Exploration COMSOL in Modeling RLSA^{TM} CVD Processes

Ar+H_2+SiH_4+C_2H_6 and Dopant Gas

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TOKYO ELECTRON

COMSOL CONFERENCE
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outline

- Radial line slot antenna (RLSA)
- Microwave plasma in semiconductor processing tool
- Coupling and operation modes
- Major challenges – plasma tools
- Model – implemented in Plasma Module by COMSOL – user experience
- Conclusion remarks

Conclusion remarks

- The creation of SW discharges is clear example of a self-consistent nonlinear problem and it represents strongly coupled stiffy system

- Solving large number of equations with complex chemistry and coupled wave-plasma physics at the scale of real reactor represents challenge

- **COMPLEXITY OF REACTIVE PLASMA STILL PRESENT!**

- Plasma Module has great capabilities for fast development, modifications, easy GUI, adaptation for new input data and postprocessing

Radial line slot antenna plasma source

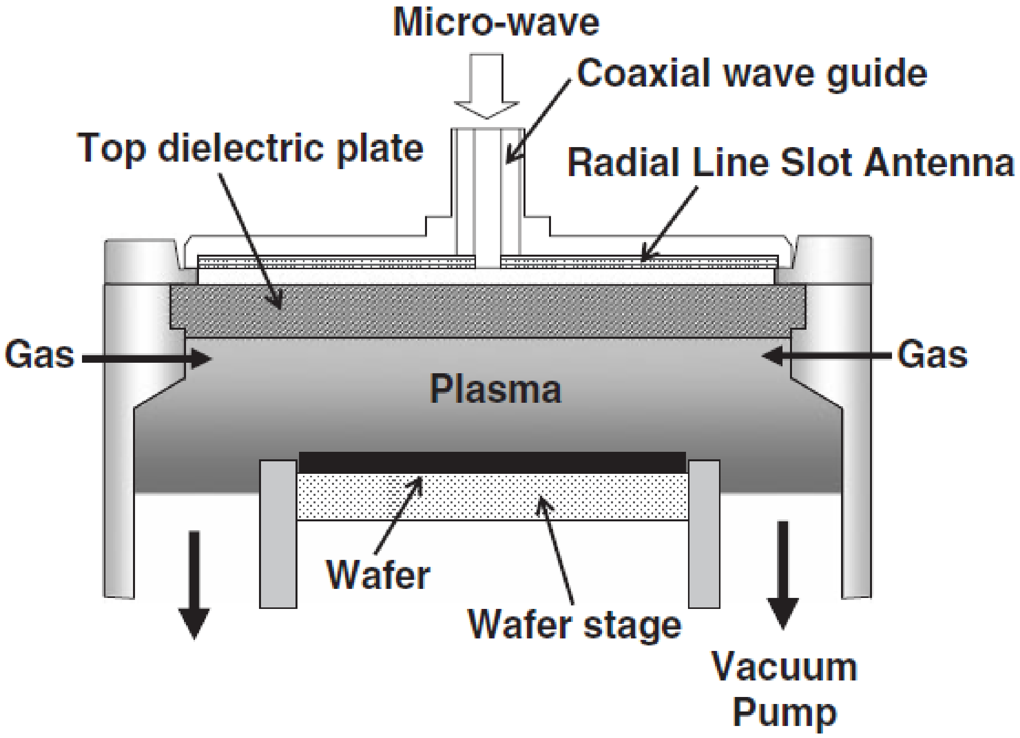
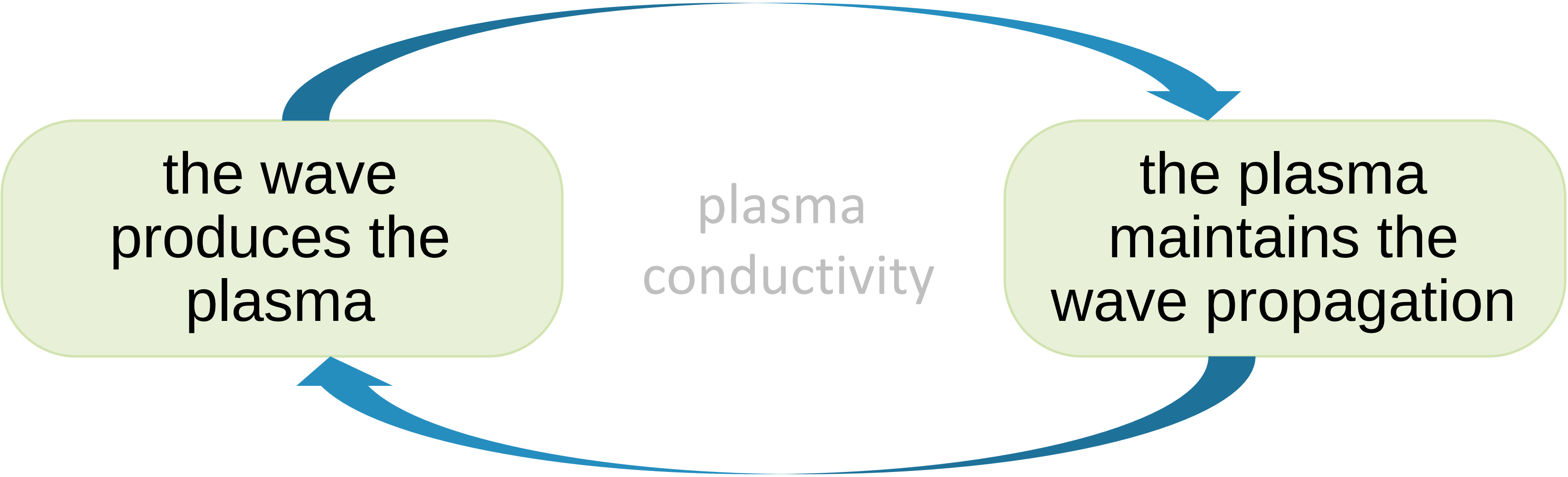


Fig. 1. A cross-sectional view of RLSA PECVD reactor.

Plasma is sustained by 2.45 GHz EM wave distributed by antenna and propagating trough processing gas

Physics background

- SW-sustained discharges are structures which unify wave-fields and gas-discharge plasmas



the wave produces the plasma

plasma conductivity

the plasma maintains the wave propagation

- The discharge behavior is simultaneously governed by electrodynamics and gas discharge physics

Plasma spatial distribution

Operation modes

Surface wave mode

Transitional mode

Resonant mode

motivation

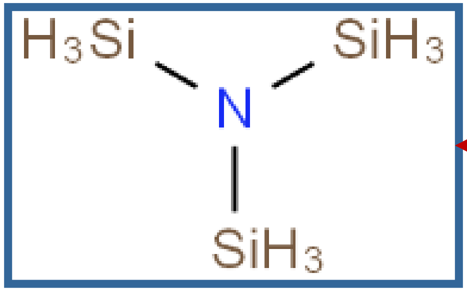
- New materials, gas mixtures, scale leading to technological process expansion
- Non obvious and predictable process outcome

