NUMERICAL MODELING OF ION PRODUCTION IN ECRIS BY USING THE PARTICLE-IN-CELL METHOD

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Outline

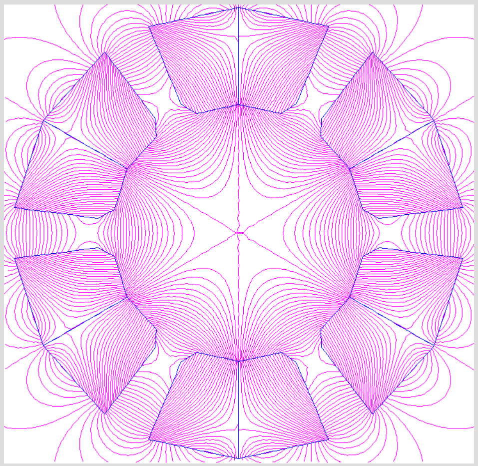
1. Introduction
2. KVI A-ECRIS
3. Code Description
4. Results
5. Conclusions

We develop the 3D Particle-in-Cell Monte-Carlo Collisions Code. The key ingredient is

ponderomotive barrier confinement

- *Numerical modeling of ECRIS allows better understanding of the physical processes in ECRIS plasmas*
- *Some experimentally observed effects can be explained*
- *Could help in finding out how to optimize the source performance*

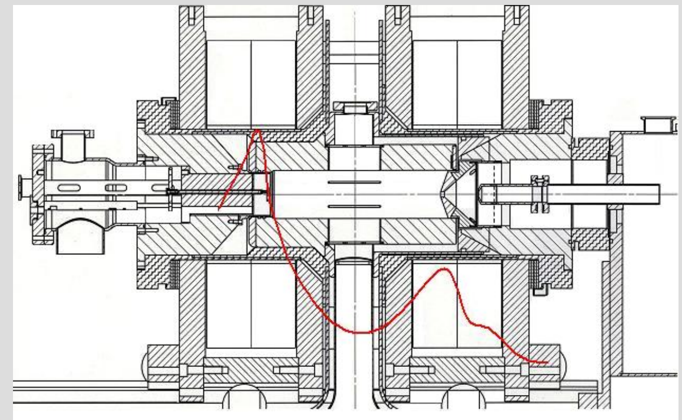
KVI A-ECRIS layout and performance



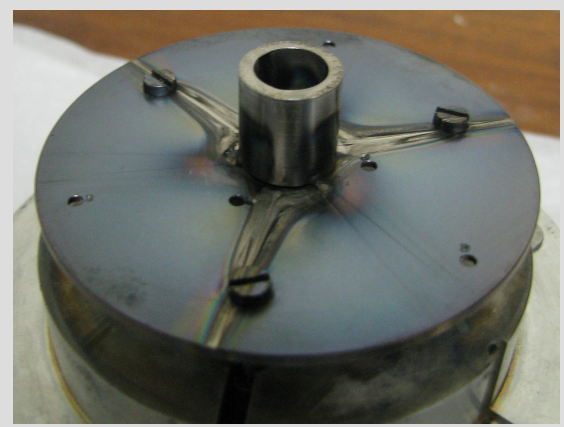
Al plasma chamber, hexapole with the slits for better pumping of the chamber.

RF frequency 14+(11-12.5) GHz

- B_{inj}=2.1 T, B_{min}=0.36 T
- B_{ext}=1.1 T, B_{rad}=0.86 T
- Chamber length 30 cm
- Chamber diameter 7.6 cm
- Extraction aperture 0.8 cm



Q	C eμA	O eμA	F eμA	Ne eμA	Ar eμA	Q	Pb eμA
1	11		67	105	55	23	19
2	40		134	158	69	24	25
3	270		159	245	61	25	29
4	187	-	183	394	75	-	-
5	61		188	590	119	27	26
6	~5	700	107	446	174	28	19
7		110	55	224	275	29	16
8				87	488	30	9
9					250	31	5
10					-		
11					20		



Code Description (1)

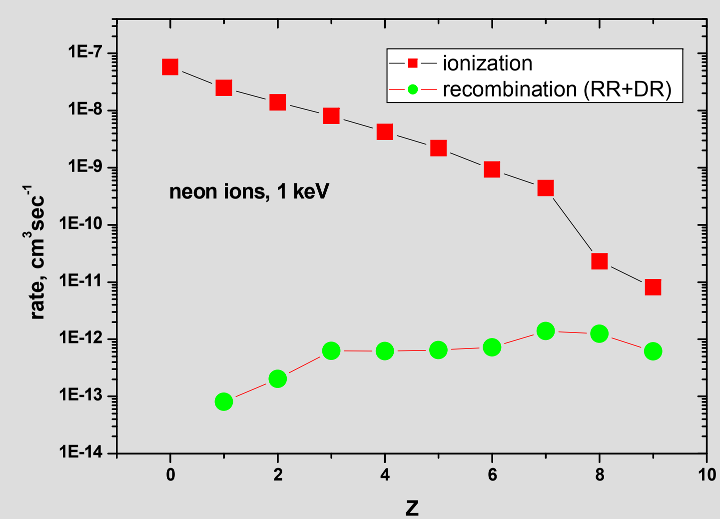
Uniformly distribute 50% neutral neon atoms and 50% Ne1+ in the volume.

