Texture Development and Abnormal Grain Growth in Thin Films

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(and a bunch of students at MIT and Dartmouth)

• Why texture matters (with a focus on MEMS)
• Structure evolution during film formation
• Texture evolution during film growth
• Texture evolution during annealing
  - normal and abnormal grain growth
  - strain, surface and interface energy
Some Applications of Polycrystalline Thin Films

• Hard, Decorative, and Optical Coatings
• Electronic Devices and Systems
  - Conductors in devices and circuits
  - Device materials - thin film transistors
• Magnetic Devices and Systems
  - Continuous and patterned storage media
  - Read/Write devices
• Photonic Devices and Systems
  - Micromirrors
  - Waveguides
• Microelectromechanical Devices and Systems
  - Micromirrors, microcontacts, actuators, biomedical devices, …

The grain structure and texture of polycrystalline films affect performance and reliability in all cases.
Surface Micromachining for Microelectromechanical Devices and Systems

Grow or

Deposit & pattern oxide  Deposit & pattern poly  Sacrificial etch

Dry Etch  Dry Etch  Wet Etch

Oxide  Poly-Si  Anchor  Cantilever

Si substrate  Si substrate  Si substrate

W. Tang - DARPA
**Accelerometer**

- Anchor
- Folded spring
- Position Sense Region (42 cells)
- Self-Test Region (12 cells)
- Shuttle motion (proof mass)

(Senturia)

**Micro-Contact Switch**

- Position Sense Region (42 cells)
- Self-Test Region (12 cells)
- Shuttle motion (proof mass)

(Novasensor)

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Ni/Au

http://www.ece.neu.edu/edsnu/zavracky/mfl/programs/relay/relay.html
Texture and Mechanical Properties of Films

In actuation applications, the mechanical response generally depends on the biaxial modulus of the film

isotropic materials: \[ \tilde{E} = \frac{E}{1 - \nu} \]

real cubic materials:
\[ \tilde{E}_{(hkl)} = c_{11} + c_{12} + K - \frac{2(c_{12} - K)^2}{c_{11} + 2K} \]
\[ K = H(h^2k^2 + k^2l^2 + h^2l^2) \]
\[ H = 2c_{44} - c_{11} + c_{12} \]
\[ h^2 + k^2 + l^2 = 1 \]

(h, k, and l are direction cosines)

[ isotropic for (111) and (100), dependent on cantilever orientation for other textures]
Texture and Mechanical Properties of Films

In actuation applications, the mechanical response generally depends on the biaxial modulus of the film.

Generally:

- $\tilde{E}_{(100)}$ has the minimum value
- $\tilde{E}_{(111)}$ has the maximum value

<table>
<thead>
<tr>
<th></th>
<th>$\tilde{E}<em>{(100)} / \tilde{E}</em>{(111)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>0.872</td>
</tr>
<tr>
<td>Au</td>
<td>0.416</td>
</tr>
<tr>
<td>Cu</td>
<td>0.440</td>
</tr>
<tr>
<td>Si</td>
<td>0.786</td>
</tr>
</tbody>
</table>
Texture and Mechanical Properties of Films

Inelastic yield affects the range of applications and reliability

Biaxial stress $\sigma$

$\phi = \text{angle between the substrate surface normal (z) and the slip plane normal (N)}$

$\lambda = \text{angle between the slip direction (Burgers vector b) and the substrate surface normal (z)}$

Resolved shear stress $\tau = \sigma \cos(\lambda) \cos(\phi)$

$\sigma_y = \text{yield stress}$

$b = \text{Burgers vector}$

$\text{h = film thickness}$

$W_i = \text{energy of interface dislocation}$

$$\sigma_y = \frac{W_i \sin(\phi)}{b \cos(\lambda) \cos(\phi) \text{ h}}$$
\[ \sigma_y = \frac{(W_L + W_i)}{b \cos(\lambda) \cos(\phi)} \frac{\sin(\phi)}{h} \]

**Yield Stress "Map"**

fcc metals

for \{111\} slip planes

Burgers vectors <110>

(Carel, Ph.D. Thesis)
Structure Evolution During Polycrystalline Film Formation

Polycrystalline Film Formation via Volmer-Weber (Island) Growth

Equiaxed Grain Structure
Other Characteristics of Polycrystalline Structures

Plan-view TEM of bimodal Ge Film

Cross-section of equi-axed poly-Si

Cross-section of columnar poly-Si

Grain Size Distribution

Grain Shape

Crystallographic Texture
Shadowing • Growth Velocity Anisotropy

nucleation and growth

coalessence

• Shadowing
• Growth Velocity Anisotropy

Grain Growth

low $T_{dep}/T_m$ high $T_{dep}/T_m$

Grain Growth

• Shadowing
• Growth Velocity Anisotropy

(coalescence)

nucleation and growth

low $T_{\text{dep}}/T_m$

high $T_{\text{dep}}/T_m$

Type 1

Type 2

Grain Growth

UHV Sputter-Deposited Al
Grain Growth to Stagnation During Deposition

Room Temperature
\( \sim 0.3T_m \)

• Shadowing
• Growth Velocity Anisotropy

nucleation and growth

coalescence

Grain Growth

low \( T_{\text{dep}}/T_m \)  
high \( T_{\text{dep}}/T_m \)