Challenge

Complex process chemistry

Scaling plasma sources

Reaction models → prediction on process



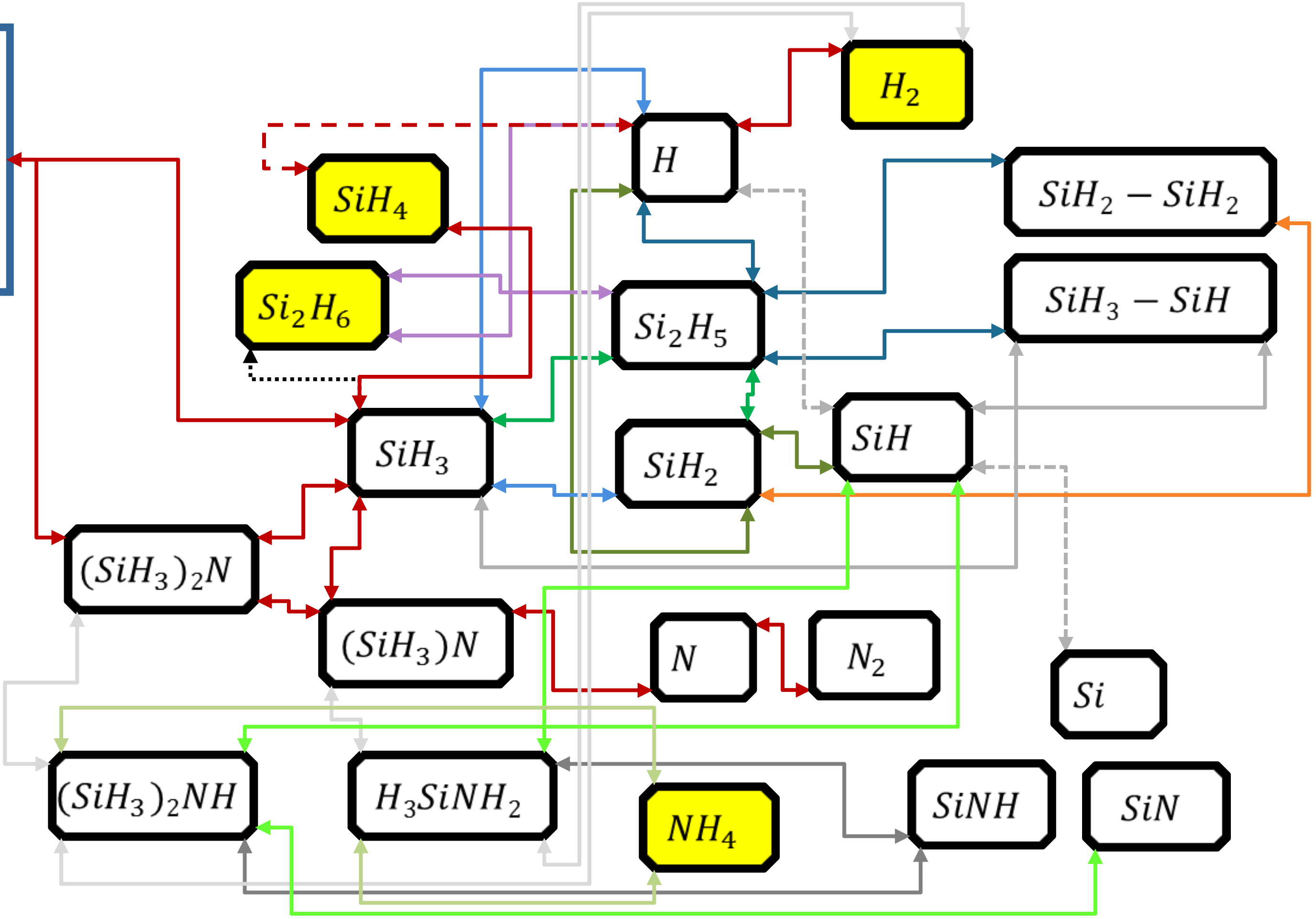
plasma e^-

+ ionized

+ excited

+ surface reactions

Trisilylamine (TSA)



H_2

H

SiH_4

Si_2H_6

Si_2H_5

SiH_2-SiH_2

SiH_3-SiH

SiH_3

SiH_2

SiH

$(SiH_3)_2N$

$(SiH_3)N$

N

N_2

Si

$(SiH_3)_2NH$

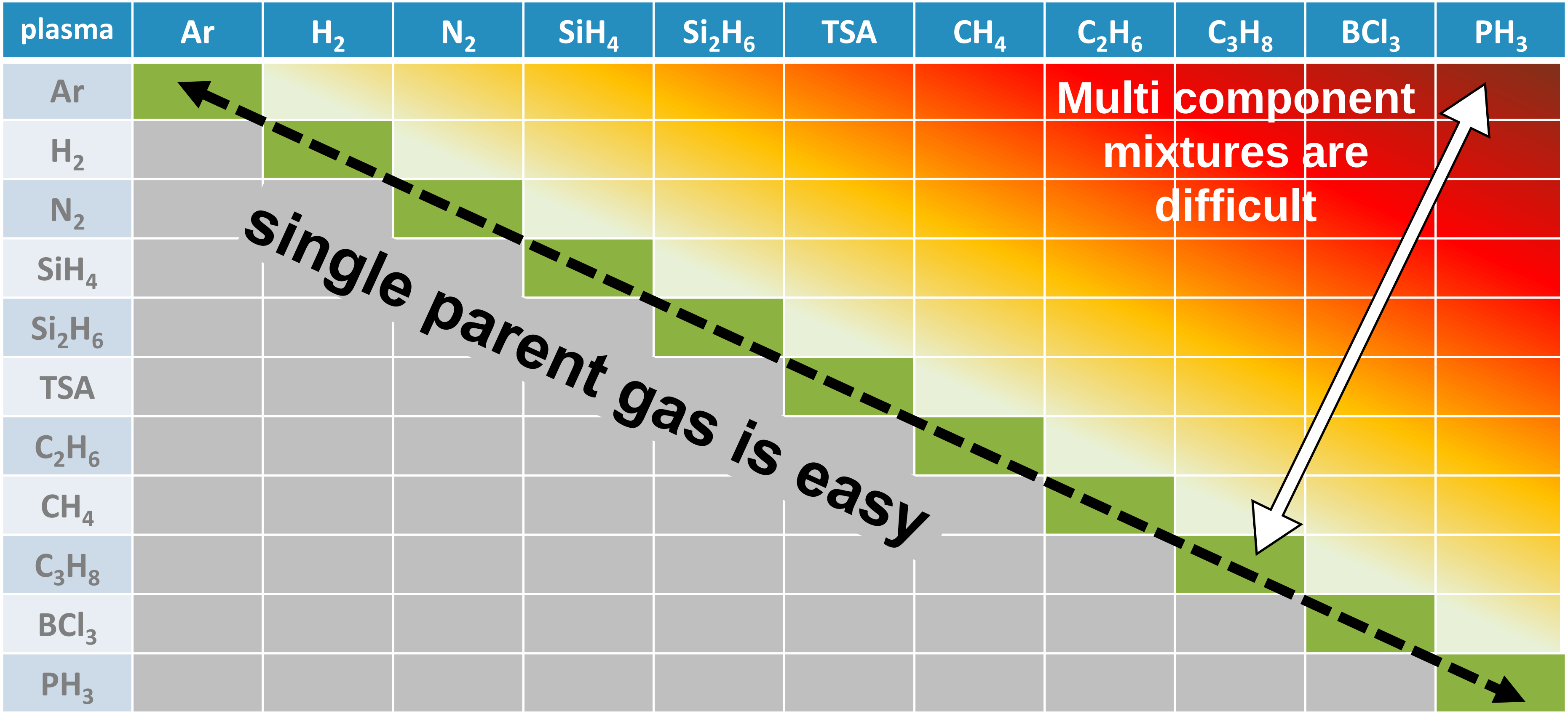
H_3SiNH_2

NH_4

$SiNH$

SiN

multispecies and reactions



plasma	Ar	H_2	N_2	SiH_4	Si_2H_6	TSA	CH_4	C_2H_6	C_3H_8	BCl_3	PH_3
Ar	🟩										
H_2		🟩									
N_2			🟩								
SiH_4				🟩							
Si_2H_6					🟩						
TSA						🟩					
C_2H_6							🟩				
CH_4								🟩			
C_3H_8									🟩		
BCl_3										🟩	
PH_3											🟩

