Vékonyrétegek előállítása és alkalmazásai

2010. október 4.

Dr. Geretovszky Zsolt

The role of film density

Lowered film density has a deleterious influence on optical, mechanical, electrical and magnetic properties, similar to the degradation of film adhesion and chemical stability.

The measurement of film density requires a simultaneous determination of both film mass per unit area and thickness.

Observed tendencies:

- The density of both metal and dielectric films increases with thickness and reaches a plateau value which asymptotically approaches that of the bulk density. Deposition method and experimental conditions affect the threshold/critical film thickness.
- Metal films tend to be denser then dielectric ones, because of the larger void content in the latter. The quantitative measure of void content is the packing factor, *p*

$$p = \frac{\text{volume of solid}}{\text{total volume of film (void + solid)}} \qquad p \leq 1$$

p can be increased with raising T_s.

- Thin films usually have excess vacancy/micropore concentration. Typically an order of magnitude larger than in bulk.

Microporosity

Microporosity on a scale much finer than imaged in zones 1 and T has also been detected (at densities of about 10^{17} cm^{-3})! They are present both at grain boundaries and in grain interior!

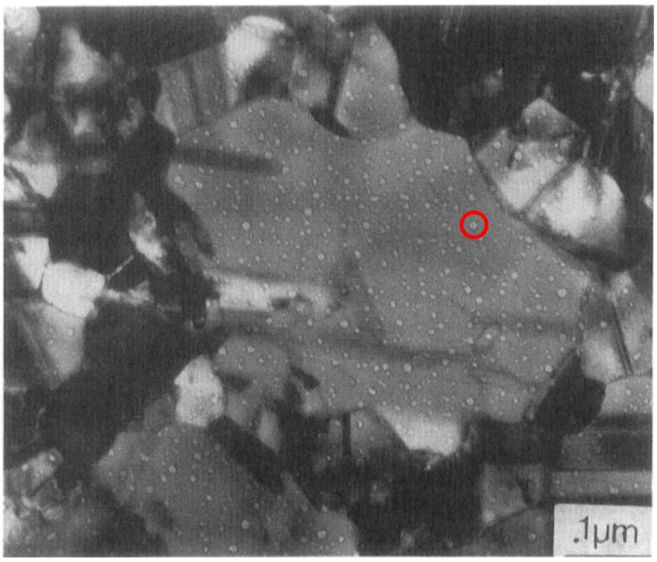


Figure 9-7 Transmission electron micrograph showing microvoid distribution in evaporated Au films. (Courtesy of S. Nakahara, AT&T Bell Laboratories.)

Computational simulations

A continuum of computer approaches was introduced to model the film growth process. The major variables that must be accounted for are the energy, size and composition of the depositing species, and the temperature and nature of the substrate. All simulations reflect the spirit of statistical mechanics.

The energy of the depositing species often establishes the division as to what will be modeled and how.

- for low energies the equilibrium structural morphology and the arrangement of atoms is evaluated through the combinations of geometric and probabilistic approaches. (i.e. lattice-gas and solid-on-solid ***Monte Carlo simulations***)
- ***molecular dynamics*** (MD) is used for modeling the effects of impinging particles having higher energy

