

### Unintended gas breakdowns in narrow gaps of advanced plasma sources for semiconductor fabrication industry

Willca Villafana<sup>1</sup>, Sung Hyun Son<sup>1</sup>, Geunwoo Go<sup>2</sup>, Igor D Kaganovich<sup>1</sup>, Alexander Khrabrov<sup>1</sup>, Hyo-Chang Lee<sup>3</sup>, Kyoung-Jae Chung<sup>4</sup>, Gwang-Seok Chae<sup>4</sup>, Seungbo Shim<sup>5</sup>, Donghyeon Na<sup>5</sup>, and June Young Kim<sup>6\*</sup>

<sup>1</sup> Princeton Plasma Physics Laboratory, Princeton, NJ, USA
 <sup>2</sup> Department of Nuclear Engineering, Seoul National University, Seoul, South Korea
 <sup>3</sup> Department of Electronics and Computer Engineering, Korea Aerospace University, Goyang, South Korea
 <sup>4</sup> Department of Semiconductor Science, Engineering and Technology, Korea Aerospace University, Goyang, South Korea
 <sup>5</sup> Samsung Electronics Co. Ltd., Hwaseong, South Korea
 <sup>6\*</sup> Department of Al Semiconductor Engineering, Korea University, Sejong, South Korea



#### Talk Overview

- 1. Context and motivation
- 2. Kinetic modeling via Particle-In-Cell simulation using EDIPIC-2D
- 3. Results and discussion
- 4. Modeling capabilities and expertise at PPPL via PCRF



#### Talk Overview

- 1. Context and motivation
- 2. Kinetic modeling via Particle-In-Cell simulation using EDIPIC-2D
- 3. Results and discussion
- 4. Modeling capabilities and expertise at PPPL via PCRF

#### Context and Motivation





#### Context and Motivation



#### **Classical Paschen law**

# $V_{b} = \frac{Bpd}{\left\lceil \ln\left(Apd\right) - \ln\left\{\ln\left(1 + 1/\gamma_{SE}\right)\right\} \right\rceil}$

#### A,B : Gas dependent constants

#### $\gamma_{SE}$ : Ion induced SEE coefficient

 $\rightarrow$  Assumes 1D Townsend discharge (Which is very simple)

#### Table 3. Representative studies of the modified Paschen curve.

	Author	Research method	Features	Gas	Pressure (Torr)	Gap (mm)	Configuration
	Lisovskiy <i>et al</i> (reference [58])	Experimental	Long tube discharge	N <sub>2</sub> , O <sub>2</sub> , Ar. air	0.01-10	5-100	Plane to plane (diameter: 9–100 mm)
More complex	Lisovskiy <i>et al</i> (reference [93])	Experimental and theoretical	Non-uniform electric field	N <sub>2</sub>	0.05-100	3-300	Plane to plane (diameter: 12 mm)
<b>c</b> • • •	Schoenbach <i>et al</i> (reference [99])	Experimental discharge	Hollow cathode	Ar	56-896	0.25	Plane to hollow (hollow hole
configuration		C C					diameter: 0.2-0.7 mm)
C	Xu et al	Experimental and	Anisotropic scattering	He	N/A (0.35 < pd	14	Plane to plane
	(reference [133])	theoretical	and fast atoms of ions		(Torr cm) < 0.6		(diameter: 150 mm)
	Meng et al	Experimental	Pulsed discharge	Air	760	0.001 - 0.025	Sphere
	(reference [120])	and theoretical					to sphere
	Brayfield et al	Experimental	Electrode-	Air	760	0.001 - 0.01	Pin
	(reference [123])		surface condition				to plate
	Marić et al	Experimental	Asymmetric	Ar	N/A ( $0.1 < pd$	0.5 - 1.5	Plane to step
	(reference [124])	electrode			(Torr cm) < 6		or central hole
	Torres and Dhariwal	Experimental	Field emission	Air	0.3-760	0.0005 - 0.025	Sphere to plane,
	(references [107, 108])	dominated discharge					cylinder to plane
	Go et al	Theoretical	Independent treatment of	Air	760	0.003 - 0.02	Plane
	(reference [35])		field emission and secondary emission				to plane
	Lisovskiy and	Experimental	RF voltage amplitude within	H <sub>2</sub> , Ar, air	0.01-20	6.5-70	Plane to plane
	(reference [27])	and theoretical	the range 0-1000 V				(diameter of 5-100 mm)
	Moon et al	Experimental	Driving frequencies	Helium	760	3	Plane to plane
	(reference [79])		in the range 1.86–27.1 MHz				(diameter of 60 mm)