single parent gas is easy

Multi component mixtures are difficult

surface	Ar	H_2	N_2	SiH_4	Si_2H_6	TSA	C_2H_6	CH_4	C_3H_8	BCl_3	PH_3
-Si-O-C-H-											

Chemistry included in current model

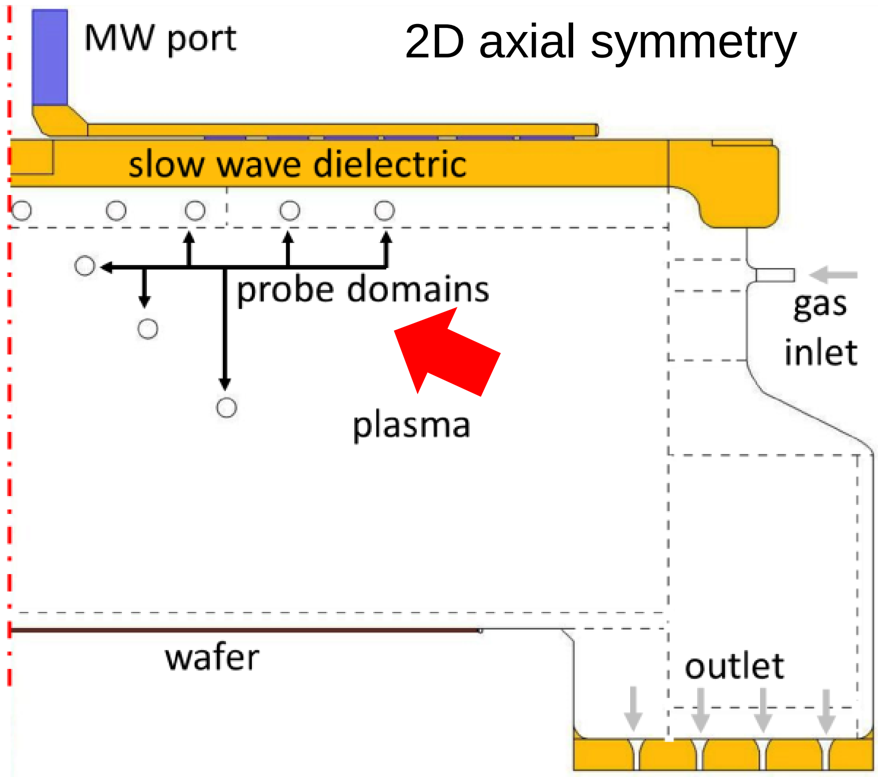
	Ar	**H_2**	**C_2H_6**	**Si** **precursor**	**Dopants** **PH_3** **BCl_3**	**TOTAL**
Number of species	5	25	16	~ 10		~ 56
Plasma reactions	4^e (39)	21^e +	~25	19	5	~ 73
Homogeneous reactions						~ 5
Surface reactions	2	21 +				~ 23

(e) - primary collisions with electron

- Model becomes substantially larger
- Still some simplifications – grouping similar reactions, excitation levels
- Upgrading chemistry not final - TBD

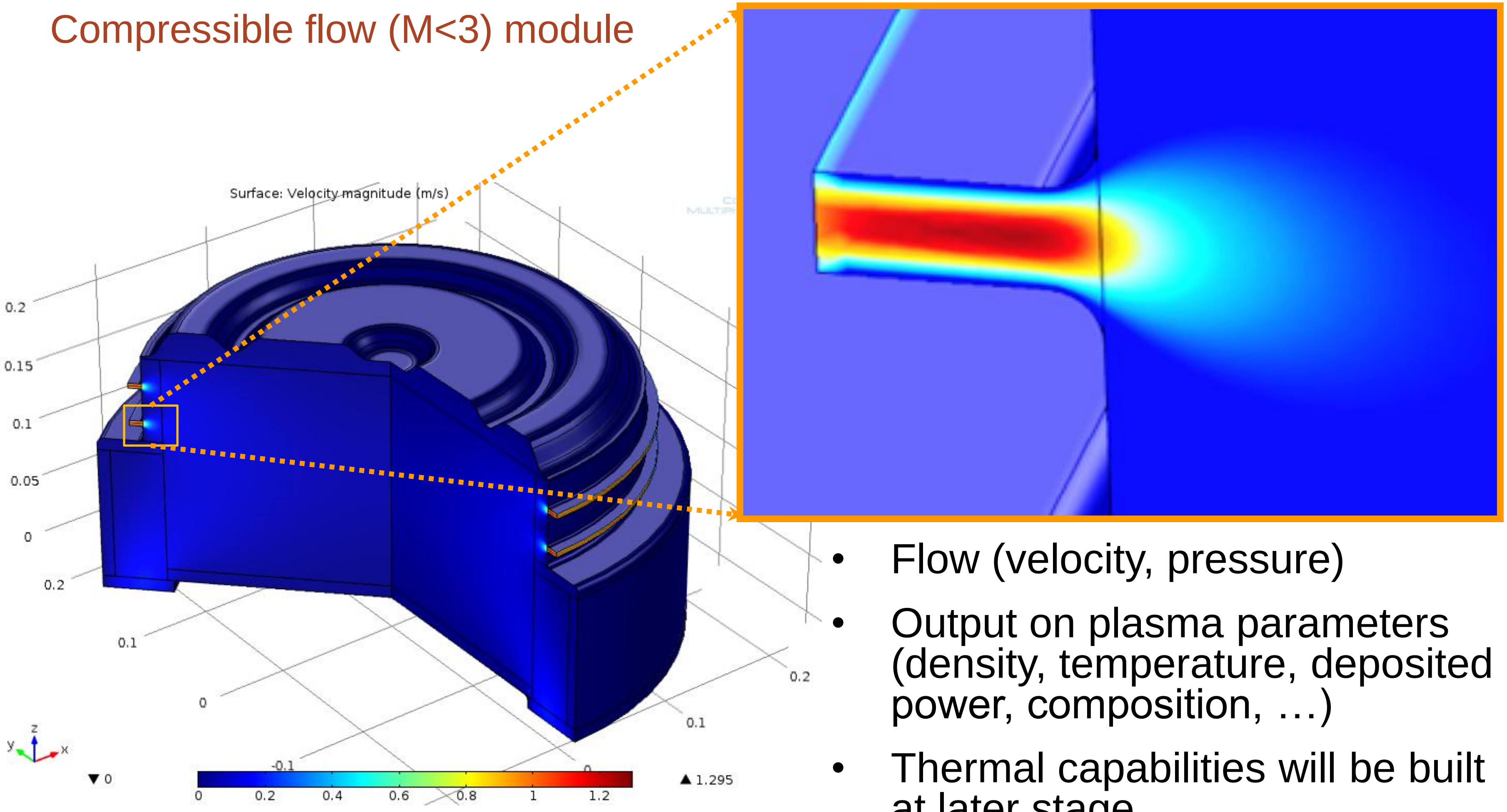
Model geometry and computational environment

- Plasma Module in COMSOL Multiphysics suite ver.4.3.b
- Memory in individual cases is in range from 10 to 50 GB
- Computational time from 4 hours to over 100 hours per case
- Individual transient cases converged typically in range $10^{-3} – 10^{-2}$ s



Gas flow

Compressible flow (M<3) module



- Flow (velocity, pressure)
- Output on plasma parameters (density, temperature, deposited power, composition, …)
- Thermal capabilities will be built at later stage

Mostly used cross-sections as input

(flexibility to explore EEDF)

- www.lxcat.laplace.univ-tlse.fr
  - *J. Phys. D: Appl. Phys.* 46 334001 (2013)
  - *J. Phys. D: Appl. Phys.* 46 334002 (2013)
  - *J. Phys. D: Appl. Phys.* 46 334003 (2013)

  – Data were not always ready to be automatically transformed
  – Certain letters used in database may triggered change in data formatting in Comsol, for example, symbol (’) triggers “d” and crashing or missinterpretation data …

  – More specific reactions from scientific publications (mostly as reaction rate constants)

  – Choosing approach with uploading rather individual cross section data instead of block of cross sections

SW upgrades – check frequently!

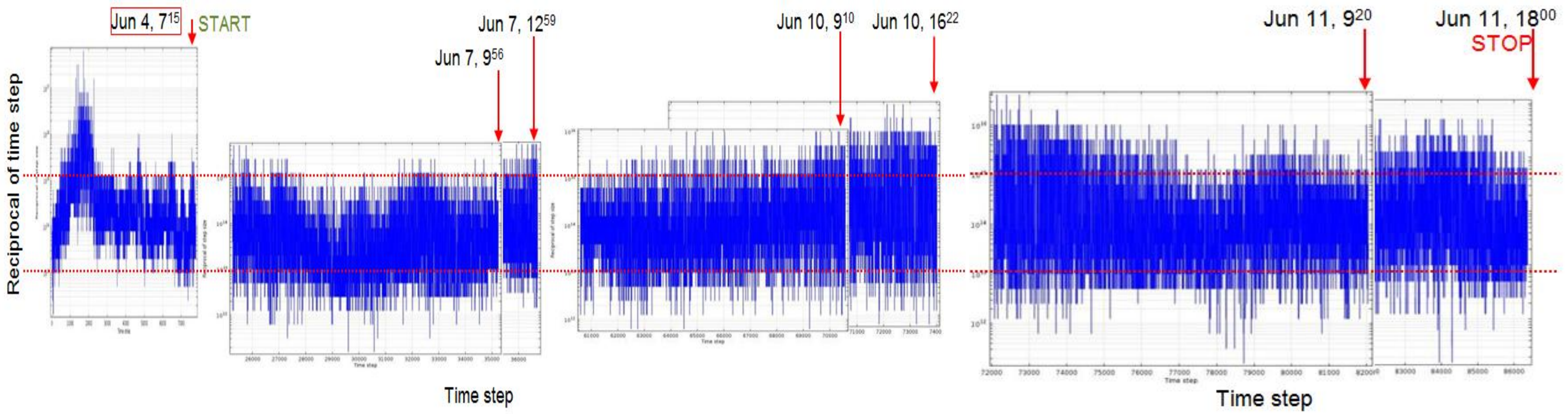
- This work used v.4.3.2.152 and it was upgraded only on Aug 29, 2013 into update v.1.3.2.189
- Upgrade released in end of July 2013

“MWP now works correctly when used with electromagnetic solver !”

