Physical Simulations in the Semiconductor Industry

- a survey -

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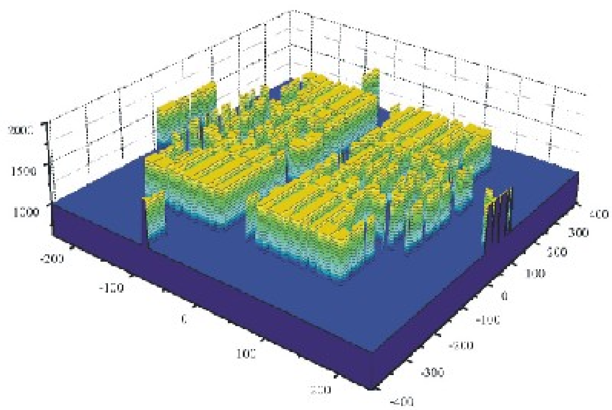
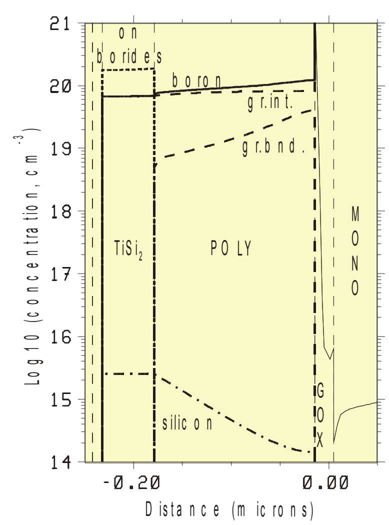
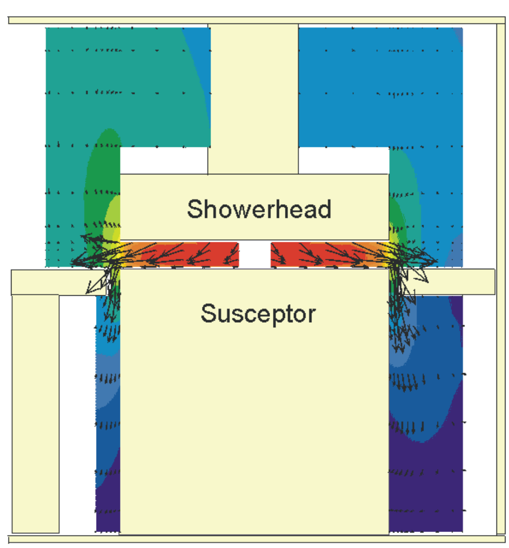
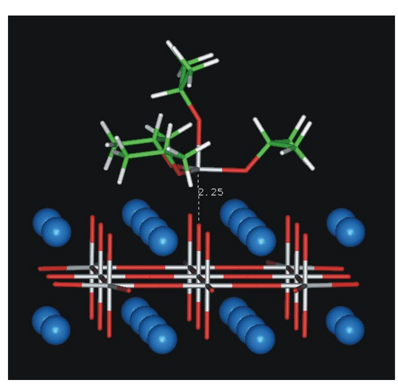
MP PTS









content

- motivation / benefits
- simulations at Infineon MP PTS
- project examples
  - high density plasma CVD
  - stability of EPI markers
- summary & notes

motivation / benefits

challenges:

- very fast product cycles
- extremely high expenses
- tough competition
- limit of current technology
- complex interactions
- no model systems
- ...

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simulation:

- yields more detailed insights
- often only way to get information otherwise not available
- fast & inexpensive (hopefully)
- (is fun)
- ...

simulation at MP-PTS

process:

- development of physical models like dopant distribution, defects...
- process optimization
- ...

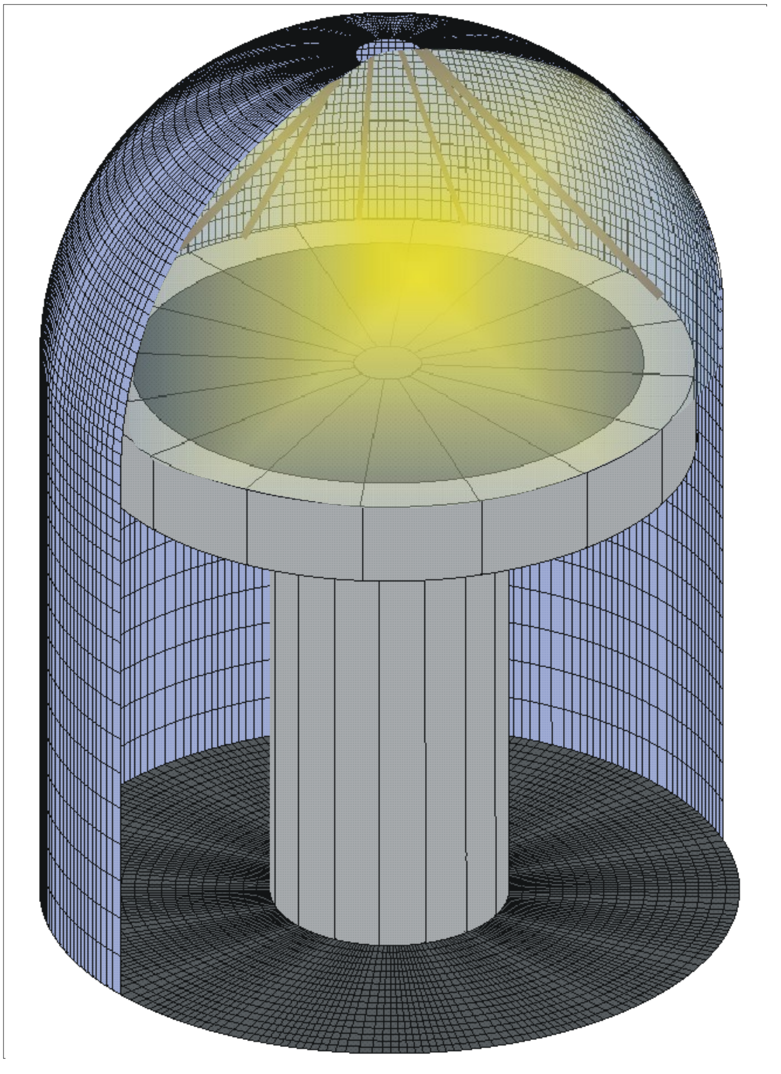
device:

- microscopic field distributions
- electron transport simulations
- scaling of devices
- ...

equipment:

- support process-engineers
- solve DE of flow, heat, & chemistry
- MC modelling of radiative heating
- ...

HDP-CVD



task:

- identify uniformity problems
- increase deposition rate
- improve gap-fill (feature scale)

goals:

- develop chemistry / plasma model
- identify relevant processes in reactor
- find reason for non-uniformity in SiO_2 films
- optimize recipe for deposition/etching

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challenges:

- gas flow
  - low pressure → possible breakdown of continuum fluid-dynamics
  - non-trivial geometry, complicated gas flow
- chemistry
  - complex plasma chemistry
  - experiments difficult

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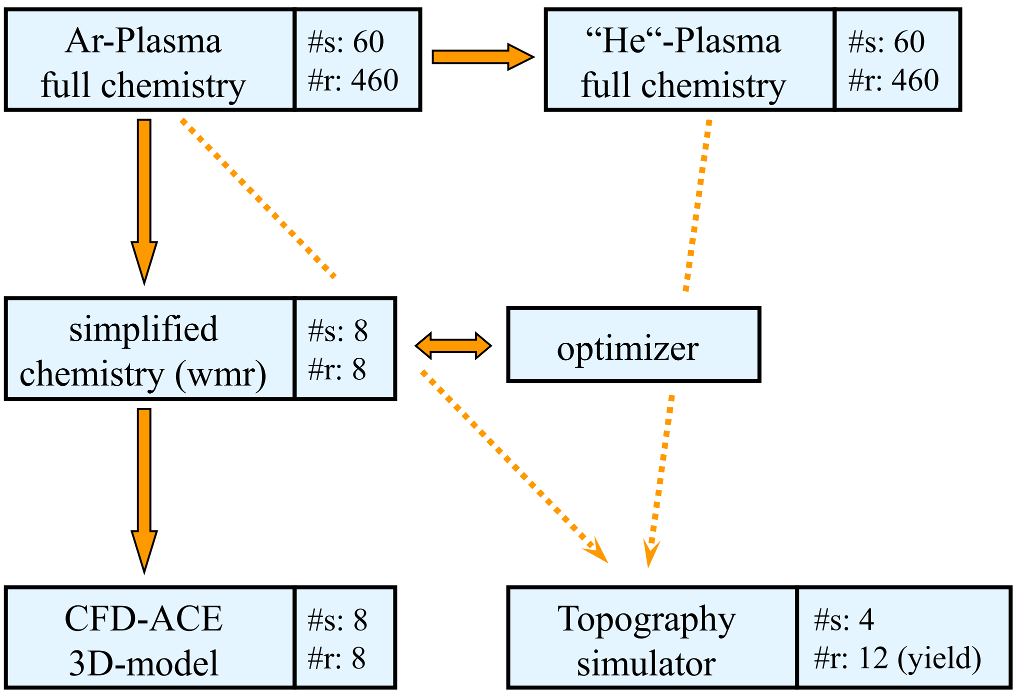
benefits:

- fast diffusion → similar to wmr

HDP-CVD activities



different complexities & scales:

- complicated chemistry using well-mixed reactor simulations
- simplified chemistry for Ar-process using custom wmr-simulator
- full 3D computational fluid dynamics simulations with simplified chemistry
- microscopic model for HDP-CVD

HDP-CVD chemistry

thermal ≈ 0.1 eV ↔ electron ≈ 5 eV
⇒ complicated chemistry!!!

Meeks et al., J.Vac.Sci.Techn. A 16(2) pp 544:

T is in Kelvin.