Modified Paschen law[1]

#### Narrow gap breakdown even more complex; e.g., presence of background plasma

#### We conduct experiments and simulations to investigate the breakdown



#### Talk Overview

- 1. Context and motivation
- 2. Kinetic modeling via Particle-In-Cell simulation using EDIPIC-2D
- 3. Results and discussion
- 4. Modeling capabilities and expertise at PPPL via PCRF

**OPPPL** 

Use of EDIPIC-2D code, based on earlier 1D version [1]

- ✓ Comprehensive 2D Cylindrical/Cartesian explicit PIC code.
- State-of-the art collision models. FFT methods or PETSc library for Poisson solver. External circuits. Inner objects
- ✓ Verified in international benchmarks [1,2,3,4]
- ✓ Numerous users from academia and industry

#### More info at poster session!



Princeton Collaborative Research Facility

Open source and portable code able to simulate a wide variety of low temperature plasma physics problems

https://github.com/PrincetonUniversity/EDIPIC-2D

[1] Sydorenko, PhD thesis, (2006)

- [2] T. Charoy, et al., Plasma Sources Sci. Technol. 28(10), 105010 (2019).
- [3] W. Villafana et al., Physics of Plasmas 30(3), 033503 (2023)
- [4] M.M. Turner et al., Physics of Plasmas 20(1), 013507 (2013).



### Configuration and numerical setup [1]



Experimental setup performed at SNU. (a) ICP schematic. (b) Breakdown during operation (c) inner surface after several discharges.

[1]S.H. Son, *et al.* Applied Physics Letters **123**(23), 232108 (2023)

[2]J.R.M. Vaughan, IEEE Trans. Electron Devices **36**(9), 1963–1967 (1989)

- Electron-induced Secondary Electron Emission is based on Vaughan's model [2]
- ✓ Ion-induced Secondary Electron Emission
- ✓ Initial conditions: Uniform Argon plasma, density  $n_0$ , Maxwellian distribution, temperatures  $T_{e,0}$  &  $T_{i,0}$
- ✓ Bias cathode voltage  $V_{cat}$



#### Talk Overview

- 1. Context and motivation
- 2. Kinetic modeling via Particle-In-Cell simulation using EDIPIC-2D
- 3. Results and discussion
- 4. Modeling capabilities and expertise at PPPL via PCRF

#### 2D results when breakdown occurs





Dramatic increase of the plasma density, the potential is screened out
 Propagation of the breakdown inside the hole

#### 1D results at centerline x = 0







 $V_{cat} = -150V$ :No breakdown





 ➤ An insufficient bias voltage does not trigger an electron avalanche
 ➤ Breakdown criterion: n<sub>i</sub> ↑ + n<sub>i</sub> ≈ n<sub>e</sub>

#### Final Paschen curve



Pressure (Torr)



plasma sources for semiconductor fabrication industry



#### Talk Overview

- 1. Context and motivation
- 2. Kinetic modeling via Particle-In-Cell simulation using EDIPIC-2D
- 3. Results and discussion
- 4. Modeling capabilities and expertise at PPPL via PCRF



More info at poster session!

### Our Development Team

Igor D. Kaganovich, PI management, benchmarking, physics models

#### LTP-PIC:

- Stéphane Ethier, co-PI porting the code to Heterogeneous CPU/GPU architectures.
- Andrew (Tasman) Powis: 3<sup>rd</sup> year postdoc, main LTP code developer.

#### **2D EDIPIC:**

- **Dmytro Sydorenko** Univ. of Alberta, original developer of EDIPIC since his Ph.D. thesis.
- Alex Khrabrov, contractor.
- Willca Villafana 2<sup>nd</sup> year postdoc















#### Electron-beam-generated plasma





 <sup>1</sup> S. Rauf, D. Sydorenko, S. Jubin, W. Villafana, S. Ethier, A. Khrabrov, and I. Kaganovich, "Particle-in-cell modeling of electron beam generated plasma," Plasma Sources Sci. Technol. **32**(5), 055009 (2023).