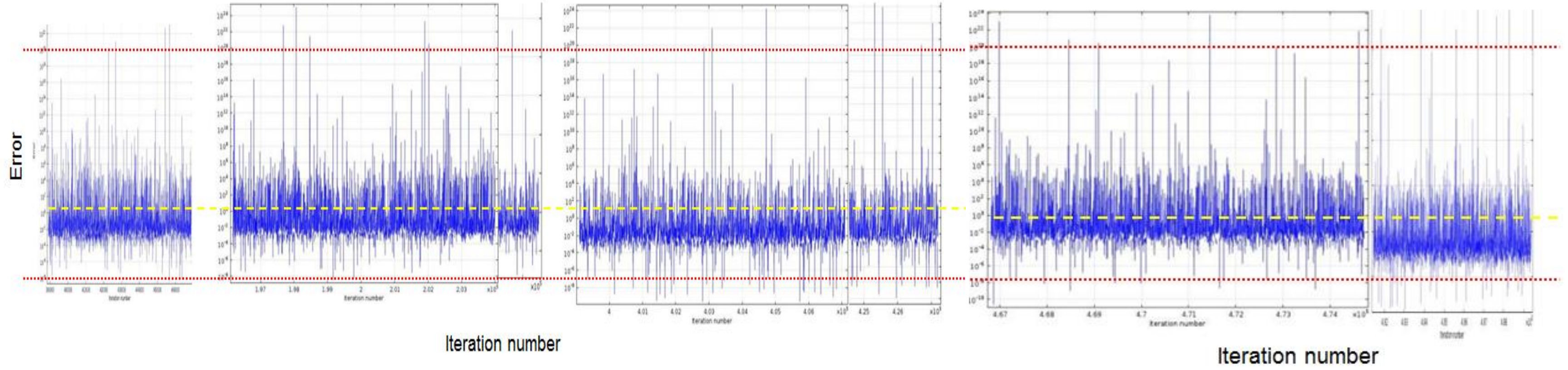
REWORK THAT COUL BE AVOIDED

NEW COMPUTATIONS → DELAY

Convergence timeline – long computations

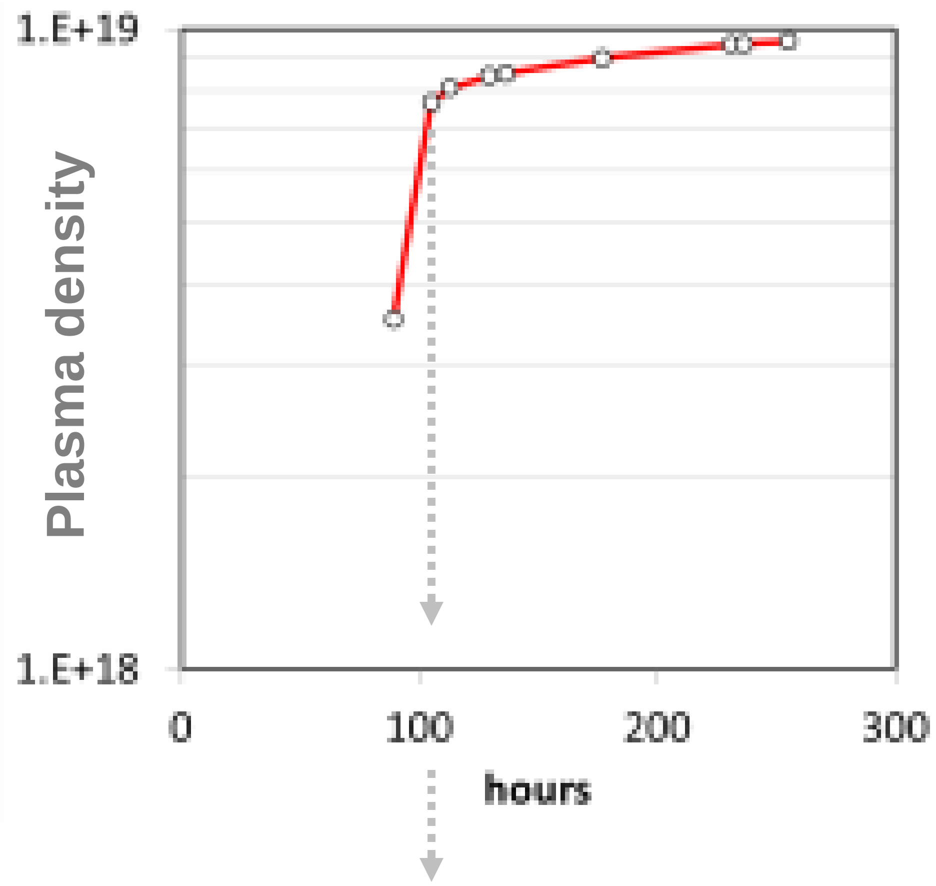


noticeable reduced error but transient computation within picoseconds steps



- **meshing and transient settings need to be optimized substantially**
- accurate but efficient numerical method is desirable in terms of computation time, especially for an optimization process

Computation time / monitoring probes



Up to several days

Pressure is critical parameter

$Ar + H_2 + SiH_4$

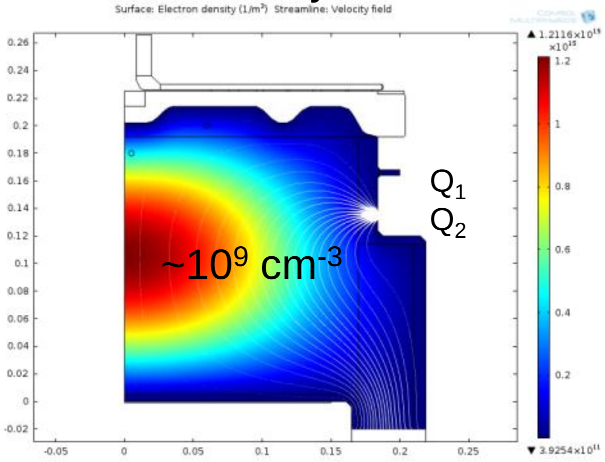
Dell Precision WorkStation T7500 (64bit Windows 7 Enterprise OS, two processors X5690 – 24 cores, RAM 96 GB)

Convergence – highly sensitive to initial values

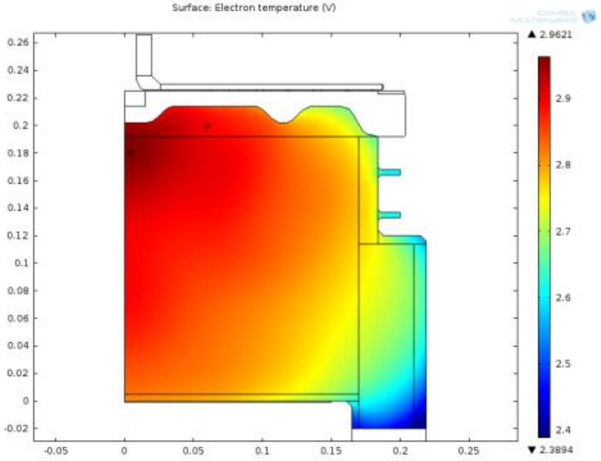
It is important wisely predict initial values to get efficient convergence

Low pressure cases – fast turnaround (several hours)