	Reaction	A	B	C	Notes	Ref.
	(Electron-impact reactions with argon)					
1.	$E+Ar \Rightarrow E+Ar^*$	1.17E−08	0.0	138 560.0		22, 23
2.	$E+Ar \Rightarrow Ar^+ +2E$	7.07E−11	0.6	187 120.0		23
3.	$E+Ar^* \Rightarrow Ar^+ +2E$	1.25E−07	0.1	60 524.0		24
	(Electron-impact reactions with oxygen)					
4.	$E+O_2 \Rightarrow O_2+E$	1.41E−04	−1.5	11 594.0	[v] $\nu_0 \rightarrow \nu_1$	25
5.	$E+O_2 \Rightarrow O_2+E$	2.41E−04	−0.9	76 827.0	[v] $\Sigma_{n=2,3,4}(\nu_0 \rightarrow \nu_n)$	25
6.	$E+O_2 \Rightarrow O_2+E$	7.13E−08	−0.1	30 812.0	[e] $a\ ^1\Delta_g$	25
7.	$E+O_2 \Rightarrow O_2+E$	2.75E−10	0.0	30 656.0	[e] $b\ ^1\Sigma_g^+$	25
8.	$E+O_2 \Rightarrow O_2+E$	2.29E−10	0.4	68 652.0	[e] $B\ ^3\Sigma_u^- + A\ ^3\Sigma_u^+ + C\ ^3\Delta_u + c\ ^1\Sigma_u^-$	25
9.	$E+O_2 \Rightarrow O+O^*+E$	4.52E−13	0.9	51 069.0		26
10.	$E+O_2 \Rightarrow O_2^+ +2E$	3.99E−14	1.1	137 580.0		25
11.	$E+O_2 \Rightarrow O+O-$	3.60E−08	−0.5	57 440.0		25
12.	$E+O \Rightarrow O^*+E$	4.30E−07	−0.3	38 431.0	[e] $2p^4\ ^1D$	27
13.	$E+O \Rightarrow O+E$	1.24E−09	0.0	60 440.0	[e] $2p^4\ ^1S$	27
14.	$E+O \Rightarrow O+E$	1.67E−09	0.0	146 940.0	[e] $3s'\ ^3D^0$	27
15.	$E+O \Rightarrow O+E$	4.36E−09	0.0	110 150.0	[e] $3s\ ^3S^0$	27
16.	$E+O \Rightarrow O+E$	1.93E−15	1.1	530 780.0	[e] O^{++}	28
17.	$E+O \Rightarrow O^+ +2E$	1.95E−11	0.6	165 410.0		27
18.	$E+O^* \Rightarrow O^+ +2E$	1.95E−11	0.6	140 000.0	g	
19.	$E+O^- \Rightarrow O+2E$	2.10E−10	0.5	39 434.0		29
20.	$E+E+O \Rightarrow O^- +E$	1.00E−30	0.0	0.0		27
	(Metastable and ion reactions in O_2/Ar)					
21.	$Ar^*+Ar^* \Rightarrow Ar+Ar^+ +E$	6.20E−10	0.0	0.0		30
22.	$O^- +O_2^+ \Rightarrow O+O_2$	2.80E−07	0.0	0.0	g	
23.	$O^- +O^+ \Rightarrow 2O$	2.80E−07	0.0	0.0		31
24.	$O^- +O \Rightarrow O_2+E$	1.40E−10	0.0	0.0		32
25.	$O^- +Ar^+ \Rightarrow O+Ar$	2.80E−07	0.0	0.0	g	
26.	$O^+ +O_2 \Rightarrow O_2^+ +O$	2.10E−11	0.0	0.0		33
27.	$O_2^+ +Ar \Rightarrow Ar^+ +O_2$	5.50E−11	0.0	0.0		33
28.	$Ar^+ +O_2 \Rightarrow +O_2^+$	4.60E−11	0.0	0.0		33
29.	$Ar^+ +O \Rightarrow O^+ +Ar$	4.60E−11	0.0	0.0	g	
30.	$O^*+O_2 \Rightarrow O+O_2$	3.20E−11	0.0	−67.0		34
31.	$O^*+O \Rightarrow O+O$	4.00E−11	0.0	0.0		35
32.	$O^*+Ar \Rightarrow Ar+O$	4.00E−11	0.0	0.0	g	
33.	$O+Ar^* \Rightarrow Ar+O$	4.00E−11	0.0	0.0	g	
34.	$O^*+Ar^* \Rightarrow O+Ar$	4.00E−11	0.0	0.0	g	
35.	$O_2+Ar^* \Rightarrow Ar+O_2$	4.00E−11	0.0	0.0	g	
	(Electron-impact reactions with silane)					
36.	$E+SiH_4 \Rightarrow SiH_4+E$	1.38E−04	−0.7	48 872.0	[v] $\nu_0 \rightarrow \nu_1,\ \nu_3$	36
37.	$E+SiH_4 \Rightarrow SiH_4+E$	4.52E−03	−1.0	21 902.0	[v] $\nu_0 \rightarrow \nu_2,\ \nu_4$	37
38.	$E+SiH_4 \Rightarrow SiH_3+H+E$	8.96E−03	−1.0	123 500.0	[d] 17%	36
39.	$E+SiH_4 \Rightarrow SiH_2+2H+E$	1.83E−03	−1.0	123 500.0	[d] 83%	36
40.	$E+SiH_4 \Rightarrow SiH_3^+ +H+2E$	3.06E−02	−1.3	184 820.0		38
41.	$E+SiH_4 \Rightarrow SiH_2^+ +H_2+2E$	2.69E−02	−1.2	179 670.0		38
42.	$E+SiH_4 \Rightarrow SiH^+ +H_2+H+2E$	1.07E−03	−1.2	189 440.0		38
43.	$E+SiH_4 \Rightarrow Si^+ +2H_2+2E$	1.58E−03	−1.3	188 260.0		38
44.	$E+SiH_4 \Rightarrow H_2^+ +SiH+H+2E$	1.89E−22	−0.4	22 610.0		38
45.	$E+SiH_4 \Rightarrow H^+SiH_2+H+2E$	9.49E−23	−0.4	20 793.0		38
	(Electron-impact reactions with hydrogen)					
46.	$E+H_2 \Rightarrow H_2+E$	1.40E−05	−0.8	22 641.0	[v] $\nu_0 \rightarrow \nu_1$	39
47.	$E+H_2 \Rightarrow H_2+E$	4.18E−12	0.6	140 680.0	[e] $B\ ^1\Sigma_u^+$	39

...