Schematic of NRL experimental set up Ar, 20 mT, xx G, 12.5 mA/m, 2 keV electron beam

#### Hollow cathode system





### Electron-beam plasma interaction

57 PIC simulations varying energy and density of the beam  $E_b$  and  $n_b$ 



**PDI** (parametric decay instability): generating backward waves (waves slightly perturb plasma)

**SWMI** (standing wave modulational instability): localized standing waves

**EMI** (*electron modulational instability*): rapidly growing standing waves (breaks quasineutrality). **NEW** 

[Haomin Sun, et al, Phys. Rev. E **106**, 035203, (2022)] Unintended gas breakdowns in narrow gaps of advanced [Haomin Sun, et al, Phys. Rev. Lett. **129**, 125001, (2022)]plasma sources for semiconductor fabrication industry



#### • Main features

- ✓ Explicit 2D-3D/3V electrostatic PIC in uniform cartesian geometry
- ✓ Written in C-C++, runs on CPUs accelerated with GPUs via OpenAcc
- ✓ Monte-Carlo model of electron-neutral and ion-neutral collisions
- ✓ Field solve via Geometric Multigrid algorithms from the Hypre package (LLNL)
- ✓ Python + *VisIt* software as post-processing tools
- Written from the ground up for scalability:
  - ✓ Inter-node parallelization via *MPI*
  - ✓ Intra-node parallelization via *MPI* and/or *OpenMP*
  - ✓ Elimination of inner loop logic to take advantage of vector registers

Portable code and soon available to the community to simulate large 2D/3D simulation domains

### 3D spoke-like activity in a Penning discharge PPPL

**Partially magnetized ExB discharges**, widely used in industry and research, often exhibit large-scale, low-frequency, coherent structures known as "spokes" [1,2].



plasma sources for semiconductor fabrication industry

214 (2010).

#### Conclusion



Princeton Collaborative Research Facility

- Breakdown: experimental and PIC study (PCRF). Background plasma and previous breakdowns facilitate future breakdowns
- EDIPIC-2D is an open source extensively verified PIC code routinely used by the industry and academia for a wide variety of LTP systems. Example of applications: CCP, ICP, e-beam, hollow cathode, ECR, Hall thruster, Penning discharge, etc ... Realistic configuration with external circuit and inner objects. 10+ publications
- LTP-PIC is a 2D/3D PIC designed for HPC aiming for whole-device modeling. Excellent scalability up to hundreds of GPUs for large and more realistic geometries.

#### **Questions?**





#### More info at poster session!

#### **Questions?**

Jac



#### > Recorded normalized energy spectrum of particles hitting the walls



Most electrons and ions hit the dielectric at low energy



> A significant portion of SEE electrons is incident electrons reflected elastically

Ion-induced SEE electrons from the cathode are less important in contrast to what is typically reported in the literature [5]

[1]D. Sydorenko, PhD thesis (2006)
[2] M. Villemant, *et al.* EPL **127**(2), 23001 (2019).
[3] A.V. Phelps, and Z.L. Petrovic, Plasma Sources Sci. Technol. **8**(3), R21–R44 (1999)

Unintended gas breakdowns in narrow gaps of advanced plasma sources for semiconductor fabrication industry

[4]S.G. Walton, *et al.*, Journal of Applied
Physics **85**(3), 1832–1837 (1999)
[5]J.Y. Kim, Plasma Sources Sci. Technol. 24 **31**(3), 033001 (2022)





> Variation of the breakdown voltage if the SEE yield is turned off



E.g., if elastic reflection in SEE is turned off,  $V_{breakdwon}$  goes up by 30% with respect to the baseline ("All SEE")

True SEE and Elastic Reflection are the most important



> Variation of breakdown voltage if SEE yield is turned off is dependent on pressure



> True SEE more important at low pressure because electrons are faster (less collisions)

### Electron-beam-generated plasma





### Rotating spokes in RF CCP





Unintended gas breakdowns in narrow gaps of advanced plasma sources for semiconductor fabrication industry

<sup>1</sup> L. Xu, H. Sun, D. Eremin, S. Ganta, I. Kaganovich, K. Bera, S. Rauf, and X. Wu, "Rotating spokes, potential hump and modulated ionization in radio frequency magnetron discharges," Plasma Sources Sci. Technol. **32**(10), 105012 (2023).



