Lecture 3:
Fundamentals of Sputter Deposition
Outline

Sputtering yield
• Linear cascade
• Correction for threshold effect
• Sputtering efficiency
• Energy of sputtered atoms
• Ion reflection

Sputtering systems
• Conventional diode sputtering
• Triode sputtering
• Magnetron sputtering
  • Discharge characteristics
  • Ion distribution at substrate
  • Reactive sputtering
  • Independent control of ion flux and ion energy
Bibliography


Ion surface interactions

Ion beam with an energy $E_i$

Positive ions are returned by the electric field

Elastic Effects

Sputtered Particles $T^0, T^+, T^n$

Reflected Particles $I^0, I^+$

Negative Ions $T^-, I^-$

Accelerated by the field

Inelastic Effects

UV/visible photons

X-rays

Secondary Electrons

Accelerated by the field

Implanted Particles $I^0$

Target

Figure after G.M. McCracken, Rep. Prog Phys. 28, 241 (1975).
Ions striking a surface interact with a number of atoms in a series of collisions. 
- recoiled target atoms in turn collide with an atom at rest generating a collision cascade. 
- The initial ion energy and momentum are distributed to among the target recoil atoms. 
- When \( E_i > 1 \text{ keV} \), the cascade is “linear”, i.e. approximated by a series of binary collisions in a stationary matrix.
Stopping cross section

\[
\frac{dE}{dx} = -NS(E) = -N\left[ S_n(E) + S_c(E) \right]
\]

\[
Range = \int_0^E \frac{dE'}{NS(E')}
\]
SRIM/TRIM simulation

Monte-Carlo simulation of ion implantation, reflection, recoil cascades, and sputtering

1 keV Ar -> Be

2 impacts

ion trajectories in red
recoils in green

1 keV Ar -> Ti

200 impacts

1 keV Ar -> W

James F. Ziegler, IBM : http://www.srim.org/
Sputtering begins at an energy threshold and increases rapidly. As the energy increases the curve levels off.

Sigmund’s linear cascade formula for $Y(E)$

$$Y(E) = \frac{0.04}{U} \alpha(M_t/M_i) S_n(E)$$

$\alpha$ - dimensionless coefficient  
$S_n(E)$, collisional energy at the surface  
(nuclear energy loss function)  
$U$ – sublimation energy

$$S_n(E) = 85 \frac{Z_i Z_t}{(Z_i^{2/3} + Z_t^{2/3})^{0.5}} \frac{M_i}{M_i + M_t} s_n(\varepsilon)$$

$s_n(\varepsilon)$ – function of the reduced energy which is the same for all ion-target combination

$$s_n(\varepsilon) = \frac{3.441 \sqrt{\varepsilon} \ln(\varepsilon + 2.718)}{1 + 6.355 \sqrt{\varepsilon} + \varepsilon (6.882 \sqrt{\varepsilon} - 1.708)}$$

$$\varepsilon = \frac{0.03255}{Z_i Z_t (Z_i^{2/3} + Z_t^{2/3})^{0.5}} \frac{M_t}{M_i + M_t} E$$

P. Sigmund, Physical Review. 184, 383 (1969)
0.1 < E < 1kV, Sigmund derives a remarkably simple formula

\[ Y(E) = \frac{3}{4\pi^2} \alpha \left( \frac{M_t}{M_i} \right) \gamma E \]

\[ \gamma = \frac{4M_iM_t}{(M_t + M_i)^2} \]
Sputtering Threshold ($E_{TH}$)

Sputtering begins at an energy threshold that depends on the efficiency of momentum transfer to the target. This depends on the mass match. It also depends on the surface binding energy of atoms in the target.

Y. Yamamura et al introduced a correction for $E_{TH}$

$$Y(E) = \frac{0.04}{U} \alpha(M_t / M_i) Q S_n(E) \left( 1 - \left( \frac{E_{TH}}{E} \right)^{0.5} \right)^2$$

$$Q = \frac{q_T}{1 + s_e(\varepsilon)}$$

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“Simple” Y(E) formula
for E < 1 keV , M_i > 15 amu

\[ Y(E) = \frac{1.8}{U} \alpha \left( \frac{M_t}{M_i} \right) \frac{(Z_i Z_t)^{0.5}}{(Z_i^{2/3} + Z_t^{2/3})^{0.5}} \frac{(M_i M_t)^{0.5}}{(1 + M_t / M_i)^{0.5}} E^{0.5} \left( 1 - \left( \frac{E_{TH}}{E} \right)^{0.5} \right)^2 \]

Eqn. A

\[ Y(E) = \frac{3}{4\pi^2} \alpha \left( \frac{M_t}{M_i} \right) \frac{\gamma E}{U} \]

\[ \gamma = \frac{4M_i M_t}{(M_t + M)^2} \]

\[ E_{TH} = \frac{1}{\alpha} \left( \frac{\gamma E}{U} \right) \]
Energy efficiency of sputtering

Power of the ion beam - \( P_{\text{ion flux}} = J \times E \)