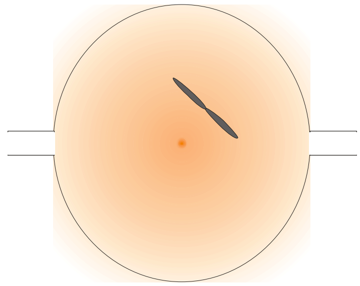
Σ = 460 reactions; 60 species

⇒ no chance for CFD-simulator...

well-mixed model

diffusion fast compared to chemistry (“well mixed reactor“)

⇒ 0-dim set of 460 coupled ODE‘s for 60 variables



pro:

- gas pressure low → diffusion fast ($D \approx 10\ m^2/s$); chemistry slow
- fast ion-diffusion ($D_{plasma} \approx 100 \cdot D_{gas} \approx 10^3\ m^2/s$)

con:

- oxidation of SiH_4 <u>very</u> fast
- no spatial depencies included (heating, pressure, T_{el}, [e],...)

use wmr simulator (“Chemkin“, ReactionDesign) for detailed HDP chemistry study...

...before using simplified chemistry model for CFD

wmr results

- complex dependencies, sometimes counterintuitive!
- good agreement with experiment
- Ar^+ sputtering needed for deposition (activation)
- other simulation results:
  - plasma density $\approx 7 \times 10^{10}$ cm^{-3}
  - electron temperature $\approx$ 3.5 eV
  - neutral gas temperature $\approx$ 700 K
  - [e] and T_d decrease with O_2 flux (electronegative)
  - [e] and T_d increase with SiH_4 flux (electropositive)
- ...

nice results...

BUT

for full simulation, CFD and WMR

have to be combined...

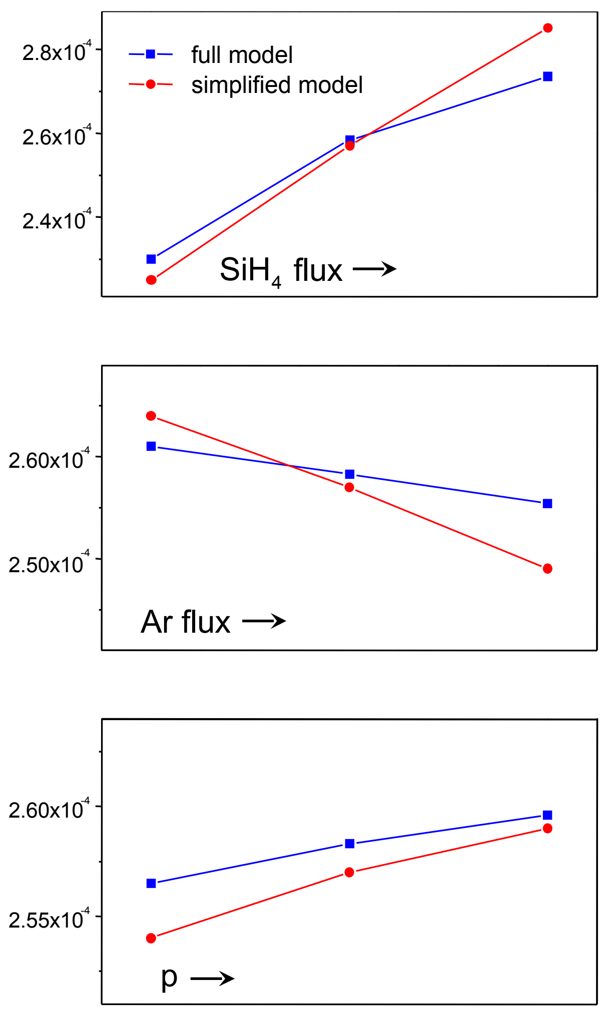
simplified chemistry

plasma:

$$SiH_4 \Rightarrow SiH_2 + H_2$$
$$O_2 \Rightarrow 2O$$
$$Ar \Rightarrow Ar^+$$
$$\ldots$$

wafer:

$$SiH_2 + 2O \Rightarrow SiO_2^B + H_2$$
$$SiO_2^B + Ar^+ + H_2^{\alpha=0} \Rightarrow SiH_2 + O_2 + Ar$$
$$\ldots$$



→ very good agreement. Simplified chemistry ready for incorporation into CFD!

CFD breakdown?

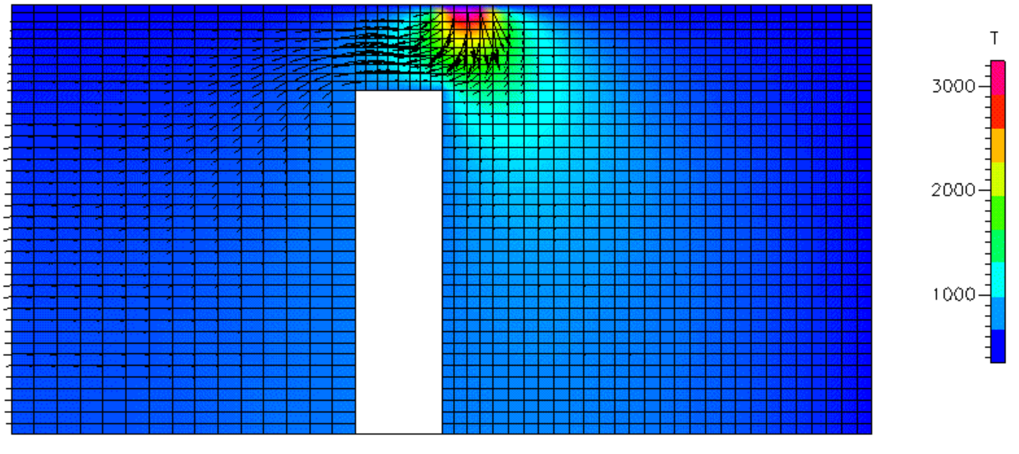
MC: + correct results even for low *p*
- slooowww... (days - weeks)