A Monte Carlo simulation

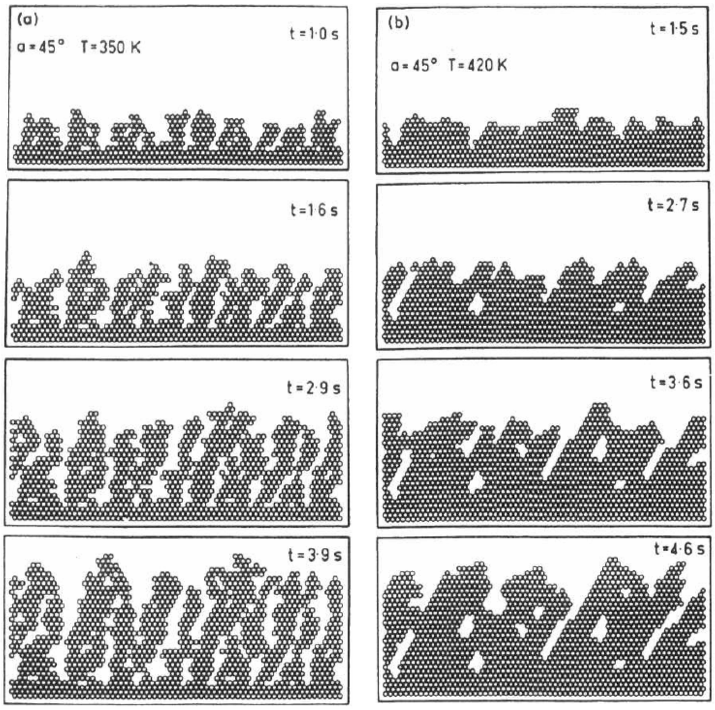
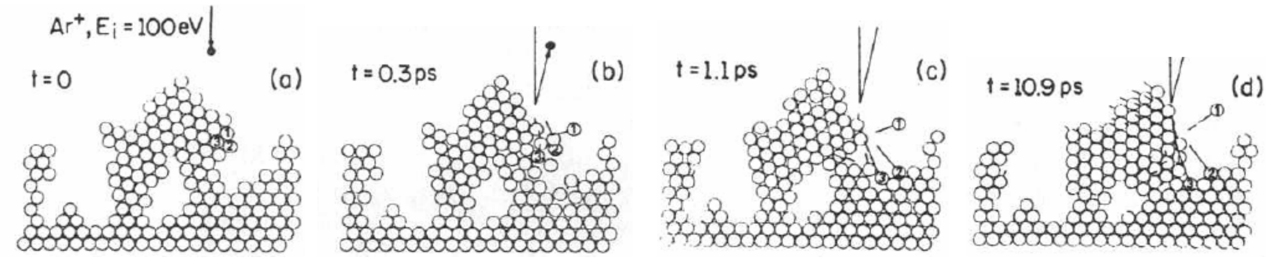


Figure 9-9 Computer-simulated microstructure of Ni film during deposition at different times for substrate temperatures of (a) 350 K and (b) 420 K. The angle of vapor deposition α is 45°.

Ion bombardment of films

molecular dynamics

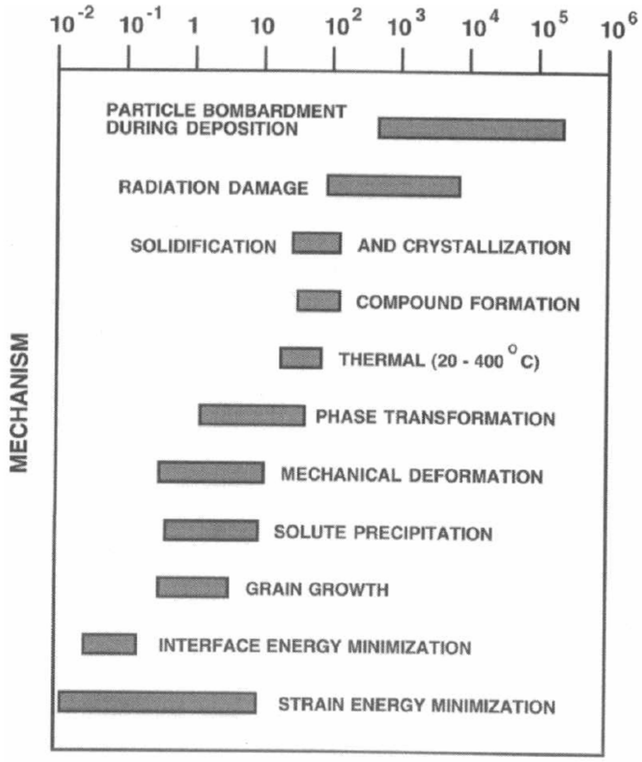


MD simulation confirms the densification of films during ion bombardment.

It was also confimed that

- greater structural densification occurs as the kinetic energy of atoms incident on a growing film increases;
- film density rises as the ratio of the ion flux to vapor flux increases. This effect is enhanced at higher ion energy; and
- at higher ion energies the tensile stress decreases.

Energetics of microstructural change



In plane structure

Now we shall explore how the grain structure of films, seen ***in plane view***, evolves during deposition and/or postdeposition processing. Issues are applicable to all polycrystalline thin film.