Power used for sputtering - \( P_{\text{sp}} = U \times J \times Y(E) \)

Sputtering efficiency \( \eta = P_{sp} / P_{\text{ion flux}} \)

\( \eta = U \times Y(E) / E \)

Yamamura formula: \( \eta_{\text{max}} \) at \( E = 7 \times E_{\text{th}}^{0.8 \eta_{\text{max}}} \)

For \( 3E_{\text{TH}} \leq E \leq 10E_{\text{TH}} \), \( \eta \geq 0.8 \eta_{\text{max}} \)

Typical example:

\( U = 4 \text{ eV}, E_{\text{TH}} = 30 \text{ eV}, \eta_{\text{max}} \) at \( E = 210 \text{ eV} \)

\( 0.8 \eta_{\text{max}} E = 90 - 300 \text{ eV} \)
Energy efficiency of sputtering

The maximum sputtering efficiency between 0.5 and 5%.

Ar provides high sputtering efficiency for a large number of metal targets (from Al to La).

Ne has ~ 20% advantage for Be and C.

Kr ~ 40-60% advantage for targets heavier than Ta.

Sputtered atom energy has a maximum at ~ U/2 (several eV) and tail extending to tens and hundreds of eV, depending on the ion energy.

Energy (Thompson) distribution:

\[ F(E) \propto \frac{E}{(E + U)^3} \left( 1 - \left( \frac{E + U}{\gamma E_{ion}} \right)^{1/2} \right) \approx \frac{E}{(E + U)^3} \]
Sputtering Yield: Other Species

Distribution of types of sputtered species:  
[Example for Ar sputtering of Cu]

- Single atoms sputtered: 100
- Diatoms: 1
- Resputtered trapped gas: 5
- Single ions: 0.1
- Diatomic ions: 0.001
- Reflected incident species: 3
- Secondary electrons: 10
Reflection of Primary Ions

Incident ions may be reflected from the target surface.
Reflection coefficient = \#reflected ion/\#incident ion

Case study: TRIM simulation of 500 eV Ar ion scattering

Both reflection coefficient and the average energy of the reflected ions increase when the target atom is heavier than the ion
Reflection of Primary Ions, cont.

Incident ions may be reflected from the target surface.

Reflection coefficient = \( \frac{\text{#reflected ion}}{\text{#incident ion}} \)

Case study: TRIM simulation of 500 eV, Xe, Ar, and N ion scattering

Both reflection coefficient and the average energy of the reflected ions for a given target decrease when heavier ions are used.
Reflection of Primary Ions, cont.

Case study: TRIM simulation of 500 eV, Xe, Ar, and N ion scattering

A significant fraction of the incident ion energy (> 10%) is reflected back when ions are much lighter than the target atoms.
Variations of sputtering systems
Magnetron sputtering
Unbalanced magnetrons
Diode sputter deposition system
Components and typical parameters

$V_T \sim 2-5 \text{ kV}$
$J_T \sim 1 \text{ mA/cm}^2$
$p \sim 50-80 \text{ mTorr}$
$\lambda \ll d_{TS}$
Triode sputter deposition system
Components and typical parameters

\[ V_T \sim 1 \text{ kV} \]
\[ J_T \sim 5 \text{ mA/cm}^2 \]
\[ p \sim 10-20 \text{ mTorr} \]
\[ \lambda \sim d_{TS} \]

Independent control of ion flux and energy
The presence of a hot filament hampers reactive deposition
**Triode sputter deposition system**

**Components and typical parameters**

- $V_T \sim 0.3-0.5 \text{ kV}$
- $J_T \sim 10-100 \text{ mA/cm}^2$
- $p \sim 2-20 \text{ mTorr}$
- $\lambda > d_{TS}$, $\lambda < d_{TS}$

ExB field near target enhances ionization efficiency, thus reducing both $V_T$ and $p$
ExB configurations

Magnetron discharge characteristics

DC magnetron discharge characteristics

Example: 50 mm Vanadium target, planar magnetron

\[ I_T = 0.3 \, \text{A} \]

\[ p = 1 \, \text{Pa (7.5 mTorr)} \]
Thermalization of sputtered species

In typical pressure range for magnetron sputter deposition, both collisionless and diffusive transport are effective

Reactive sputtering

I. Petrov, A. Myers, J.E. Greene, and J.R. Abelson, JVST A 12, 2846 (1994)
Ion distribution at the substrate

Relative ion fluxes

- \(\text{Ar}^+\)
- \(\text{Ar}^{2+}\)
- \(\text{Ti}^+\)
- \(\text{N}^+\)
- \(\text{N}_2^+\)
- \(\text{TiN}^+\)

Ti Target
- \(P_T = 3\) mTorr
- \(I_T = 0.2\) A

I. Petrov, A. Myers, J.E. Greene, and J.R. Abelson, JVST A 12, 2846 (1994)
Independent control of ion flux and ion energy

\[ E_i = e(V_{\text{plasma}} - V_{\text{bias}}) \]
\[ J_i = f(B_{\text{ext}}) \]