Type 1

Type 2

anneal

Abnormal Grain Growth in Germanium
(h~300A, annealed for 1 hr. at 900C)

- Shadowing
- Growth Velocity
- Anisotropy

(nucleation and growth)

coalescence

low $T_{dep}/T_m$  

high $T_{dep}/T_m$  

Grain Growth

Move boundary points with a velocity proportional to the local curvature

\[ v = m \gamma_{gb} \kappa = \mu \kappa \]

Move triple junctions to maintain a force balance

STABLE STATE GRAIN SIZE DISTRIBUTION

(W.Fayad, C.V. Thompson, and H.J. Frost, Scripta Mater 40, 1199, 1999)
Lognormal Grain Size Distributions

300Å Ge Film annealed 5 hrs. at 915°C (2126 grains)

Evaporated Ge

Sputtered Al

Sputter-Deposited Al (Tracey et al)
Best fit for steady state distributions (from simulations)

(W. Fayad, C.V. Thompson, and H.J. Frost, Scripta Mater 40, 1199, 1999)
Following Mullins, stagnation will occur if: \( \theta_i < \theta_0 \) or \( \kappa < \frac{\gamma_{gb}}{\gamma_s h} \)

Modeling Grain Growth Stagnation

Normal grain growth: $v =$

Normal grain growth with stagnation:

\[ v = \begin{cases} \frac{\gamma_{gb}}{\gamma_{sh}h} & l > 0 \\ 0 & l > 0 \end{cases} \]

\[ \kappa_{cr} = \frac{\gamma_{gb}}{\gamma_{sh}h} \]

Fig. 8. Distributions of $\sqrt{A}$ for the grains in the stagnant structure and a steady-state structure, plotted on both linear and logarithmic scales.

Abnormal Grain Growth in Germanium
(h~300A, annealed for 1 hr. at 900C)

Abnormal Grain Growth

Surface and Interface Energy:
\[ \Gamma_{s/i} = \left( \frac{\Delta \gamma_s}{h} \frac{\gamma_{gb}}{} \right) + \left( \frac{\Delta \gamma_i}{h} \frac{\gamma_{gb}}{} \right) \]
\[ \Delta \gamma_s = \gamma_{s,av} - \gamma_{s,min} \]
\[ \Delta \gamma_i = \gamma_{i,av} - \gamma_{i,min} \]

Strain Energy:
\[ \varepsilon = \left( \alpha_{\text{substrate}} - \alpha_{\text{film}} \right) \Delta T \]
\[ \Gamma_{\varepsilon} = \left( \bar{E}_{\text{min}} - \bar{E}_{\text{av}} \right) \varepsilon^2 / \gamma_{gb} \]

the surface and interface energy depend on the crystallographic orientation of a grain

the biaxial modulus depends on the crystallographic orientation of a grain
Abnormal Grain Growth

Driven by: Interface Energy Minimization
Surface Energy Minimization
Strain Energy Minimization

Abnormal Grain Growth

Surface and Interface Energy:

\[ \Gamma_{s/i} = \left( \frac{\Delta \gamma_s}{h \gamma_{gb}} \right) + \left( \frac{\Delta \gamma_i}{h \gamma_{gb}} \right) \]

\[ \Delta \gamma_s = \gamma_{s,av} - \gamma_{s,min} \]

\[ \Delta \gamma_i = \gamma_{i,av} - \gamma_{i,min} \]

Strain Energy:

\[ \varepsilon = \left( \alpha_{substrate} - \alpha_{film} \right) \Delta T \]

\[ \Gamma_{\varepsilon} = \left( \tilde{E}_{min} - \tilde{E}_{av} \right) \varepsilon^2 / \gamma_{gb} \]

The surface and interface energy depend on the crystallographic orientation of a grain.

The biaxial modulus depends on the crystallographic orientation of a grain.
Comparison of Ag/(001)Ni Experiments and Simulations

Cu films 0.5-10mm thick Annealed on Polyimide at 330°C
(Max-Planck for Metals)

P. Sonnweber-Ribic, P. Gruber, G. Dehm, and E. Arzt,
Super Secondary Grain Growth in Cu Films
(IMEC, Hasselt University)

(SGG = abnormal grain growth)

Abnormal Growth of Giant Grains in Ag Films
(Max Planck Institute for Metals)

Initial texture (111), Giant grains (100)
Both on and off the substrate.

Abnormal Growth of Giant Grains in Ag Films
(Max Planck Institute for Metals)

Abnormal Growth of Giant Grains in Ag Films
(Max Planck Institute for Metals)

When grain sizes are significantly smaller than the film thickness, the analysis is more complex.
Summary

• When polycrystalline films form through the Volmer-Weber mechanism (island nucleation and growth) all of the following can be texture selective:
  i) island nucleation
  ii) island growth
  iii) grain growth during island coalescence, during thickening of continuous films, and during post-deposition annealing
  iv) competitive processes at the surface of a growing continuous films

• Mechanism iii) dominates for high mobility materials (e.g. fcc metals) even down to 0.2T<sub>m</sub>

• Models for 2D grain growth generally do not describe behavior in thin films well

• Models that include the effects of grain boundary trapping, surface energy anisotropy, and strain energy anisotropy do better.

• Some unanswered questions:
  - What triggers “giant” grain growth or “SSGG”?
  - Are there multiple mechanism that lead to (100) texture?
  - Are recrystallization, grain rotation.... important?