Two main topics are *grain size* and *texture*.

1. Grain growth *in thin films* is generally more complex.
2. In thin films the grain growth is said to be abnormal, i.e. is often caracterised by a bimodal size distribution (even 2 orders of magnitude difference in size).
3. Abnormal grain growth leads to an evolution in the average crystallographic orientation of the grains. This effect is more pronounced for thinner films.
4. Grain growth in thin films often stagnates when the grain size is 2 to 3 times the film thickness. Solute segregated at grain boundaries often acts as a drag that inhibits growth.

Texture

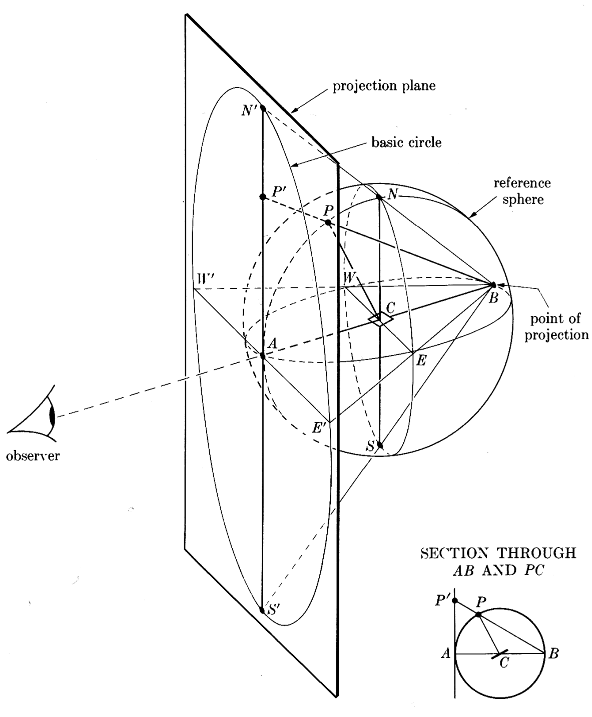
Texture is the distribution of crystallographic orientations of a sample. A sample in which these orientations are fully random is said to have *no texture*. If the crystallographic orientations are not random, but have some *preferred orientation*, then the sample has a *weak, strong, or moderate texture*. The degree is dependent on the percentage of crystals that have the preferred orientation. Texture is seen in almost all engineered materials, and it can have a great influence on material properties.

Texture can be determined by different methods. Among the quantitative techniques the most widely used is X-ray diffraction using texture goniometers, followed by EBSD-method (electron backscatter diffraction) in Scanning Electron Microscopes. For qualitative analysis it can be done by Laue photography, simple X-ray diffraction or with the polarized microscope. neutron and synchrotron high-energy X-ray diffraction allow to access textures of bulk material and in-situ whereas laboratory x-ray diffraction instrument are more appropriate for thin film textures.
Texture is often represented using a pole figure, in which a specified crystallographic axis (or pole) from each of a representative number of crystallites is plotted in a stereographic projection, along with directions relevant to the material's processing history such as the rolling direction and transverse direction or the fiber axis (see below).

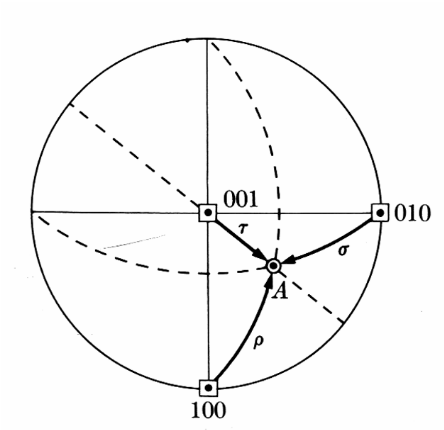
The texture is usually introduced in the fabrication process and affect the material properties by ***introducing structural anisotropy***.