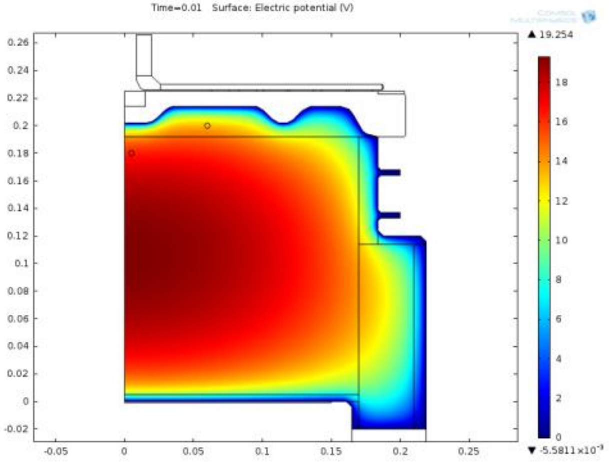
Electron density



Electron temperature



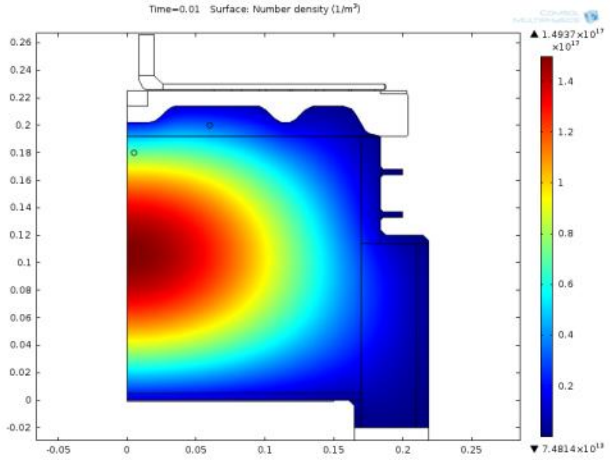
Plasma potential



Ar - 15 mTorr - 1 kW - Q_2/100 sccm

- Low pressure cases – fast turn around (several hours)
- Enhanced chemistry may produce even longer computational times
- Transitional or resonant mode

Argon excited / density

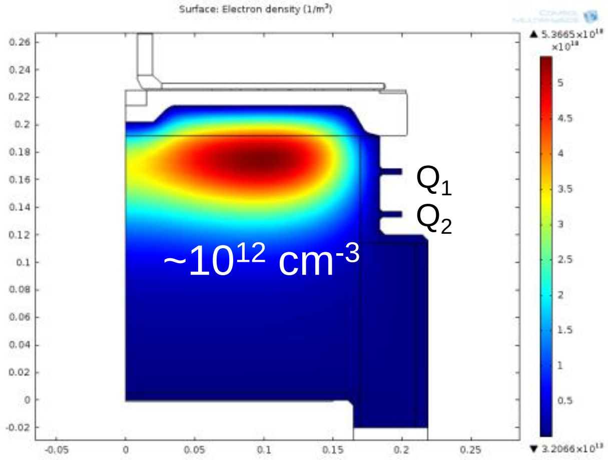


Increased pressure

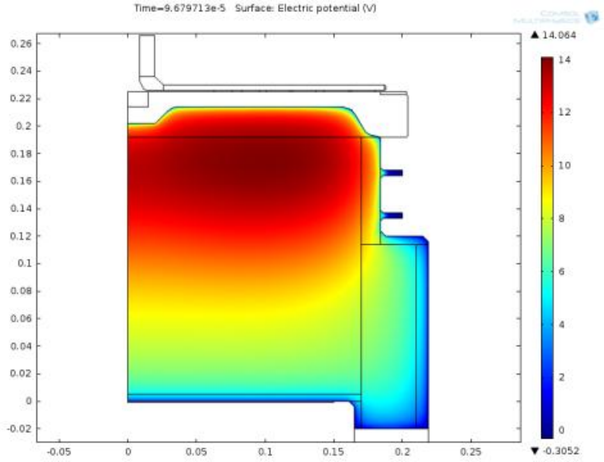
longer convergence (>24^+ hours)

Ar - 100 mTorr - 5 kW - Q_1/50 sccm - Q_2/50 sccm

Electron density



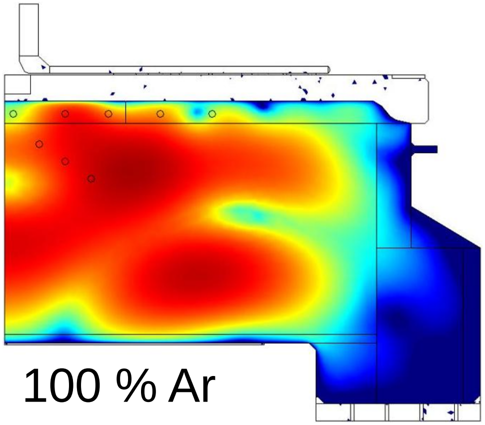
Plasma potential

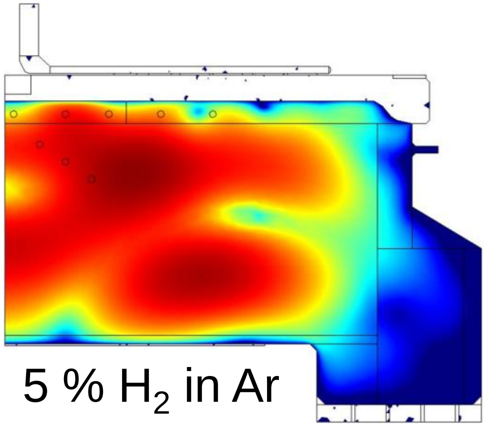


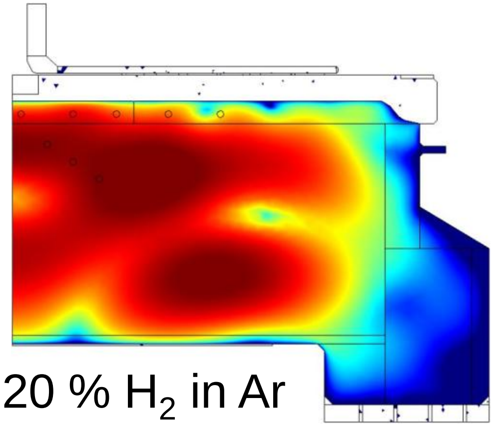
shown results are not final (10^{-4} s)

