Validation and benchmarking of two particle-in-cell codes for a glow discharge

Johan Carlsson[1], Alexander Khrabrov[1], Igor Kaganovich[1], Timothy Sommerer[2] and David Keating[3]

[1]Princeton Plasma Physics Laboratory
[2]General Electric Global Research
[3]Department of Physics, University of California at Berkeley

44th International Conference on Plasma Science

05/25/2017

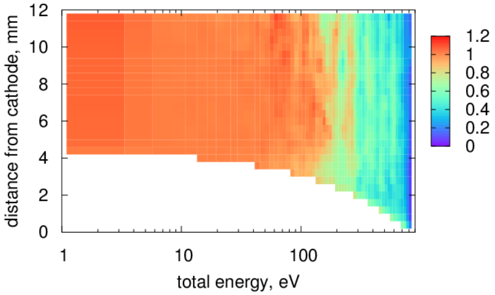
PPPL PRINCETON PLASMA PHYSICS LABORATORY

Motivation and introduction

- The two particle-in-cell codes EDIPIC and LSP were used to simulate a plasma-based power-electronics device
- To reconcile differences, a code benchmarking / validation exercise was performed
  - verification: are the equations of the physics models solved correctly?
  - validation: are the physics models sufficient to reproduce relevant physics of real device?
  - benchmarking: how do different codes compare?
- This talk will cover validation and benchmarking only
- Inherent conflict between benchmarking and validation:
  - benchmarking facilitated by few and simple physics models
  - validation requires complete set of physics models
- We first did validation, and then benchmarking, as the need arose

Glow discharge as a validation target

- We particularly wanted to benchmark / validate the collision models of respective code
- A glow discharge is a discerning validation target for collision models, including their anisotropy
- The plot shows a contour plot of the anisotropy parameter for a glow discharge very similar to the validation target
- The anisotropy parameter $a = \langle \frac{2}{3} \sin^2 \theta \rangle$, where θ is the angle between the velocity vector and the discharge axis



The challenges of simulating a glow discharge

Conceptually simple system, but with

- non-local kinetics
- non-Maxwellian electron velocity distribution
- strong anisotropy
- strong inhomogeneity
  - electron energy and density vary by about three orders of magnitude between the cathode-fall and the negative-glow regions
- severe temporal multiscale problem (picosecond to millisecond – nine orders of magnitude)
- sensitive dependencies on only approximately known parameters that are hard to measure in a reproducible way

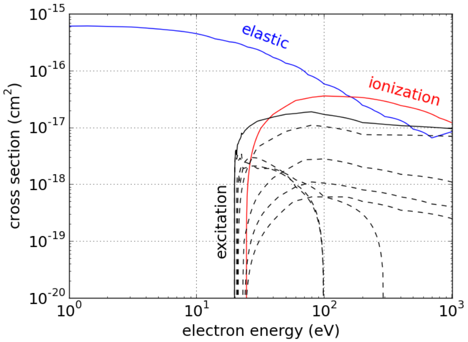
PRINCETON PLASMA PHYSICS LABORATORY

Simulation model

- Both LSP and EDIPIC are PIC-MCC codes
- EDIPIC has a null-collision model but it was disabled to facilitate benchmarking
- Short glow discharge in helium at 3.5 Torr, operated in the moderately abnormal regime
- Cold aluminum electrodes, located 0.62 cm apart
- 1D simulation with only axial direction resolved
- Electrostatic approximation used for electric field
- 10 μm cell size and 2 *ps* time step
- Electrons produced at cathode primarily by ion secondary electron emission with yield $\gamma_{eff} \approx 0.3$
- Voltage drops of 211 V and 600 V were simulated
- γ_{eff} adjusted for each code to match experimental discharge current

Collision models

- Coulomb collisions for electrons on electrons
- Charge exchange of ions on neutrals
- Elastic, excitation and ionization for electrons on neutrals
  - Excitation collisions are modelled with a consolidated cross section (solid black graph in plot below)



Anisotropy models for collisions

- Elastic, excitation and ionization collisions all anisotropic
- For elastic and excitation collisions, an anisotropy model based on energy-dependent screened-Coulomb scattering is used [Khrabrov&Kaganovich, PoP **19** (093511) 2012]:

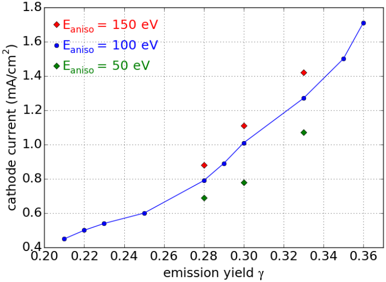
$$\frac{1}{\sigma(E)}\frac{d\sigma}{d\Omega}(E,\theta) = \frac{1}{4\pi}\frac{1+\varepsilon}{\left(1+\varepsilon\sin^2\frac{\theta}{2}\right)^2},$$

  where the normalised energy ε is defined as $8E/E_{aniso}(E)$ and E_{aniso} is the anisotropy parameter
- For ionization, the same screened-Coulomb model is applied, but with a constant screening length treated as an adjustable parameter that determines the anisotropy level