CFD: + fast (hours - days)
- not valid at low *p*:

criterium Knudsen number: $K := \frac{l}{L} \overset{!}{<} 0.01$

$$l = \frac{k_B T}{\sqrt{2}\, p \sigma} \approx 1\ \text{cm};\ L \approx 10\ \text{cm} \Rightarrow K \approx 0.1\ !!!$$

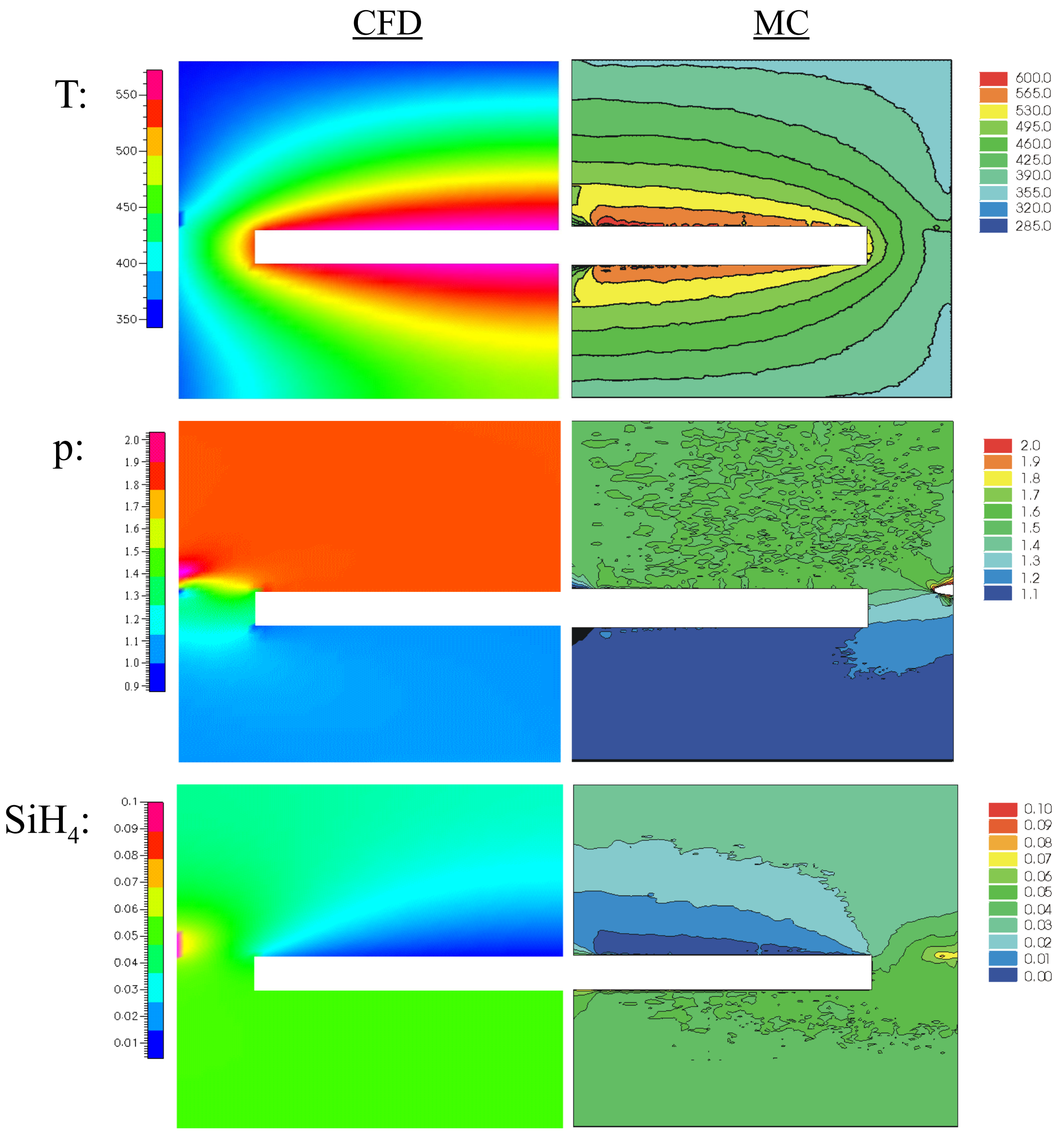
check...



... breakdown!