For each macro-particle, define in which cell it is now (rectangular mesh 38x38x64). Calculate n_i and get n_e from quasi-neutrality requirement.

Group the particles in the cell in random order and calculate ion-ion elastic collisions

(Takizuka-Abe method of grouping + Nanbu model for scattering angles).

Code Description (2)

Calculate electron-ion heating. T_e=1 keV everywhere, free parameter Martin et al. X-ray spectroscopy of 14 GHz ECRIS arXiv:0909.2393v1	$V_{x,y,z} = V_{x,y,z} + \delta \times (n_e(ix,iy,iz) \times 15. \times dt \times Z^2 \times 6.11 \times 10^{-9} / m)^{0.5}$
Calculate ionization probability; if yes, Z=Z+1 Rates are from P.Mazzotta, et al., Astron. Astrophys., Suppl. Ser., **133**, 403 (1998). Recombination processes are negligible.	

Code Description (3)

Calculate charge-transfer and ion-atom elastic scattering rates. Scale it as Z (Langevin). $\sigma_{Langevin} = Z \times 2\pi a_0^2 \times (\alpha Ry / \varepsilon)^{0.5}$

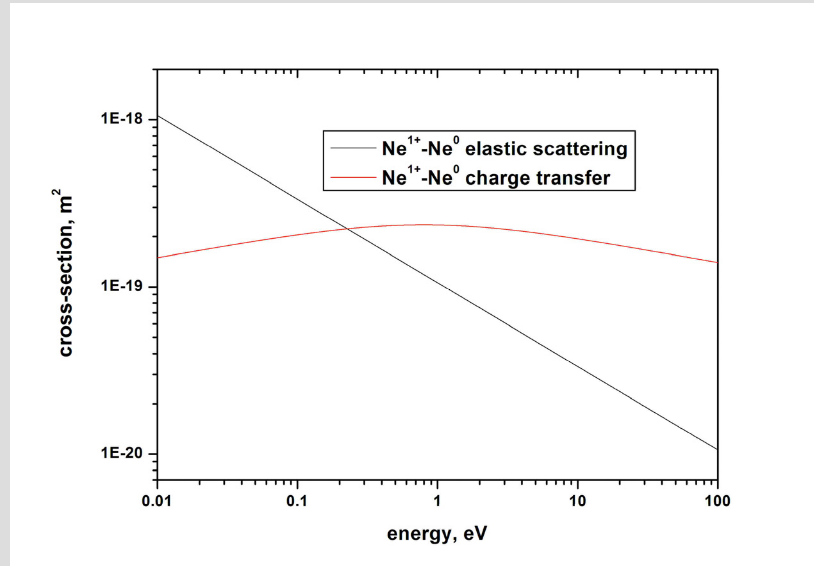
Energy release with Q around 10 eV!

Analytical expressions for the Ne^+-Ne cross sections as a function of relative energy are

$$Q_b = 2.8 \times 10^{-19} / \varepsilon^{0.15} / (1 + 0.8/\varepsilon)^{0.3} \qquad (7)$$

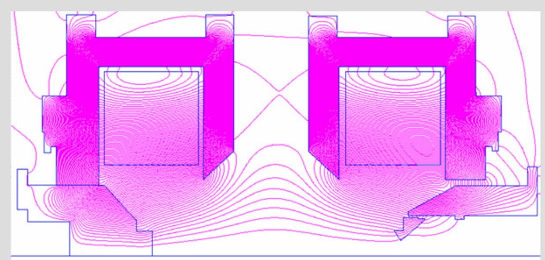
and from Eq. (3) with $\alpha = 2.67$ a.u. [22],

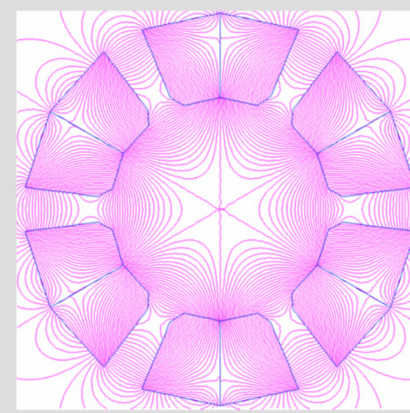
$$Q_{iso} = 1.059 \times 10^{-19} / \varepsilon^{0.5}. \qquad (8)$$



Move ion in the static B and E fields defined analytically.