PRINCETON PLASMA PHYSICS LABORATORY

Uncertainty quantification for secondary-emission yield and anisotropy parameter

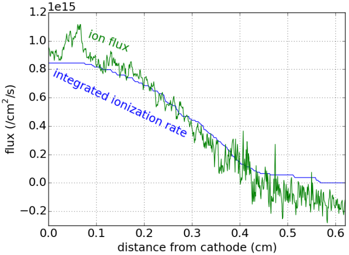
- Several versions of anisotropy model for ionization exists
- Here we use the one proposed by Okhrimovskyy
- Plot shows discharge current computed with LSP vs. secondary-emission yield γ for three different values of the E_{aniso} anisotropy parameter
- Large error bar for γ (and E_{aniso}) is amplified for current



PPPL PRINCETON PLASMA PHYSICS LABORATORY

Simulations are ran until approximate steady state is reached

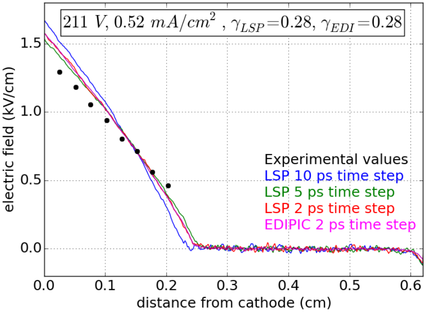
- Simulations are almost in steady state after about 100 μs (10^8 time steps)
- The exception is the very slow accumulation of sub-eV electrons in the negative glow, which has a millisecond time scale
- The plot compares the ion flux (green graph) with the integral of the ionization rate (blue) from EDIPIC
- The graphs overlap, except in negative glow ($x > 0.35\ cm$)



PRINCETON PLASMA PHYSICS LABORATORY

Simulations at 211 V

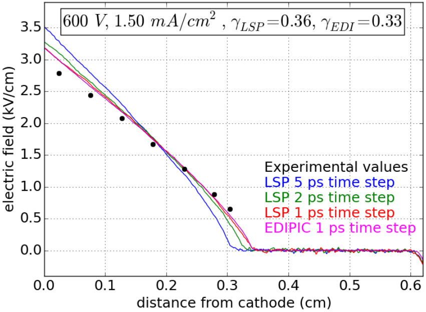
- 211 V applied and secondary-emission yield γ adjusted to 0.28 to match experimental discharge current
- Temporal convergence for 2 ps time step (restricted by cell transit time for electron in cathode fall)
- LSP and EDIPIC in excellent agreement
- Both give slightly shorter cathode fall / higher cathode electric field than experiment



PRINCETON PLASMA PHYSICS LABORATORY

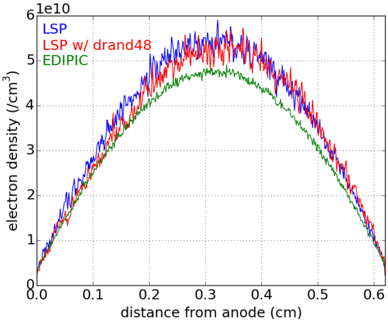
Simulations at 600 V

- 600 V applied and secondary-emission yield γ adjusted to match experimental discharge current
- Temporal convergence for 1 ps time step (due to stronger acceleration in larger cathode fall)
- LSP needs larger γ than EDIPIC to match current (0.36 vs. 0.33)
- Otherwise similar to 211 V case



Synthetic benchmarking of collision models

- To help explain the need for larger γ for LSP than for EDIPIC at 600 V, we performed a set of simplified benchmarks for the collision models in isolation
- MCC simulation of electron-beam injection into helium
- Significant difference found for anisotropic elastic and excitation collisions



Summary

- The LSP and EDIPIC code were largely succesful in reproducing experimental results for a short glow discharge
- Both codes give correct variation of cathode-fall width with voltage and sub-eV electron temperatures in negative glow (not shown here)
- EDIPIC is better at reproducing negative-glow density (presumably due to better Coulomb collisions, not shown)
- Several issues were identified:
  - Subpar pseudo random number generators (corrected in both codes)
  - Electron-electron Coulomb collisions in LSP
  - Anisotropy suppression in LSP
- Full paper available at: http://dx.doi.org/10.1088/0963-0252/26/1/014003
- The necessary data to benchmark your code available at: http://arks.princeton.edu/ark:/88435/dsp01x920g025r

Acknowledgment

- The information, data, or work presented herein was funded in part by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR00000670 (JC, AK, IK).
- The information, data, or work presented herein was funded in part by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR0000298 (TS).
- This work was made possible by funding from the Department of Energy for the Summer Undergraduate Laboratory Internship (SULI) program. This work is supported by the US DOE Contract No. DE-AC02-09CH11466 (DK).

PPPL PRINCETON PLASMA PHYSICS LABORATORY