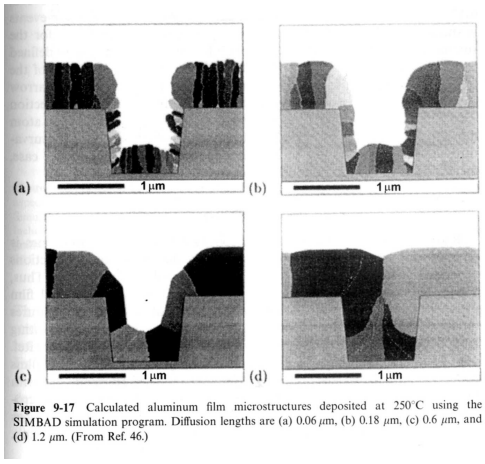
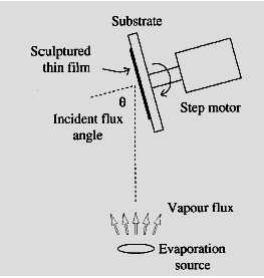
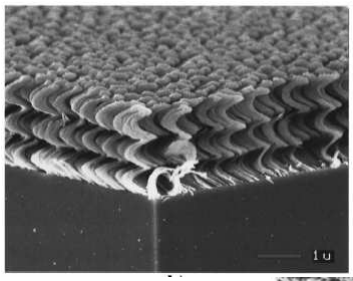


Figure 9-17 Calculated aluminum film microstructures deposited at 250°C using the SIMBAD simulation program. Diffusion lengths are (a) 0.06 μm, (b) 0.18 μm, (c) 0.6 μm, and (d) 1.2 μm. (From Ref. 46.)

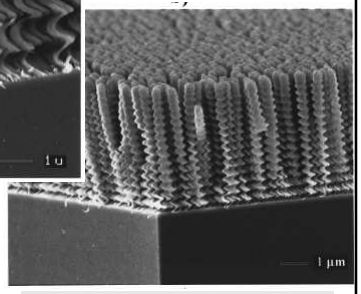
Sculptured Films

- Shadowing-dominating aggregation during oblique deposition (>75°)
- Low Ts favors Z1 columnar growth





K. Robbie[a)] and M. J. Brett



1460 J. Vac. Sci. Technol. A 15(3), May/Jun 1997

helical shaped columns with pitches comparable to the wavelengths of visible light → an artificial structurally chiral medium

Amorphous Films

- Deposition on cryogenically cooled substrates to prevent atoms diffuse. Cooling rates $>10^6$ K/s are required → limit for film thickness
- Amorphization by ion bombardment
- Properties can be very different from normal films (Bi)

Applications:
- amorphous Si in solar cells
- amorphous C for hard wear resistant coatings