B field is from POISSON-SUPERFISH calculations for KVI-AECRIS + component for the Halbach hexapole (no edge effects)





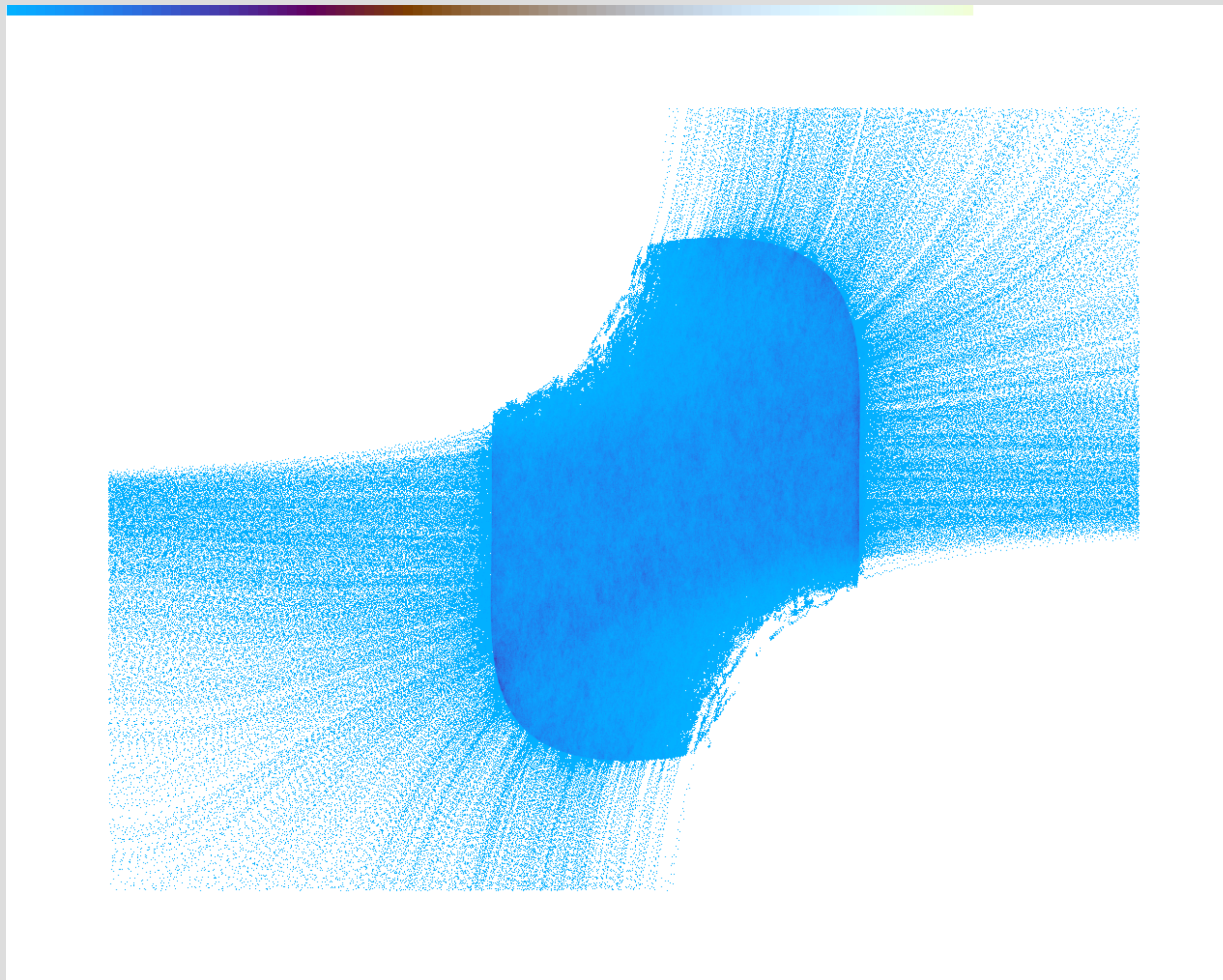
Electric field

Inside ECR zone ($B<0.5$ T) it is set to zero.

1 V/cm towards the walls outside the zone (pre-sheath). Can be varied in a wide range.

When ion crosses the ECR zone boundary, it is either accelerated to the walls, or it is reflected back if V<PB*sqrt(Z)

Ponderomotive Barrier



Ponderomotive barrier

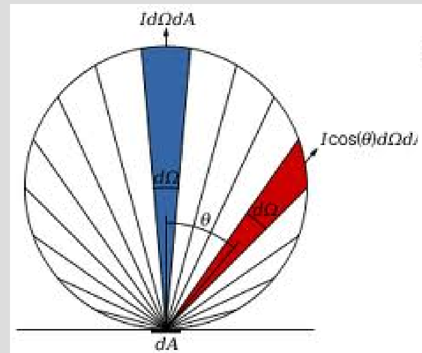
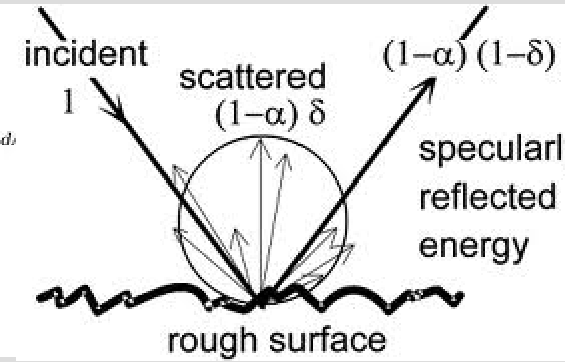
Electrons are expelled from a thin layer around ECR by the ponderomotive force, giving rise to a positive potential barrier. The potential barrier (PB) confines ions inside the ECR zone.