#### Talk Overview

- 1. Context and motivation
- 2. Modeling capabilities using EDIPIC-2D
- 3. Toward 3D whole-device modelling with LTP-PIC
- 4. Advanced algorithms

#### 3D simulation of Hall thruster channel

channel [Villafana 2023]





Fig. 1 Schematic of the simulations, with (a) showing the configuration for the modified Landmark 2a benchmark and (b) the configuration for the 3D simulations extended into the radial direction.

### 3D simulation of Hall thruster channel





Different electron transport in 3D. Influence of boundary conditions

#### Performance of LTP PIC









### Performance of LTP PIC





Domain x500 but efficiency decreases by only x1.5 = large computational domain/geometry

### Can we model the whole device?



- 10<sup>8</sup> cells (10x10x5 cm<sup>3</sup>)
- 10<sup>11</sup> simulation particles
- 10<sup>8</sup> time steps

Each time step is approximately 100 ms for a large 3D simulation

If we require  $10^8$  time steps this corresponds to a simulation > 100 days!







### Can we model the whole device?



We think a goal of 10 days is potentially useful to industry

We can improve step time in three ways:

- More resources
- Better computer science
- New algorithms



Weak scaling of LTP-PIC in 3D







#### Talk Overview

- 1. Context and motivation
- 2. Modeling capabilities using EDIPIC-2D
- 3. Toward 3D whole-device modelling with LTP-PIC
- 4. Advanced algorithms

#### Unintended gas breakdowns in narrow gaps of advanced plasma sources for semiconductor fabrication industry

#### 39

#### Fig. (a) Ion density, (b) plasma potential and (c) electron temperature at steady state



### 2D simulation of CCP

- 2D, 30 mTorr Argon discharge
- 4000 × 1000 cells, ≈ 500 particle-per-cell,
   20 million time steps
- Simulated using 256 GPUs on the Perlmutter supercomputer in 6 days

#### Fig. Simulation geometry,





### Weakly magnetized CCP in cylindrical

510



#### Weakly magnetized CCP







Plasma	confinement			where	
magnetic	field	is	parallel	to	the
walls					

Case C: eight loops  $n_i [m^{-3}]$   $v_i$   $v_i$ 

### Reducing the number of cells and time steps OPPPL



rgy-conserving Numerical heating or cooling in DI can be mitigated

<sup>1</sup> H. Sun, et al "Direct implicit and explicit energy-conserving particle-in-cell methods for modeling of capacitively coupled plasma devices," Physics of Plasmas **30**(10), 103509 (2023) s for semiconductor fabrication industry



#### INDUSTRY

- Industry invests \$billions in large, complex machines for chip manufacturing (etching and deposition)
- Machines have limited diagnostics
- Fundamental research "takes too long" and is too expensive (prefer trial-and-error)
- However, industry recognizes the benefits that theoretical and computational research can bring

#### **MODELING NEEDS**

- Fully kinetic treatment of low temperature plasmas (ICP, CCP, ECR, electron beam generated plasmas, hollow cathodes, dc and rf magnetrons, etc.)
- Complete reaction pathway of chemistry in the plasma and at the interface with surface
- Any insights on the plasma and chemical processes at play can give them a huge advantage over competition

#### EDIPIC: How to use?

 $\mathbf{O}$ 



#### **Open source: public repository** https://github.com/PrincetonUniversity/EDIPIC-2D

Search or jump to / Pull request	s Issues Marketplace Explore		
PrincetonUniversity / EDIPIC-2D Public			
↔ Code ⊙ Issues 🐧 Pull requests ⊙ Actions	🗄 Projects 🖽 Wiki 🙂 Security	🗠 Insights	
	P main →         P 3 branches         S 0 tags		Go to file Add file - Code -
	😵 dsydoren Add files via upload		7a9d5ed 20 days ago 🕚 160 commits
	Doc	Add files via upload	3 months ago
	Instructions	Updated the SLURM script for Stellar, replace	ing the openmpi library 7 months ago
	Postprocessing	Add files via upload	7 months ago
	input_data_dc_inner_object_avg	Delete removeme	3 months ago
	input_data_dc_inner_object_ion_i	Add files via upload	8 months ago
	input_data_dc_periodic_ion_indu	Add files via upload	8 months ago
	input_data_dc_semiperiodic_Heli	Add files via upload	7 months ago
	input_data_files_waveform	Add files via upload	8 months ago
	input_data_rf_external_circuit	Delete removeme	3 months ago
	input_data_sample	Add files via upload	8 months ago
	input_data_sample_periodic_SEE	Add files via upload	8 months ago
	input_data_sample_periodic_ebe	Add files via upload	8 months ago
	input_data_waveform_amplitude	Update init_bo_01_waveform.dat	last month
	src src	Add files via upload	20 days ago
		Create LICENSE	13 months ago
	C README.md	Update README.md	26 days ago