MC vs. fluid-dynamics

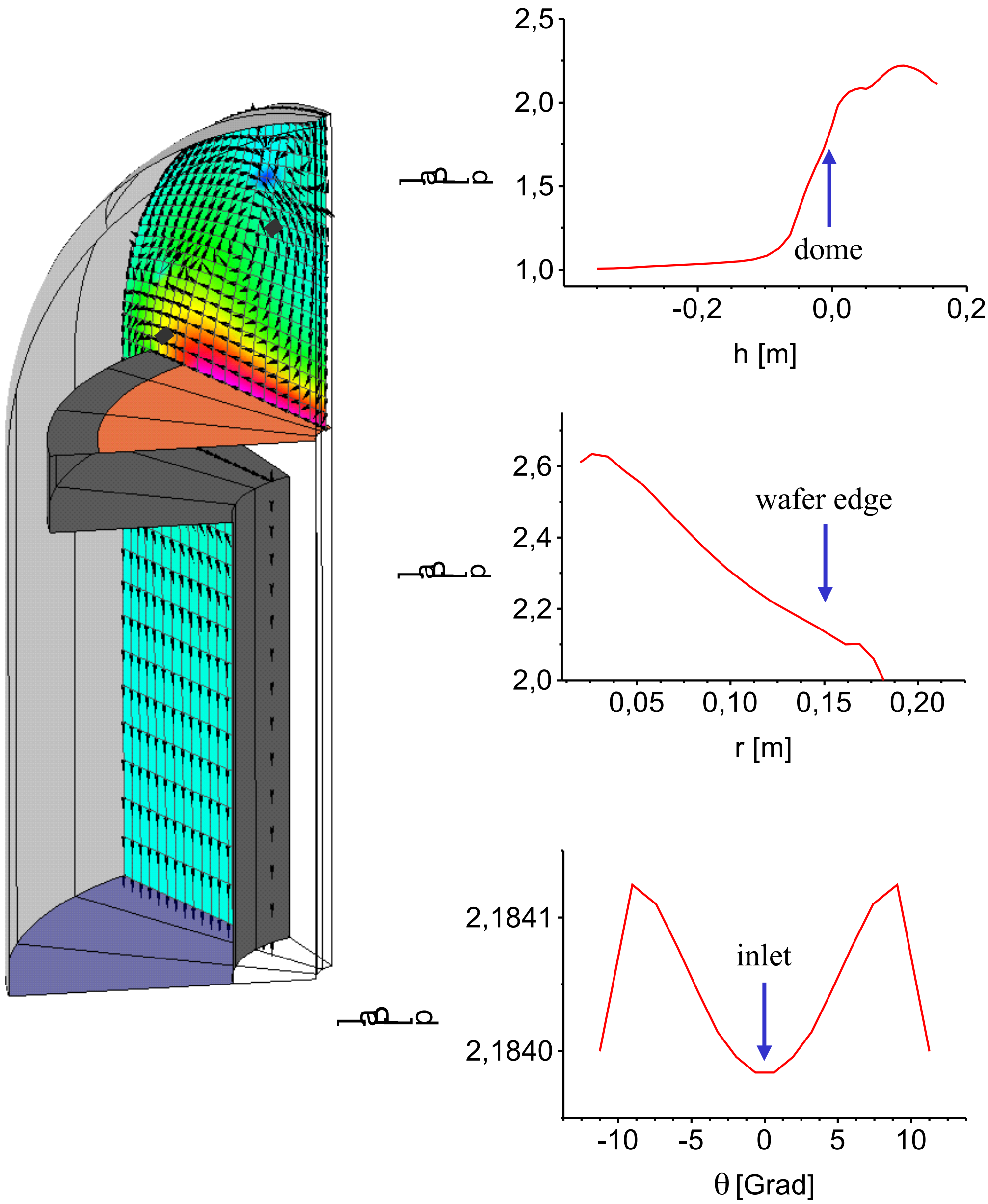
trick: switch off viscous dissipation...



→ satisfactory aggreement, even for $K \approx 0.1$

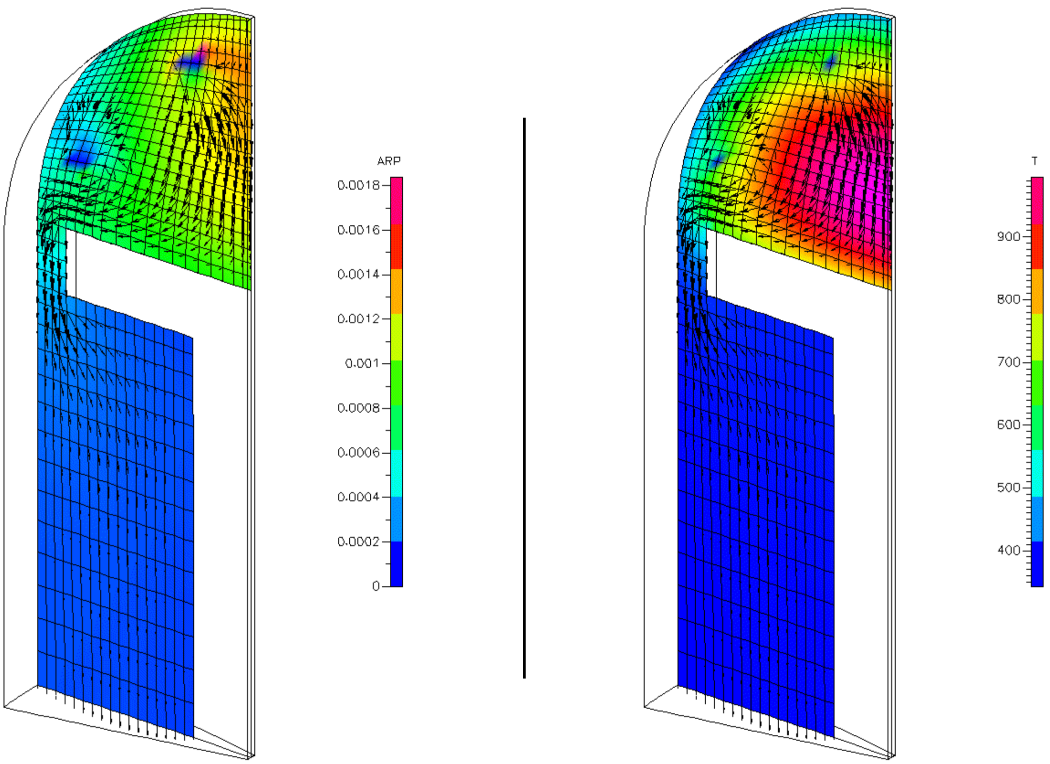
Infineon technologies

CFD: gas flow



→ large radial pressure gradients,
possible source for problems...