It is a free parameter in our calculations, varies in (0-1) V range. No spatial variations.

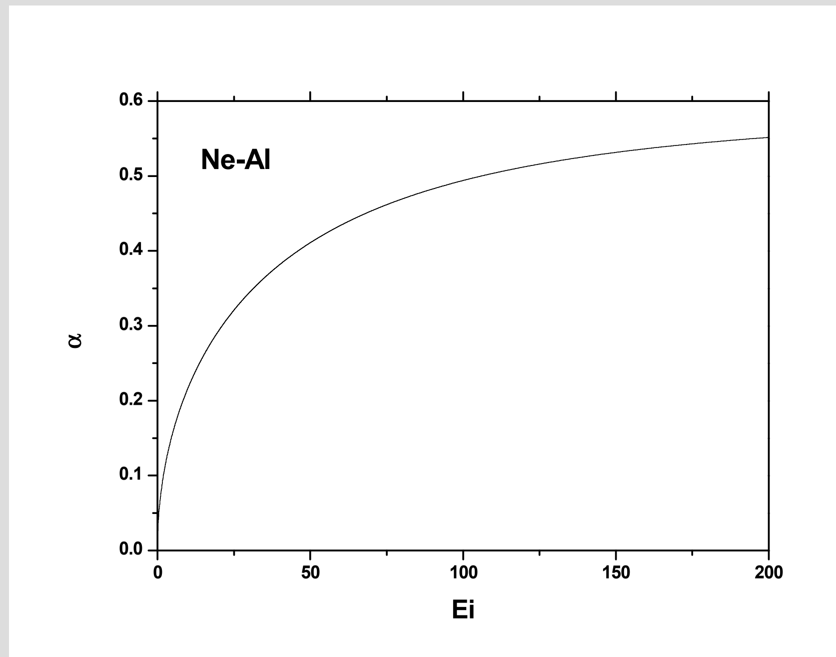
We set its height to zero if the plasma density exceeds the cut-off limit of 2.5×10^{12} cm^{-3} (for 14 GHz RF frequency)
– reflections/absorption in the plasma
– empirically observed saturation of plasma density at cut-off value.

$$\Phi = \frac{q^2}{4\,m} \frac{|E_\theta|^2}{(\omega^2 - \Omega^2)}$$

Code Description (4)

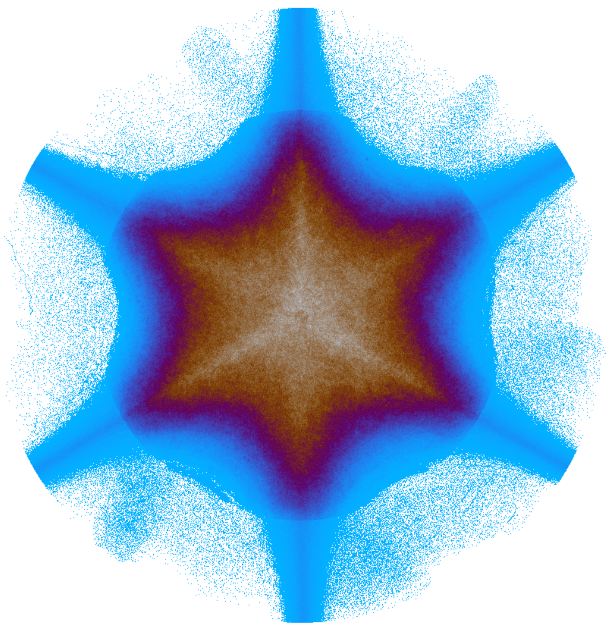
When ion hits the chamber wall, it is neutralized	Fraction of the backscattered singly charged ions is less than 1 %
If not in extraction aperture, ion is scattered back with an angular distribution according to the cosine-law (diffuse scattering)	 
Energy distribution of neutralized atoms is from the experimental data J.W.Cuthbertson, W.D.Langer and R.W.Motley, J.Nucl.Mater. **196-198**, 113 (1992).	Gaussian distribution with the FWHM around 10 eV, maximum at 10 eV independent on the initial energy

Code Description (5)

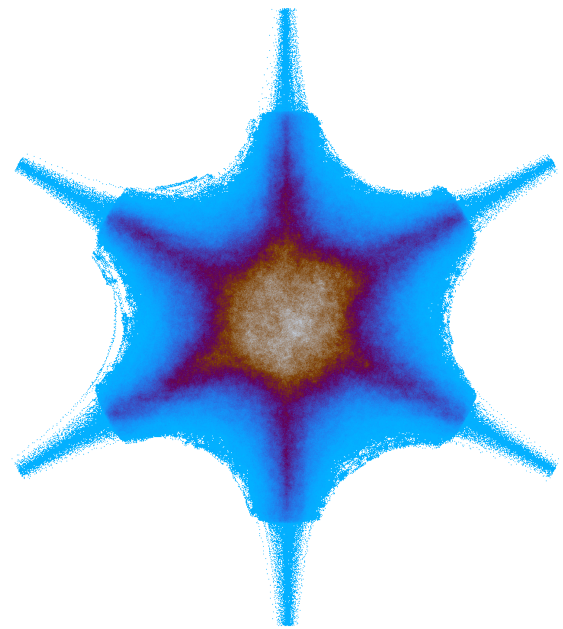
When atom hit the wall, it looses some energy. The thermal accommodation coefficient α	$E_s - E_i = \alpha\,(T_w - E_i)$
We use α(T) for Ne-Al surface collisions from *F.O.Goodman and H.Y.Wachman, J.Chem.Phys.* ***46****, 2376 (1967).* For small energies, α(T) is quite small → hot gas in the chamber Not for all elements!	