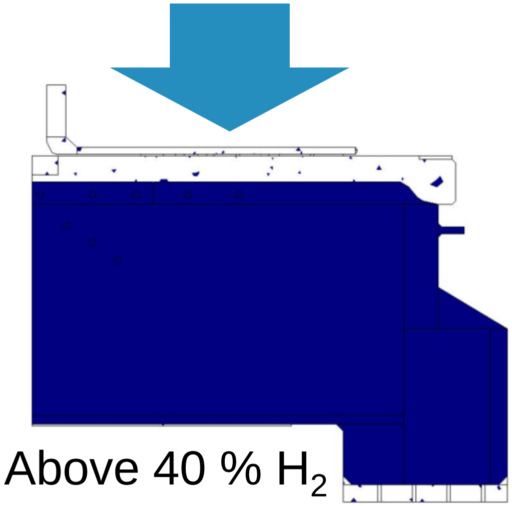
- Plasma in SW mode

Ar:H_2 resistive loss in plasma


100 % Ar


5 % H_2 in Ar


20 % H_2 in Ar


Above 40 % H_2 in Ar

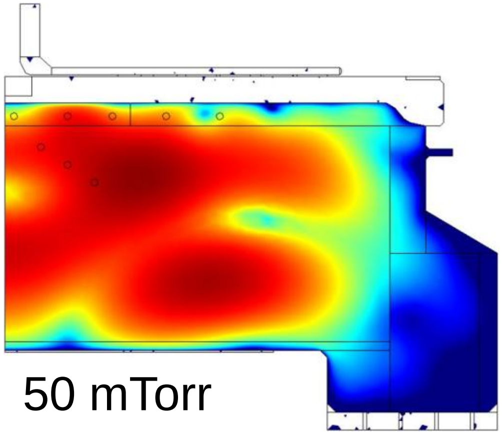
Ar+H_2 only, 50 mTorr, 3.5 kW

Adding H_2 increases the resistive loss in plasma → then convergence is lost

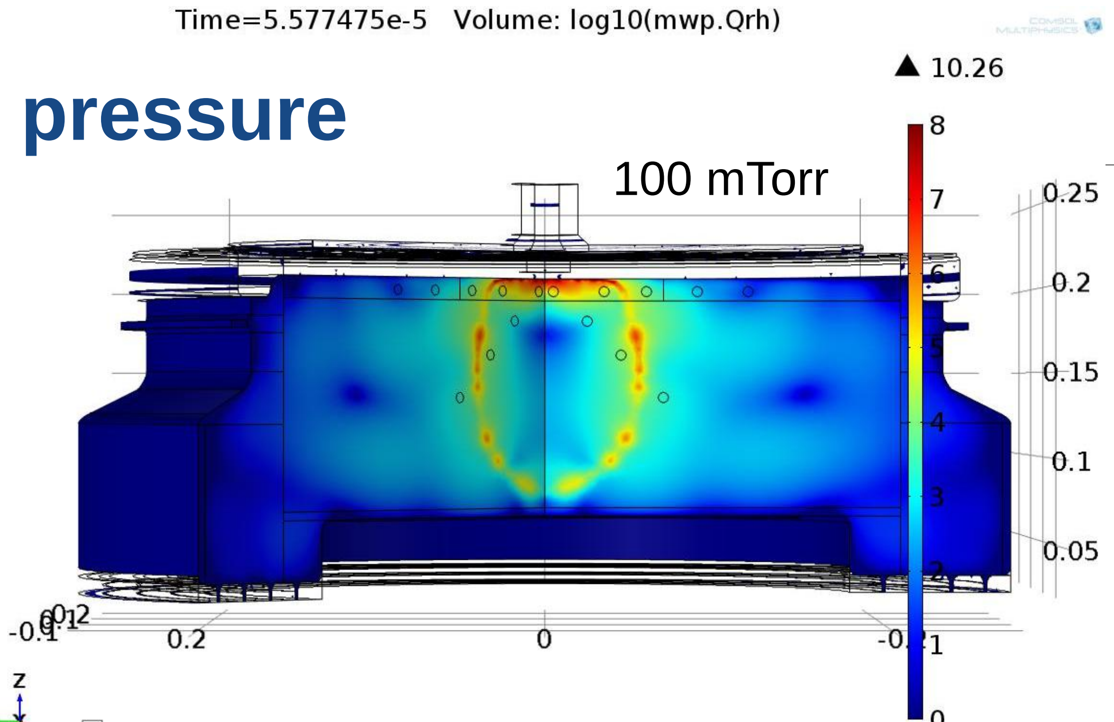
Convergence abbrupted by mode change – model settings (mesh, time step) do not allow fast transition on numerical side