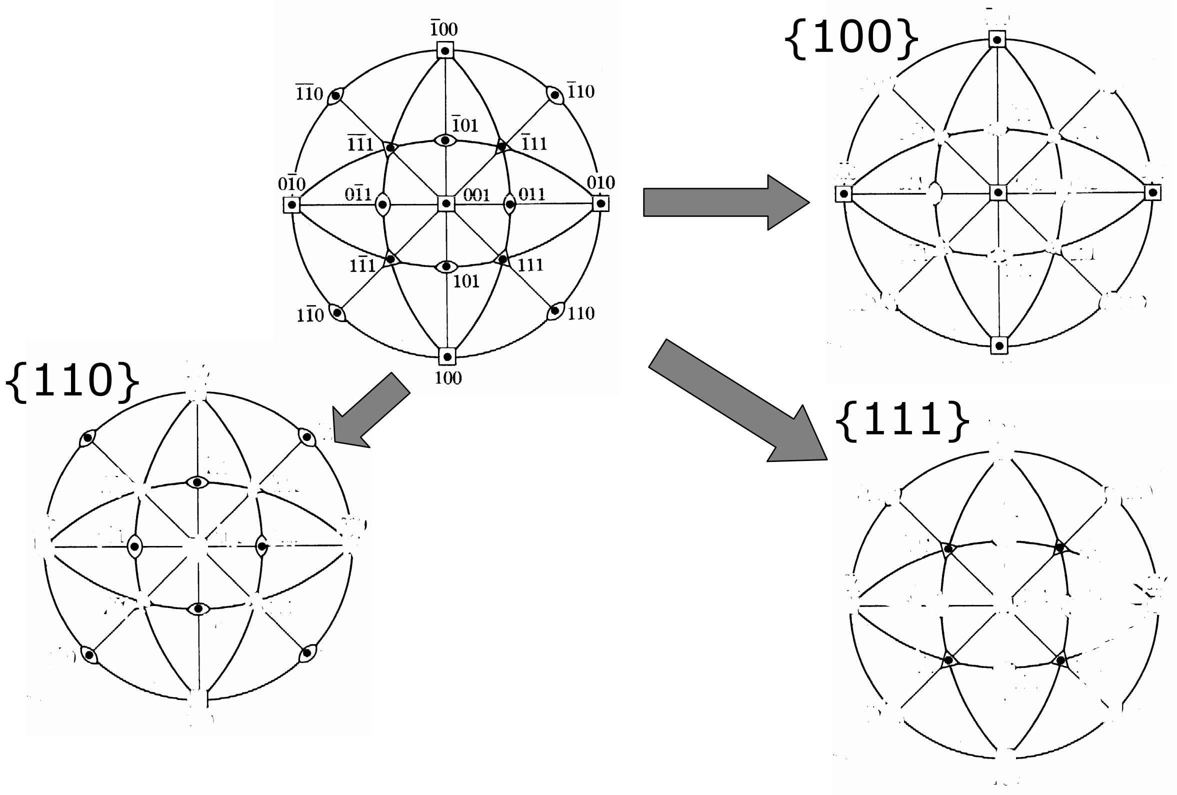
http://en.wikipedia.org/wiki/Texture_%28crystalline%29

Construction of the pole figure



Stereographic projection





Coverage

An important issue related to film uniformity is the *conformal coverage* of nonplanar substrate features.

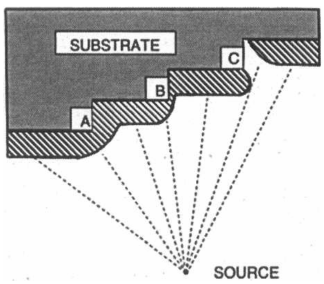
When a film of the same thickness coats the horizontal as well as the vertical surfaces of substrates, we speak of conformal coverage.

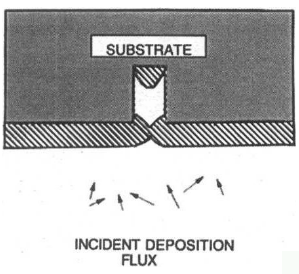
Coverage will not be uniform when physical shadowing effects cause unequal deposition on the top and side walls of the steps.

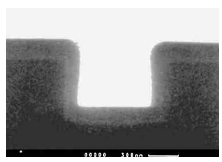
Achieving conformal coverage and filling of deep narrow (i.e. high aspect ratio (depth to width)) channels is a particular challenge.