Spatial Distributions of Ions

Ne^{1+}

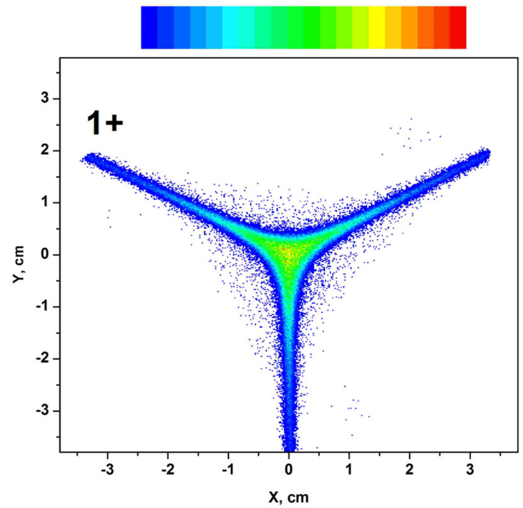


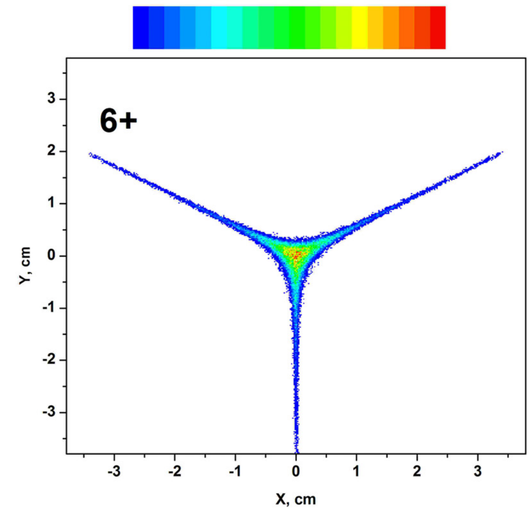
Ne^{6+}



Higher charge states are more localized on the axis

Spatial Distribution at Extraction



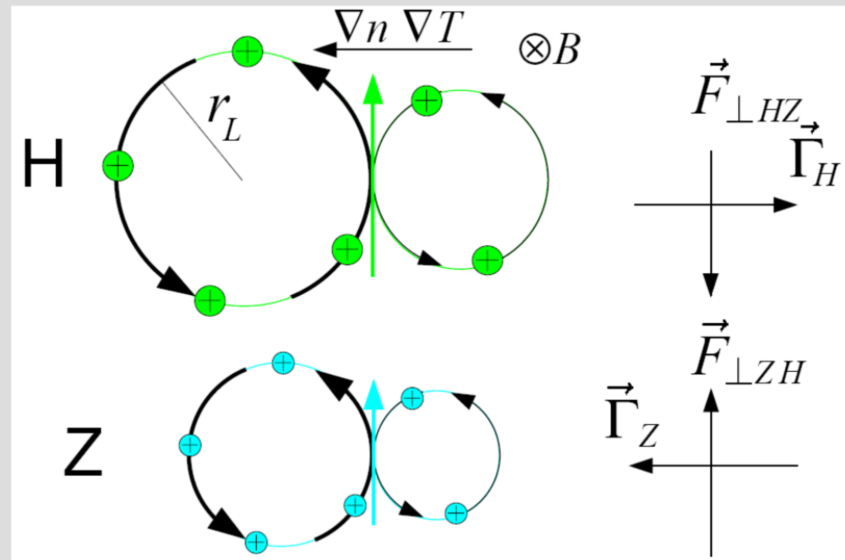


A cartoon of classical flux

$$\rho_a = \frac{v_{Ta}}{e_a B / m_a} = \frac{\sqrt{2 k_B T_a m_a}}{e_a B}$$

$$\vec{u}_{dia,a} = -\frac{\nabla p_a \times \vec{B}}{e_a n_a B^2}$$

Diamagnetic velocity depends on the charge and causes friction between different species, that drive radial fluxes.



http://www.aug.ipp.mpg.de/E2/Mitarbeiter/Zohm/PhD_Network_2010/Dux.ppt#14

The classical radial particle flux (final result)

$$\boxed{\vec{\Gamma}^a_{CL} = -\nabla n_a \sum_{b\neq a} D^{ab}_{CL} + n_a \sum_{b\neq a} D^{ab}_{CL} \frac{e_a}{e_b}\left(\frac{\nabla n_b}{n_b} - \frac{\nabla T}{T}\left[\frac{3m_{ab}}{2m_b} - 1 - \frac{e_b}{e_a}\left(\frac{3m_{ab}}{2m_a} - 1\right)\right]\right) \qquad D^{ab}_{CL} = \frac{\rho_a^2}{2}\nu_{ab}}$$