CFD chemistry



check wmr assumption:

	CFD-ACE	wmr
frac Ar	0.77	0.76
frac Ar^+	4.8e-4	4.8e-4
frac O_2	0.10	0.13
frac O	6.6e-2	4.3e-2
frac SiH_4	1.4e-2	1.3e-2
frac SiH_2	2.7e-2	3.5e-2
frac H_2	1.8e-2	1.7e-2
dep mol/(m^2 s)	3.1e-4	2.3e-4

wmr assumption good
→ chemistry rates are reliable...

microscopic HDP-CVD model

- almost no direct deposition of ions (< 2%)
- surface activated by ions
- simplified chemistry model for feature scale gained from knowledge on full chemistry

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procedure:

reactor conditions → full model → calculate fluxes → topography simulator

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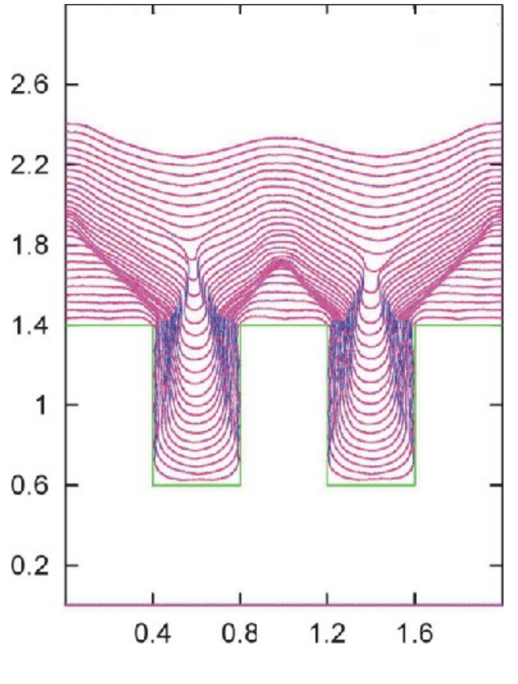
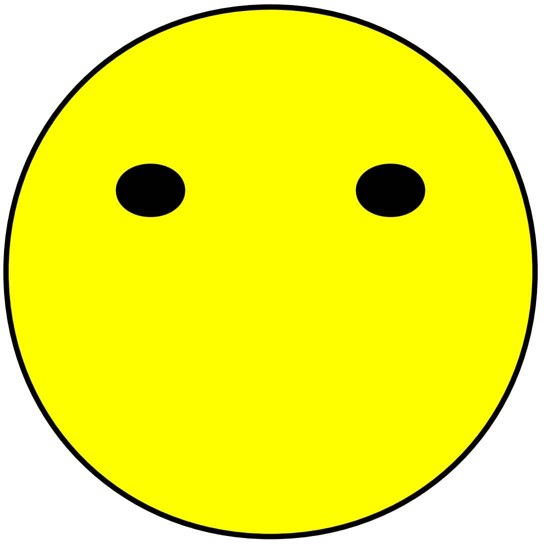
result:



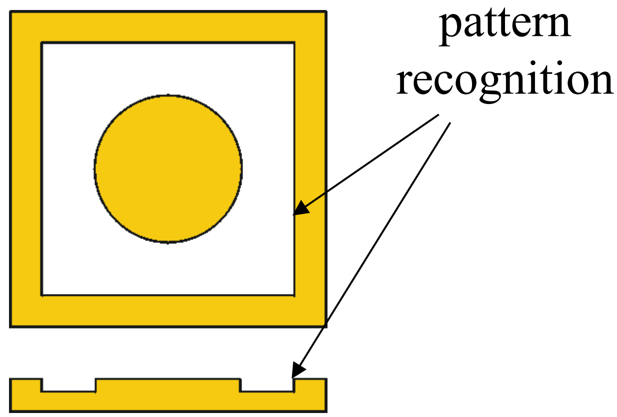
HDP-CVD summary

- Ar- & He-plasma characterized using wmr
- simplified chemistry for Ar-plasma developed
- implemented reduced chemistry into CFD
- good qualitative agreement with experiment
- first feature-scale simulations performed

