

The (in)stability of process control mechanisms in reactive DC sputtering deposition

Simulation software

RSD 2013
version 3
= balance equation model

INPUT
operation and material parameters

OUTPUT
operation process curves (with hysteresis)

System observables:
reactive gas pressure
discharge current/voltage
target/substrate state

Operation parameters:
reactive gas flow
pumping speed
discharge current/voltage

GUI + manual

SIMTRA
version 2.1.1
= test particle Monte Carlo model

OUTPUT
deposition:
number densities
energy distribution
incidence direction

INPUT
3D representation setup
target racetrack
initial energy/angular distribution
sputter gas pressure/temperature
interaction potential

GUI + manual

process curve $O(S)$

Problem : Criticality mechanisms during reactive deposition

Planar 2 inch Al DC sputtered in Ar/O₂ atmosphere

R. Schelfhout et al., Applied Physics Letters 109, 111605 (2016)

$Q_{O_2} = 1.2$ sccm

"traditional" hysteresis

higher/lower reactive gas pressure

less/more reactive gas getting by substrate

more/less target reaction

lower/higher deposition rate

Substrate driven

"double" hysteresis

higher/lower compound fraction

more/less target reaction

lower/higher erosion speed

more/less implanted reactive gas

more/less time to react

Target driven

Solution : Voltage control ?

stable Al - Al₂O₃

☺ $\gamma_{see,ox} > \gamma_{see,m}$

reactive IV-characteristic = superposition of metallic and oxidized $I = k_{m/ox}(V - V_{m/ox,0})^2$ where $k \sim \gamma_{see}$

unstable Ti - TiO₂ - ...

☹ $\gamma_{see,ox} < \gamma_{see,m}$

reactive IV-characteristic = superposition of metallic and ONE oxidized IV? No!

Different oxidation states? In-vacuo XPS determination of target composition proves existence of two additional sub-oxides TiO and Ti₂O₃ along hysteresis.

Reactive IV-characteristic is in fact a mixture of four $I = k_i(V - V_{i,0})^2$ with $i = Ti, TiO, Ti_2O_3, TiO_2$ and $k_i \sim \gamma_{see,i}$ where

$\gamma_{see,Ti} > \gamma_{see,TiO} > \gamma_{see,TiO_2} > \gamma_{see,Ti_2O_3}$