For a heavy impurity in a hydrogen plasma (collisions with electrons can be neglected):

$$\vec{\Gamma}^Z_{CL} = \frac{\rho_Z^2 \nu_{ZH}}{2}\left\{-\nabla n_Z + n_Z Z\left(\frac{\nabla n_H}{n_H} - \frac{1}{2}\frac{\nabla T}{T}\right)\right\}$$

inward outward (temperature screening)

In equilibrium the impurity profile is much more peaked than the hydrogen profile (radial flux=0)

$$\frac{\nabla n_Z}{n_Z} = Z\left(\frac{\nabla n_H}{n_H} - \frac{1}{2}\frac{\nabla T}{T}\right)$$

For a pure hydrogen plasma:

$$\vec{\Gamma}^e_{CL} = \frac{\rho_e^2 \nu_{ei}}{2}\left\{-\nabla n - n\left(\frac{\nabla n}{n} + \frac{1}{2}\frac{\nabla T}{T}\right)\right\} = \frac{\rho_e^2 \nu_{ei}}{2}\left\{-2\nabla n - \frac{n}{2}\frac{\nabla T}{T}\right\} = \vec{\Gamma}^i_{CL}$$

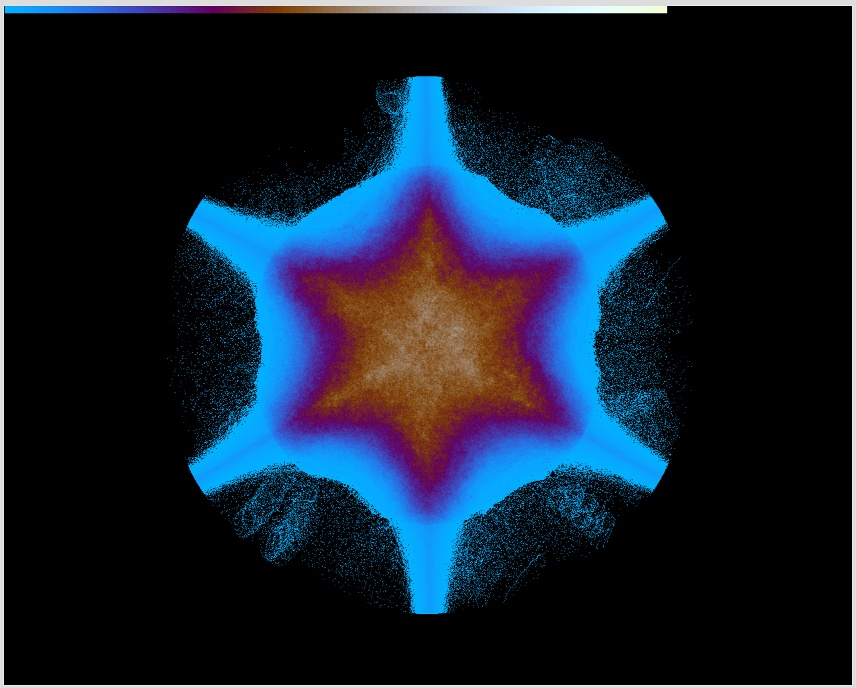
$\rho_e^2 \nu_{ei} = \rho_i^2 \nu_{ie}$ ion and electron flux into the same direction and of equal size!