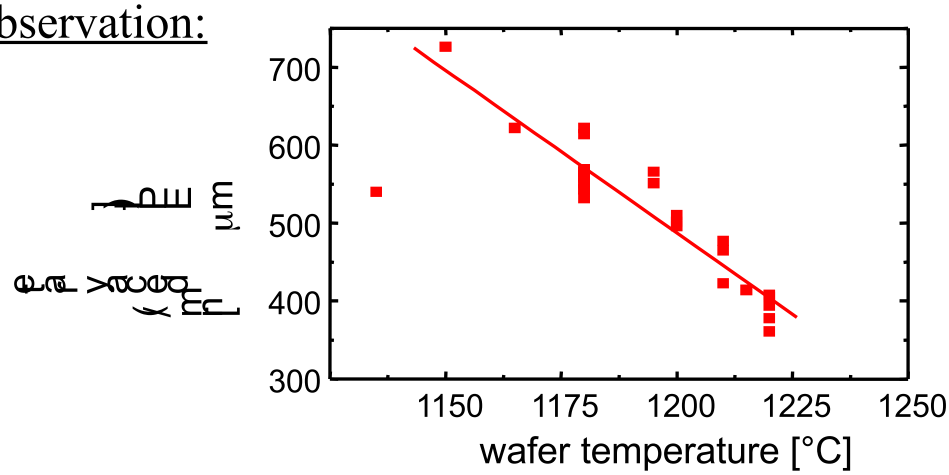


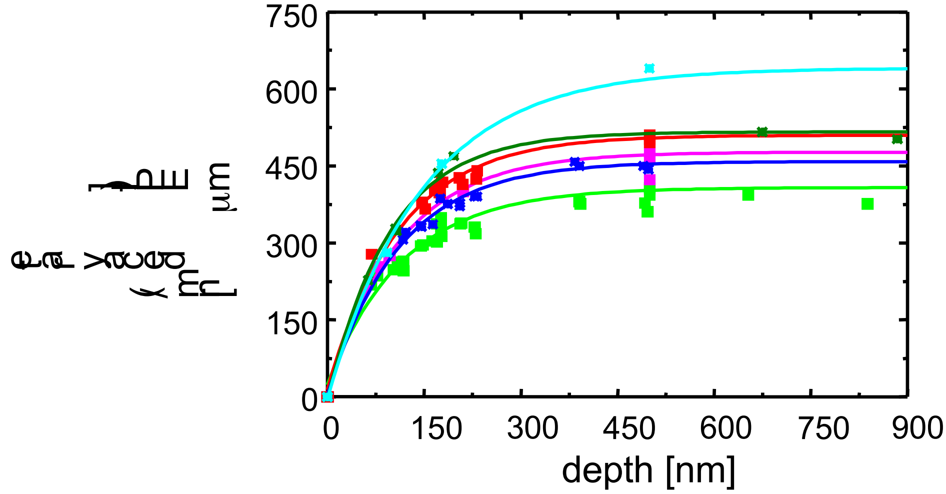
lithography marker in epitaxy

need alignment of consecutive layers
use markers for automatic recognition
problem: marker unstable during deposition



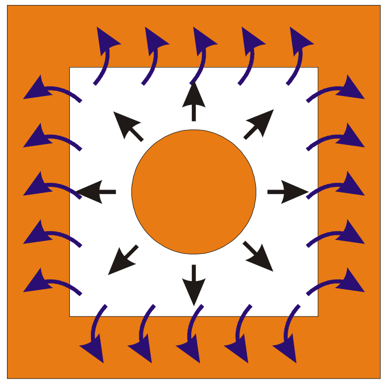
observation:





model for decay

combined Ostwald ripening of island & vacancy
(no microscopic mechanism)



- vacancy grows due to desorption/etch/...
- island decays in favor of vacancy (stabilization)

→ explains both T and depth dependency

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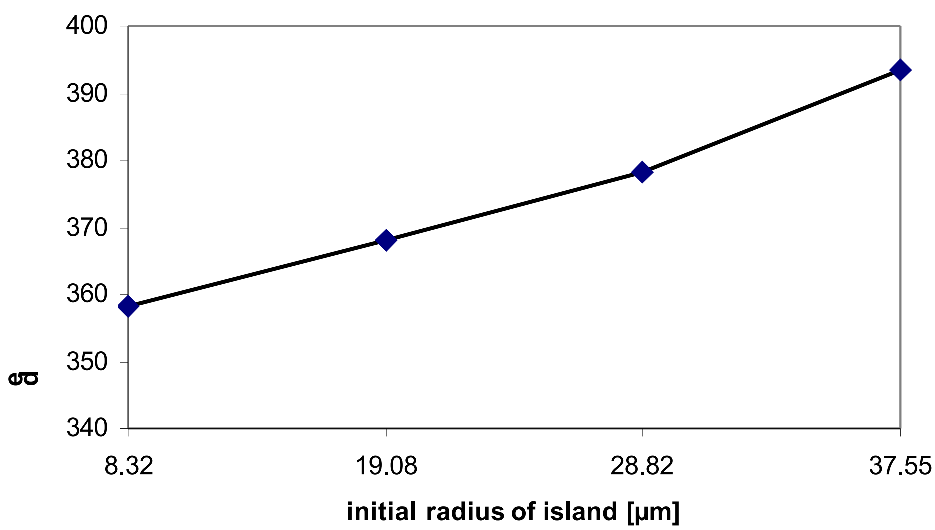
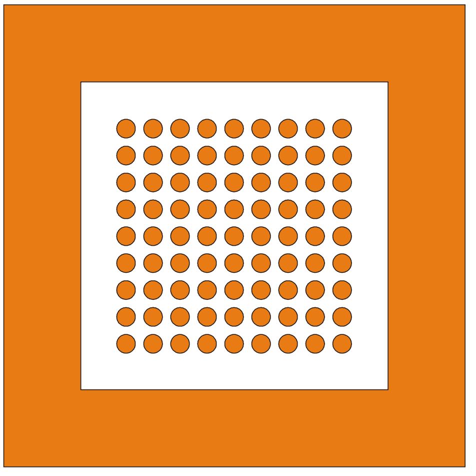
idea: enhance 2nd effect by minimizing island...

...test:



solution...



... ???

summary & notes

- simulations are a powerful tool in SC-industry
- importance increases steadily
- ongoing development of physical models
- large variety of problems

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personal impression

- emphasis of work on physics
- challenging work
- strong interaction between projects
- very good atmosphere
- high demand for physicists...