### EDIPIC: How to use?



#### Documentation:

How to install on Stellar (or any clusters):

https://github.com/PrincetonUniversity/EDIPIC-2D/blob/main/Instructions/installing\_edipic2d.md

#### Installing EDIPIC-2D

EDIPIC-2D is a Fortran code so you need access to a Fortran compiler. The current makefile works with the Intel Fortran compiler as well as with GNU gfortran. The makefile determines which compiler is being used by looking at the output of the "mpifort -show" command (see MPI section below).

EDIPIC-2D requires a few libraries in order to run. These are :

- MPI (OpenMPI, MPICH, Intel-MPI, etc.)
- PETSc
- HYPRE
- BLAS/LAPACK

How to run on Stellar (or any clusters) from templates: https://github.com/PrincetonUniversity/EDIPIC-2D/blob/main/Instructions/running\_edipic2d.md

#### **Running EDIPIC-2D**

The easiest way to get started with EDIPIC-2D is by copying one of the examples found in the top directory of the repository and modifying it to match the parameters of your system. The example directories are:

- input\_data\_sample
- input\_data\_sample\_periodic\_SEE
- input\_data\_sample\_periodic\_ebeam
- iinput\_data\_files\_waveform

### EDIPIC: How to use?

#### Documentation:

- How to post process data:
  - Via gnuplot
  - Via python scripts

https://github.com/PrincetonUniversity/EDIPIC-2D/blob/main/Doc/EDIPIC2D\_output\_data\_description\_0.pdf

Code overview and input file description:

https://github.com/PrincetonUniversity/EDIPIC-2D/tree/main/Doc

#### And we can help!



# EDIPIC-2D output data description

Dmytro Sydorenko



### Low-pressure plasma modelling challenges **OPPPL**

velocity vector

At higher pressures, the ions may collide with

particles on their way to the surface deflecting their

A low-pressure plasma is essential to maintain ion etch *anisotropy* 

He He+ He+ He+ He+ He+ He He Mask He Mask (He Silicon Silicon He Wafer Wafer Electrode Electrode

### Low-pressure plasma modelling challenges **OPPPL**

Often in gas or plasma simulations we rely on a **fluid** treatment

n(x, t) – Number density v(x, t) – Velocity vector

And if the plasma is electrostatic we can solve for:

 $\phi(\mathbf{x}, t)$  – Electric potential



X

$$x = (x, y, z)$$

$$x = (x, y, z)$$

$$n(x, t), v(x, t), \phi(x, t)$$

However, we are considering a lowpressure system, where our gas/plasma is weakly collisional

In this case we <u>cannot</u> assume that our plasma has a Maxwellian velocity distribution.

The fluid approximation breaks down and we must use a six-dimensional *kinetic* treatment



### Low-pressure plasma modelling challenges **OPPPL**



### Low-pressure plasma modelling challenges **OPPPL**

Solve kinetic equation via Particle-In-Cell simulations



# 1D cuts at radial locations

Case A: no B field

Case B: one loop

Case C: eight loops





#### Accelerating LTP-PIC with OpenACC



Assume, on a single GPU, ~10 GB per plasma species:

- This allows us to model around 10<sup>8</sup> particles, per-species, per-GPU
- Corresponding to around 10<sup>5</sup> cells per-GPU

## Such a grid is not big enough to take full advantage of the GPU



#### Accelerating LTP-PIC with OpenACC



### Reducing the number of cells and time steps OPPPL



Can obtain a significant **speed up x10** Simulations were verified with a classic momentum conserving explicit PIC schemes

<sup>1</sup> H. Sun, et al "Direct implicit and explicit energy-conserving particle-in-cell methods for modeling of capacitively coupled plasma devices," Physics of Plasmas **30**(10), 103509 (2023).

### Reducing the number of cells and time steps OPPPL



[2] Preprint available at arXiv:2308.13092