Color scale is same for all plots in range from 0 to 4 Wm^{-3}

Resistive loss vs pressure



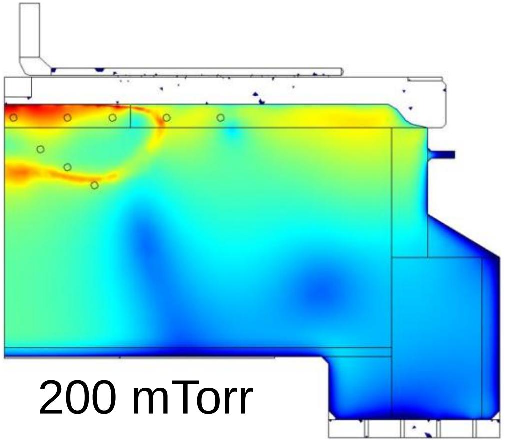
50 mTorr



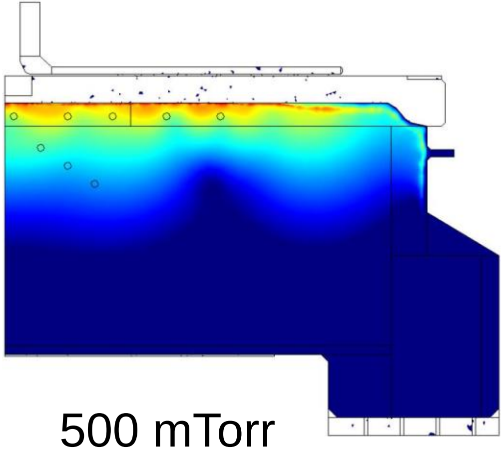
100 mTorr

5 % H_2 in Ar plasma

Conversion from transitional/resonant mode into SW mode



200 mTorr

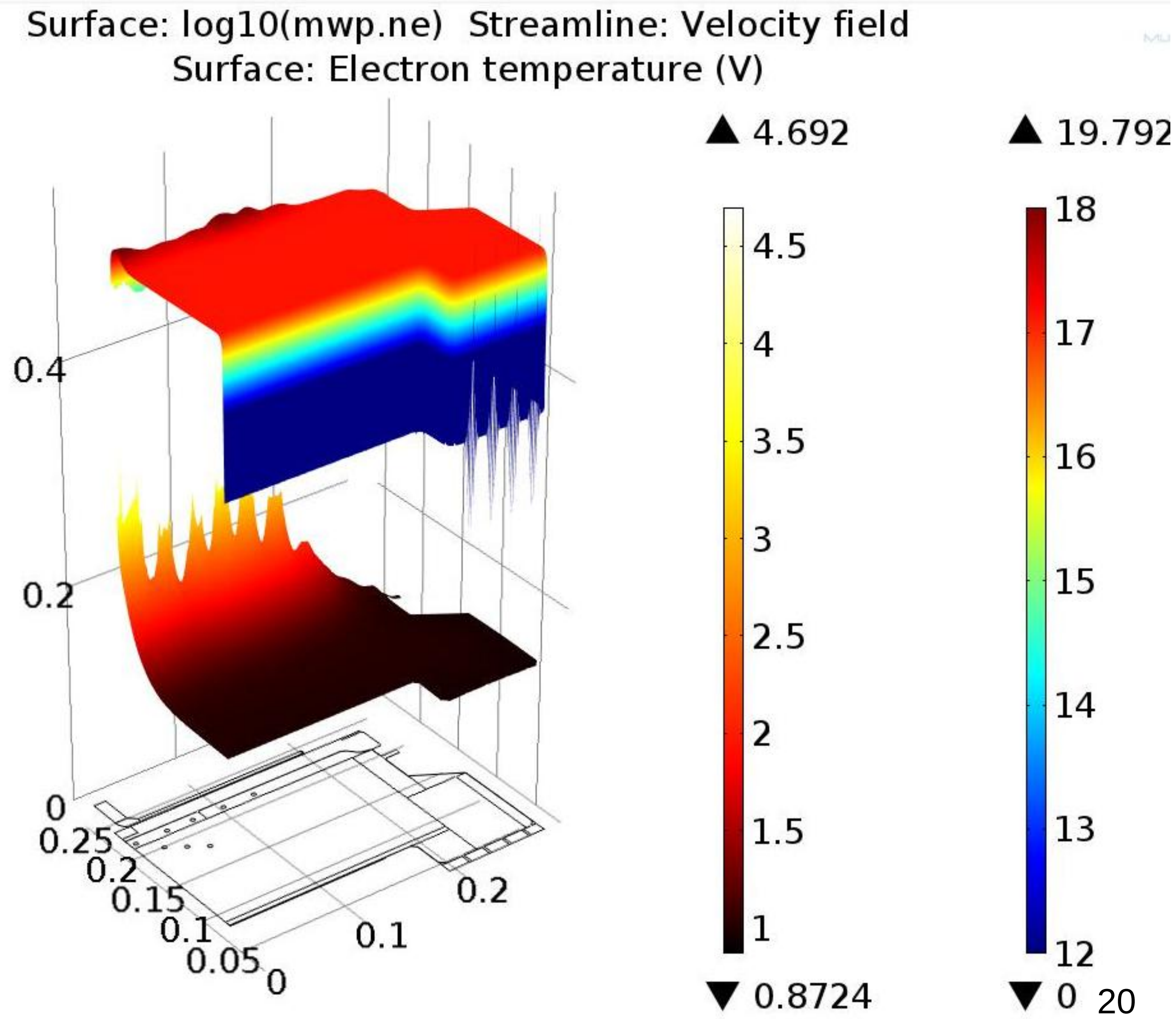


500 mTorr

Color scale is same for all plots in range from 0 to 4 Wm^{-3}

5% H_2 + Ar mixture

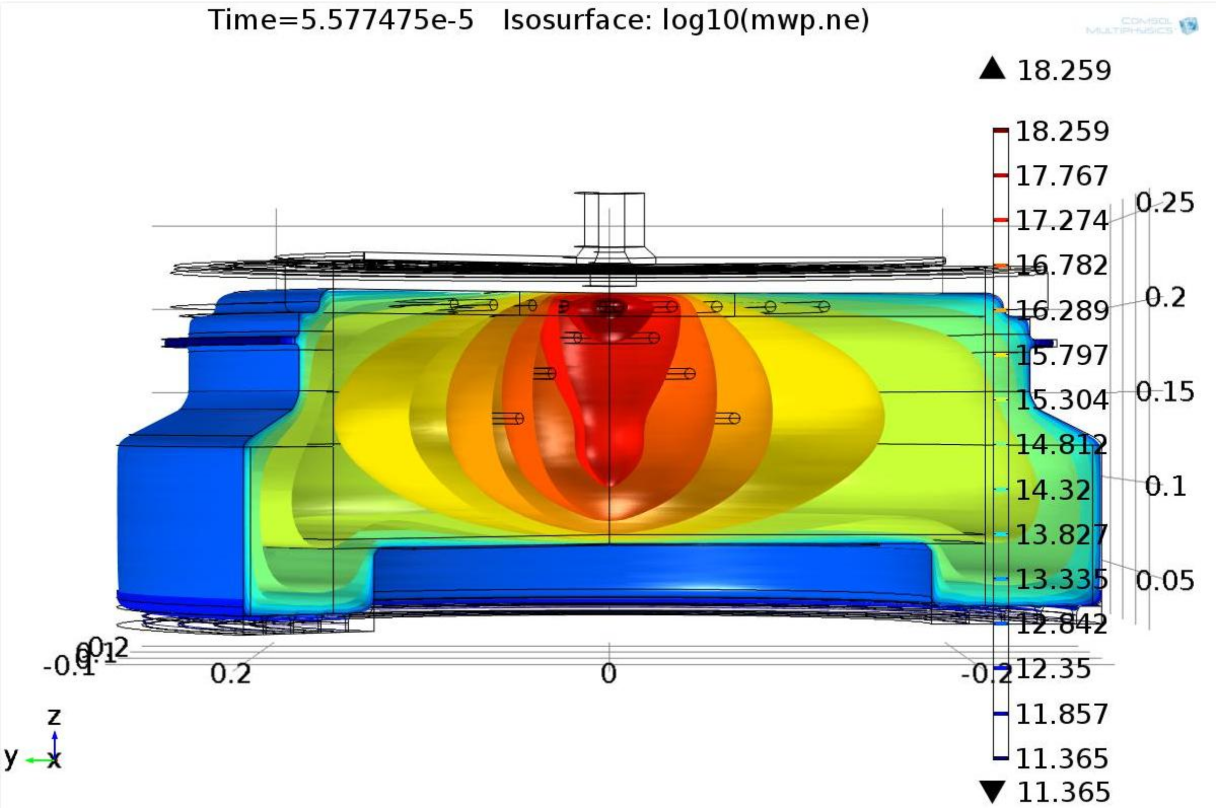
- surface plots of electron density, n_e, and electron temperature, T_e,
- total flow 400 sccm
- microwave power 3.5 kW
- 500 mTorr
- converged case



Plasma density

$Ar+H_2+SiH_4$

100 mTorr

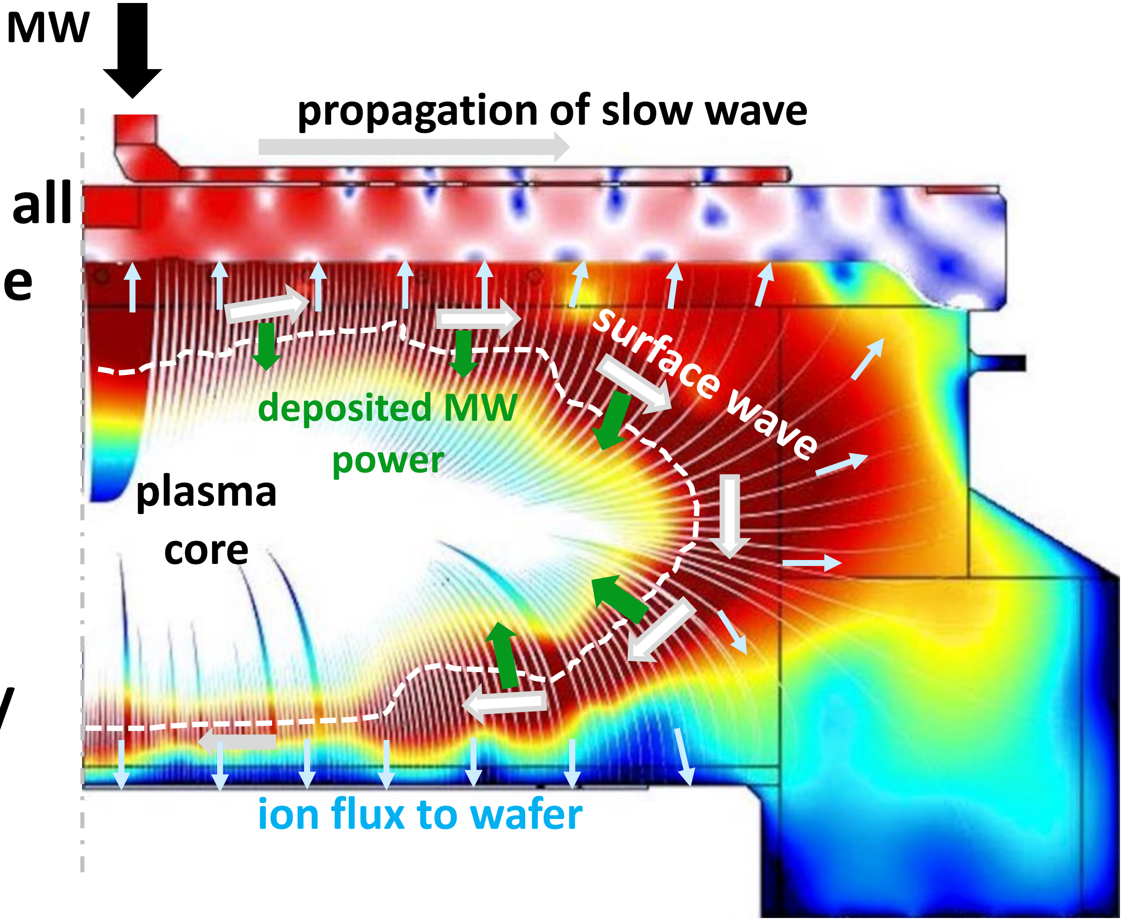


Iso-surface plot of electron density (n_e, m^{-3})

Hydrogen and silane flows were sustained at low level to enable convergence

comprehensive and approachable assessment

- To show and interpret all phenomena within one framework
- Coupled physics and chemistry
- Accessible to process / hardware engineer, marketing, customer



Final remark

- Physics modes transition due to wave-plasma coupling may creates problems that separately are solvable but in fast transient need special prevention to overcome (over-dense meshing, extremely short time steps)

Questions?

Thank you!

Plasma spatial distribution

Operation modes

Surface wave mode

OVER-DENSE PLASMA

Transfer mechanism allows generation of over-dense plasmas with electron densities beyond the critical density (above ~3x10^{17} m^{-3})

The conductivity of the plasma enables the wave to propagate along the plasma surface

The SW mode allows generation of uniform plasmas over several wavelengths of the EM wave (in vacuum $\lambda \sim$ 12.2 cm)