http://www.aug.ipp.mpg.de/E2/Mitarbeiter/Zohm/PhD_Network_2010/Dux.ppt#14

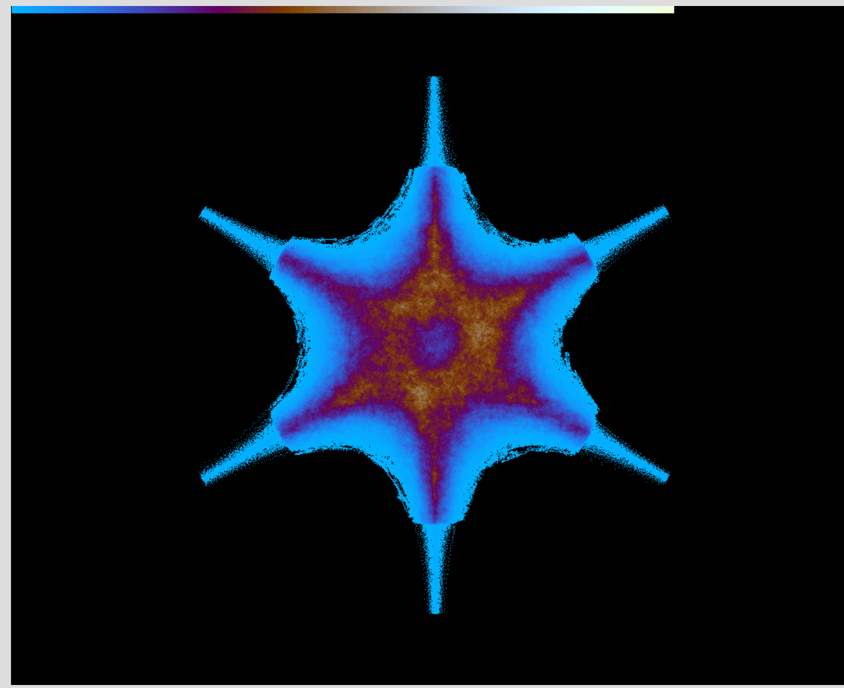
Spatial Distribution

High accomodation coefficient (cold gas) and low PB