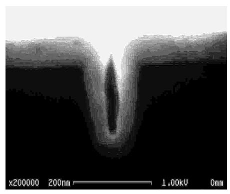
Two important needs of IC metallization are:

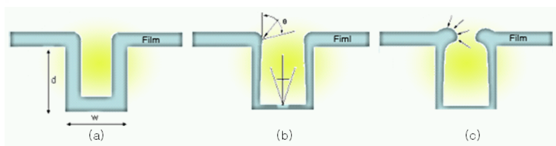
conformal coverage and completely filled trenches and vias.











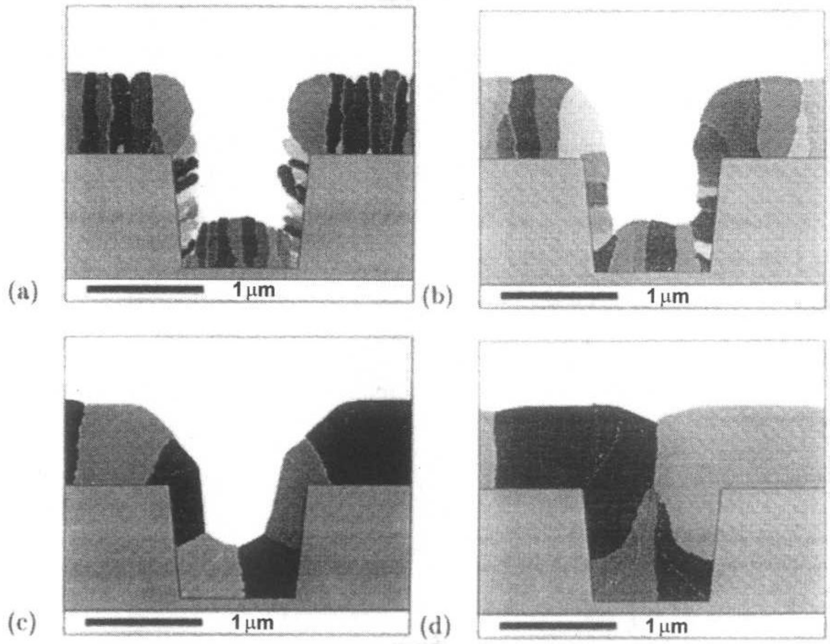


Figure 9-17 Calculated aluminum film microstructures deposited at 250°C using the SIMBAD simulation program. Diffusion lengths are (a) 0.06 μm, (b) 0.18 μm, (c) 0.6 μm, and (d) 1.2 μm. (From Ref. 46.)

Two important needs of IC metallization are:

conformal coverage and completely filled trenches and vias.

Filling may not be achieved or practical to achieve in one step, i.e. during deposition.

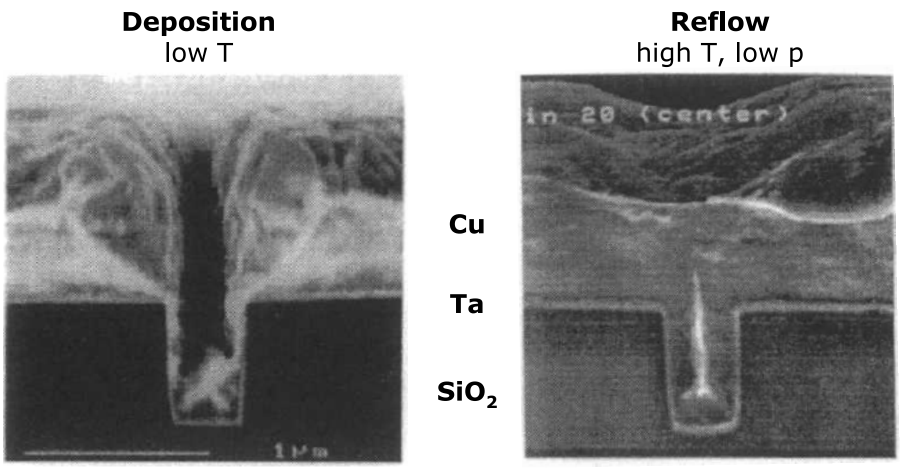


Figure 9-18 (Top) SEM images of sputtered copper microstructures in a 0.35 μm wide, 2:1 aspect ratio trench as deposited (left) and after annealing at 450°C for 25 min. (Bottom)