Transitional mode

BELOW CUT-OFF DENSITY
~ 7.5x10^{16} m^{-3}

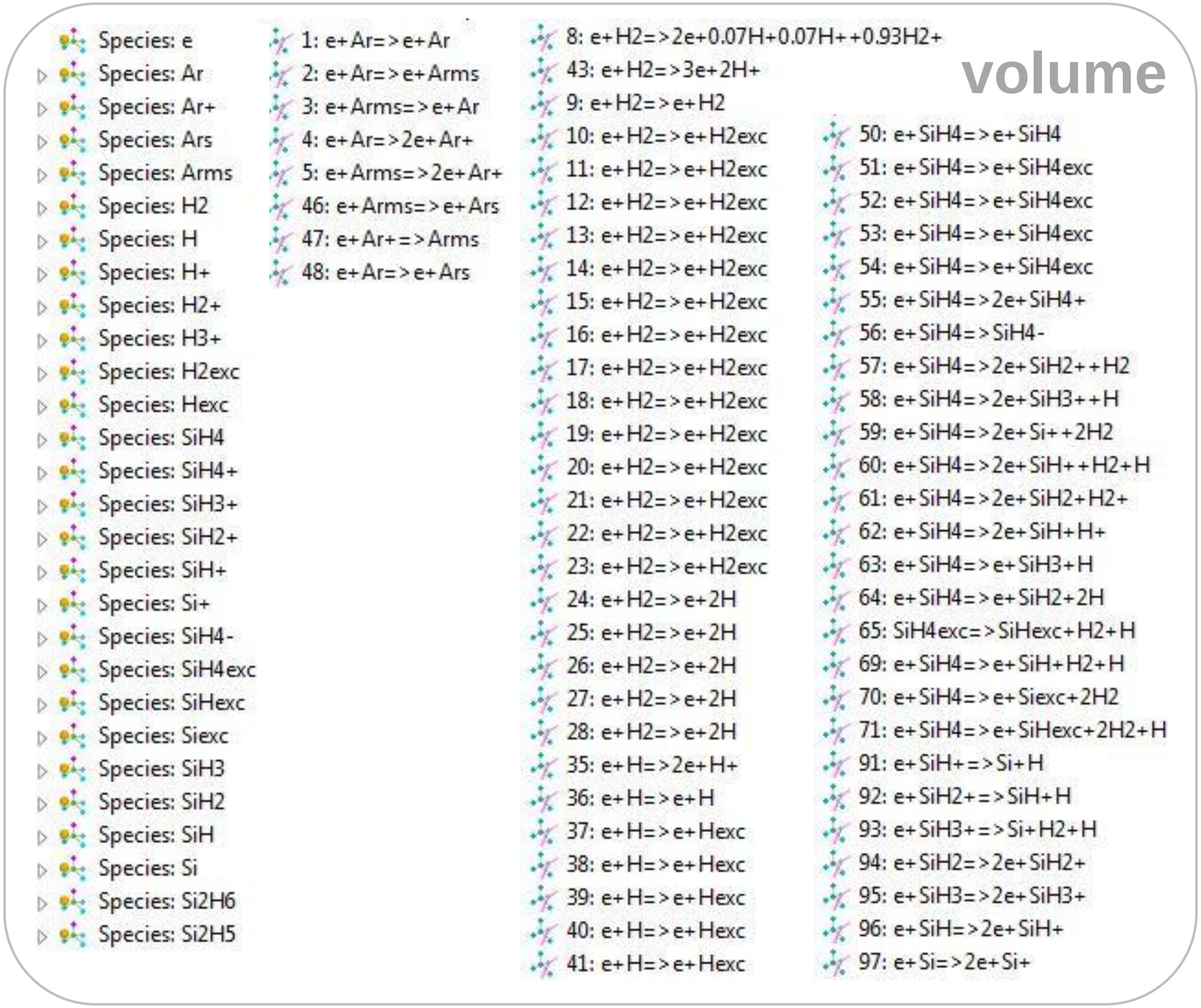
EM wave is partially traversing the plasma
Both reactor geometry and dense plasma structure interplay and form final spatio-temporal distribution

Resonant mode

VERY LOW DENSITY

When plasma density does not exceed the critical density a standing EM wave is confined by a reactor (resonator cavity) and penetrates the plasma which is sustained by wave in the regions of highest field intensity

Listing from model tree



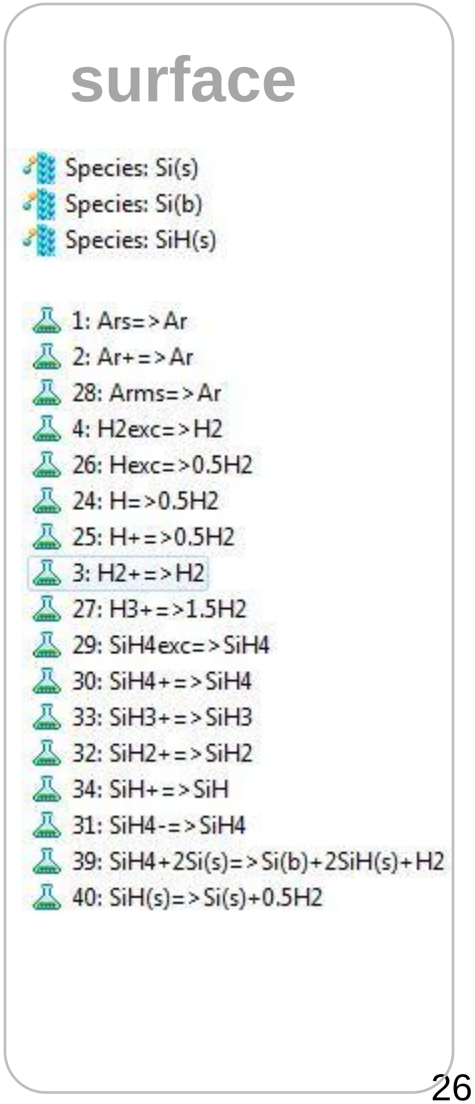
volume

Species: e
Species: Ar
Species: Ar+
Species: Ars
Species: Arms
Species: H2
Species: H
Species: H+
Species: H2+
Species: H3+
Species: H2exc
Species: Hexc
Species: SiH4
Species: SiH4+
Species: SiH3+
Species: SiH2+
Species: SiH+
Species: Si+
Species: SiH4-
Species: SiH4exc
Species: SiHexc
Species: Siexc
Species: SiH3
Species: SiH2
Species: SiH
Species: Si
Species: Si2H6
Species: Si2H5

1: e+Ar=>e+Ar
2: e+Ar=>e+Arms
3: e+Arms=>e+Ar
4: e+Ar=>2e+Ar+
5: e+Arms=>2e+Ar+
46: e+Arms=>e+Ars
47: e+Ar+=>Arms
48: e+Ar=>e+Ars

8: e+H2=>2e+0.07H+0.07H++0.93H2+
43: e+H2=>3e+2H+
9: e+H2=>e+H2
10: e+H2=>e+H2exc
11: e+H2=>e+H2exc
12: e+H2=>e+H2exc
13: e+H2=>e+H2exc
14: e+H2=>e+H2exc
15: e+H2=>e+H2exc
16: e+H2=>e+H2exc
17: e+H2=>e+H2exc
18: e+H2=>e+H2exc
19: e+H2=>e+H2exc
20: e+H2=>e+H2exc
21: e+H2=>e+H2exc
22: e+H2=>e+H2exc
23: e+H2=>e+H2exc
24: e+H2=>e+2H
25: e+H2=>e+2H
26: e+H2=>e+2H
27: e+H2=>e+2H
28: e+H2=>e+2H
35: e+H=>2e+H+
36: e+H=>e+H
37: e+H=>e+Hexc
38: e+H=>e+Hexc
39: e+H=>e+Hexc
40: e+H=>e+Hexc
41: e+H=>e+Hexc

50: e+SiH4=>e+SiH4
51: e+SiH4=>e+SiH4exc
52: e+SiH4=>e+SiH4exc
53: e+SiH4=>e+SiH4exc
54: e+SiH4=>e+SiH4exc
55: e+SiH4=>2e+SiH4+
56: e+SiH4=>SiH4-
57: e+SiH4=>2e+SiH2++H2
58: e+SiH4=>2e+SiH3++H
59: e+SiH4=>2e+Si++2H2
60: e+SiH4=>2e+SiH++H2+H
61: e+SiH4=>2e+SiH2+H2+
62: e+SiH4=>2e+SiH+H+
63: e+SiH4=>e+SiH3+H
64: e+SiH4=>e+SiH2+2H
65: SiH4exc=>SiHexc+H2+H
69: e+SiH4=>e+SiH+H2+H
70: e+SiH4=>e+Siexc+2H2
71: e+SiH4=>e+SiHexc+2H2+H
91: e+SiH+=>Si+H
92: e+SiH2+=>SiH+H
93: e+SiH3+=>Si+H2+H
94: e+SiH2=>2e+SiH2+
95: e+SiH3=>2e+SiH3+
96: e+SiH=>2e+SiH+
97: e+Si=>2e+Si+



surface

Species: Si(s)
Species: Si(b)
Species: SiH(s)

1: Ars=>Ar
2: Ar+=>Ar
28: Arms=>Ar
4: H2exc=>H2
26: Hexc=>0.5H2
24: H=>0.5H2
25: H+=>0.5H2
3: H2+=>H2
27: H3+=>1.5H2
29: SiH4exc=>SiH4
30: SiH4+=>SiH4
33: SiH3+=>SiH3
32: SiH2+=>SiH2
34: SiH+=>SiH
31: SiH4-=>SiH4
39: SiH4+2Si(s)=>Si(b)+2SiH(s)+H2
40: SiH(s)=>Si(s)+0.5H2