



Source Scale-up for Physical Vapor Deposition of Cu(InGa)Se₂ on Flexible Substrates



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INTRODUCTION

IEC Pilot-scale system

- Inline roll-to-roll physical vapor deposition (PVD) of Cu(InGa)Se₂ film onto 6" wide flexible polyimide substrates
- Typical deposition run: 10 feet substrate with web speed of 0.75"/min

Motivation

System scale-up to wider substrates (~12") and faster web speeds (~12"/min) for commercially attractive, high throughput low cost production.

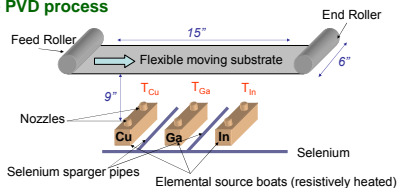
Successful scale-up requires:

- Symmetric melt surface temperature profile
- Higher effusion rate
- Low operating temperature

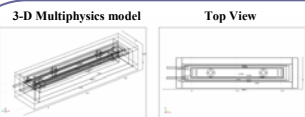
Modeling requirements:

- Source temperature profile prediction
FEMLAB modeling
- Effusion rate and flux distribution prediction
Direct Simulation Monte Carlo modeling

Co-evaporative PVD process

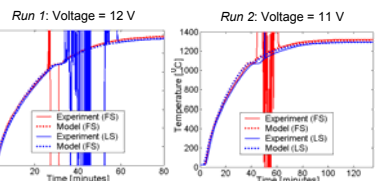


FEMLAB MODELING: Asymmetric heater



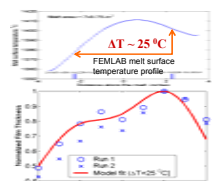
- Assumptions:**
- Good thermal contact between all the components
 - Rectangular source interior
 - Neglect convective heat transfer
- Model input:** Voltage across the heater pins
Model output: Source temperature profile

Experimental Validation: Temperature dynamics



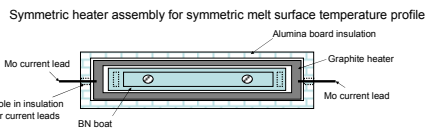
Model fits experimental data very well
FEMLAB accurately predicts source temperature dynamics

Validation: Film thickness profile



- Accurate prediction of melt surface temperature
- Asymmetric heater causes unequal nozzle effusion rates

FEMLAB MODELING: Symmetric heater



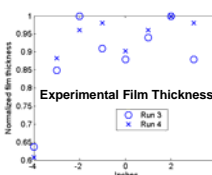
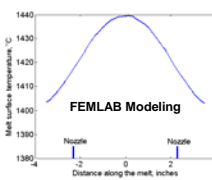
Melt surface and heater temperature profile: top view



Temperature under each nozzle is the same

Effusion rate from each nozzle is the same
 (Peak heights in the film thickness profile are equal)

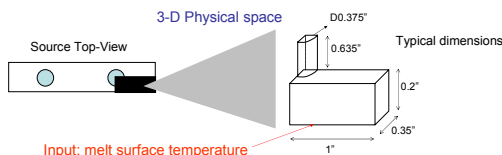
Easier to achieve film thickness uniformity



DIRECT SIMULATION MONTE CARLO (DSMC)

Direct Simulation Monte Carlo (DSMC) is a computational Monte Carlo algorithm for the stochastic simulation of rarefied gas flows

- Particle motion and inter-particle collisions are decoupled over small time intervals
- Particle motions are modeled deterministically
- Collisions are treated statistically
- Each simulated particle represents a large number of actual particles
- Physical space is divided into "cells" of fixed volume; particles located within a given cell are allowed to interact
- Average within a cell provides macroscopic flow properties at the center of the cell



Simulation parameters:

- Number of simulated particles ~ 1000
- Actual atoms per simulated particle: $F \sim 10^{11}$
- Initially all the particles are on the melt surface
- Cubic cell with dimension: $\lambda/3$, λ : mean free path
- Time interval, $\Delta t = \tau/10$, τ : mean collision time
- Particles per cell = 30

Assumptions:

- Uniform temperature throughout the physical space
- The vapor effusion properties depend on the melt temperature directly below the nozzle

Effusion flow properties

- **Vapor flow rate:** the number of particles exiting the nozzle per unit time

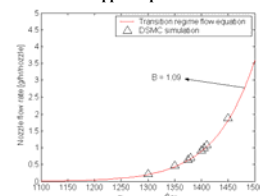
$$f = 4 \frac{N_{out} FM}{N_A t}$$

N_{out} : total # of particles that have exited the nozzle
 N_A : Avogadro number
 t : time elapsed
 M : molecular weight

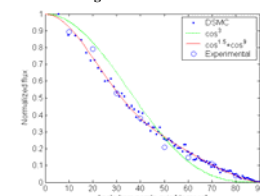
- **Angular flux distribution:** frequency distribution of the angles at which the particles exit the nozzle

Validation: Experimental and DSMC Results

Copper vapor flow rate



Angular flux distribution



Transitional regime flow equations

$$\frac{\dot{m}_{nozzle}}{A_{nozzle}} = B \left(\frac{P_{cell} - P_{nozzle}}{\sqrt{2\pi RT/M}} \right)$$

$$\frac{\dot{m}_{nozzle}}{A_{nozzle}} = \frac{D^2}{16\mu L} \left(\frac{P_{cell}^2 - P_{nozzle}^2}{RT/M} \right) \left(1 + 4 \left(\frac{2}{f} - 1 \right) \frac{L}{D} \right)$$

Experimentally fitted parameter: B
 B: Correction factor for entrance losses

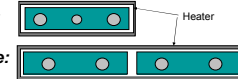
- DSMC simulation vapor flow rate prediction matches very well with the experimental data
- DSMC simulation instead of real experiments can be used to determine vapor flow rates
 - Reduces cost and development time
- DSMC angular distribution result matches with experimental data
 - $\cos^{n1}(\theta) + \cos^{n2}(\theta)$ is a better fit than $\cos^3(\theta)$

FEMLAB thermal modeling and DSMC simulations are now used to optimize source design parameters to achieve desired film thickness uniformity

SOURCE SCALE-UP

Two example designs:

- **Three nozzle single source:**



- **Four nozzle modular source:**

Designed for:

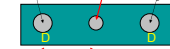
- Substrate = 12 inch wide
- Source-substrate distance (H) = 6" } 2 μm film thickness
- Thickness non-uniformity < 10%

Procedure:

1. Optimize nozzle-to-nozzle separation and nozzle flow rates for desired film thickness uniformity
2. Determine melt surface temperature profile using FEMLAB
3. Determine nozzle diameter using DSMC to obtain desired effusion rates

3-Nozzle Single Source

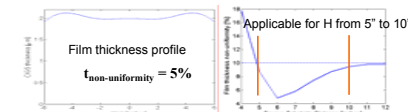
1. **Center nozzle flow rate (f_c)?**



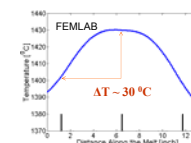
For given:
 Outer nozzle diameter = D, and
 Web speed

Nozzle-to-nozzle separation (d_{NN})?

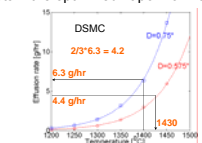
Optimize for f_c and d_{NN} to achieve $\pm 5\%$ thickness non-uniformity.



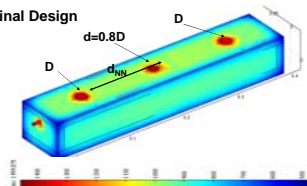
2. FEMlab modeling



3. Determine center nozzle diameter to obtain the optimized vapor flow rate

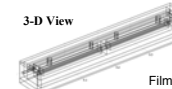


Final Design

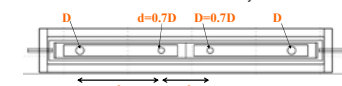


Film thickness = 2 μm
 Web speed = 1 foot/min
 Thickness non-uniformity = 5%
 Material utilization efficiency = 65%
 Source operating temperature under outer nozzle = 1400 °C

4-Nozzle Modular Source



Film thickness = 2 μm
 Web speed = 2 inch/min
 Thickness non-uniformity = 5%
 Material utilization efficiency = 66%



Source operating temperature under the outer nozzle = 1375 °C