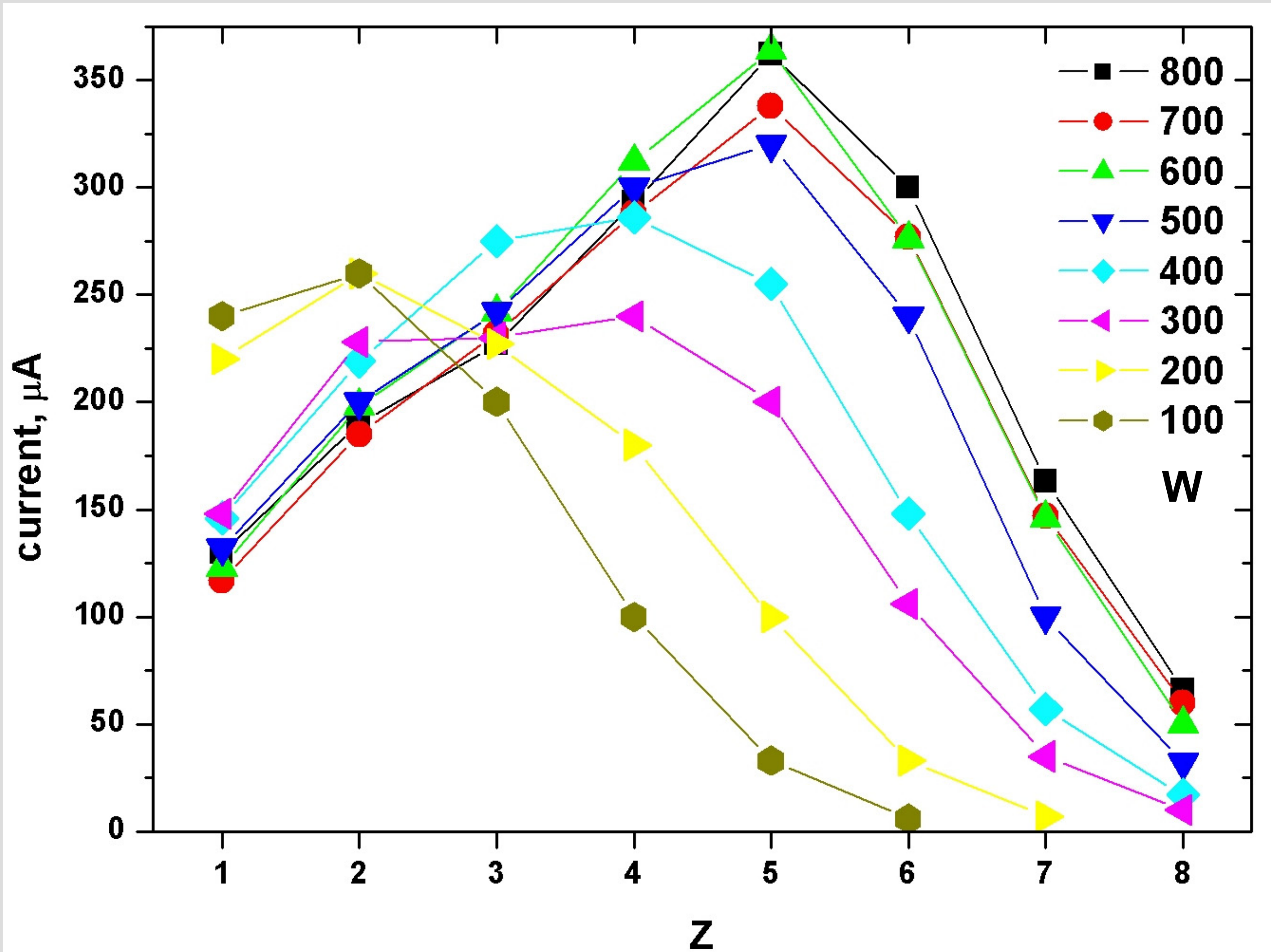
Ne^{1+}



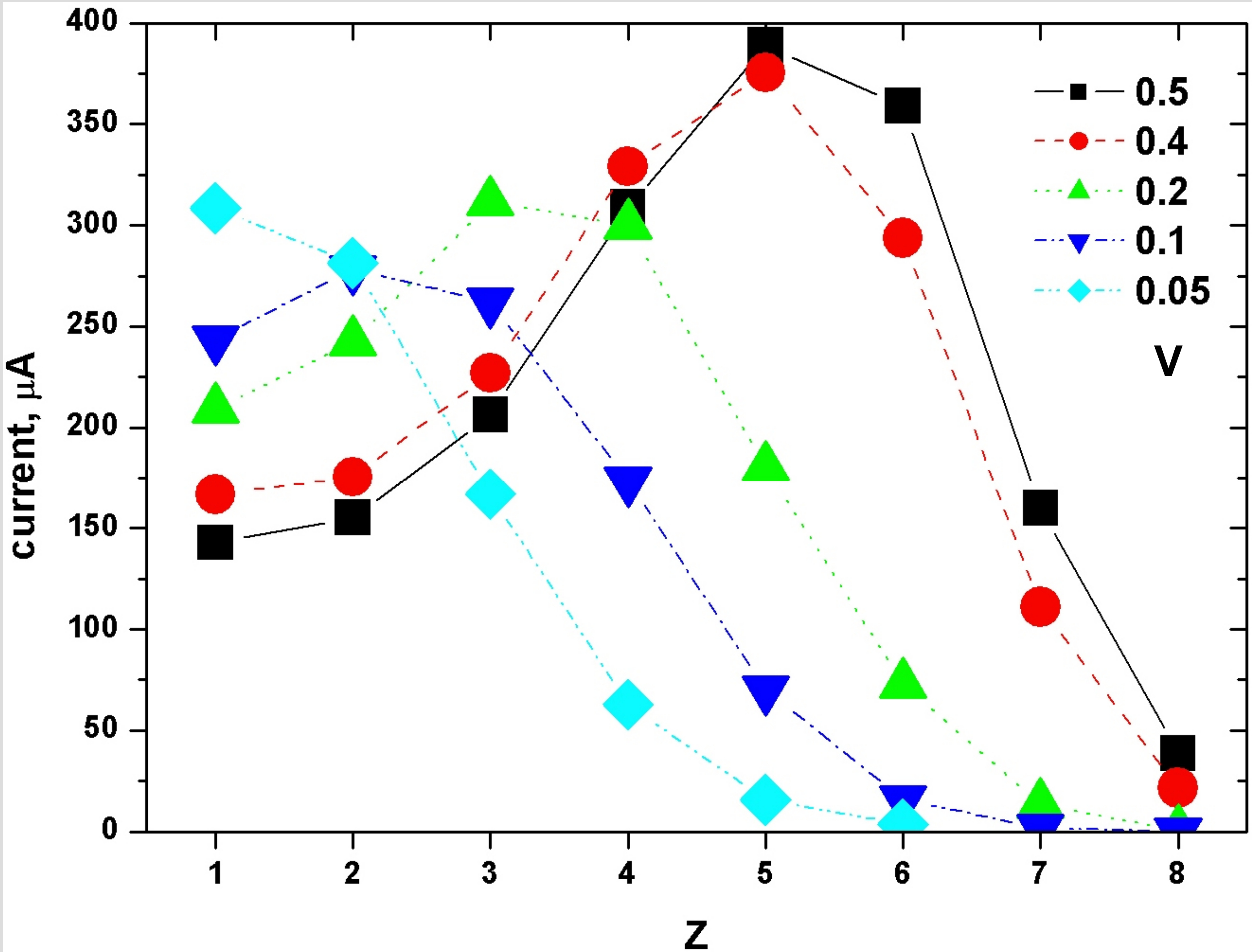
Ne^{6+}

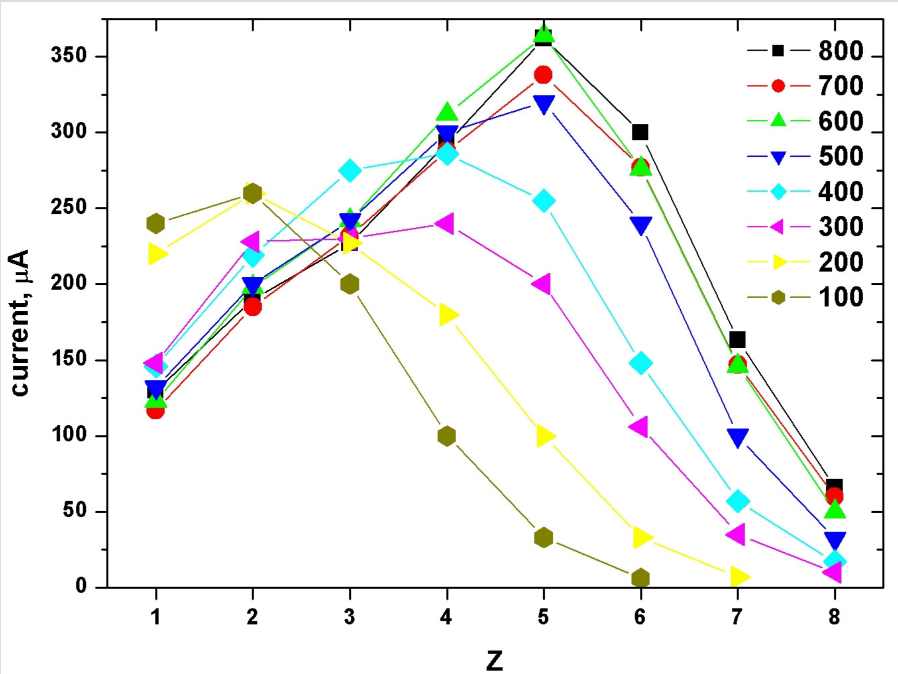


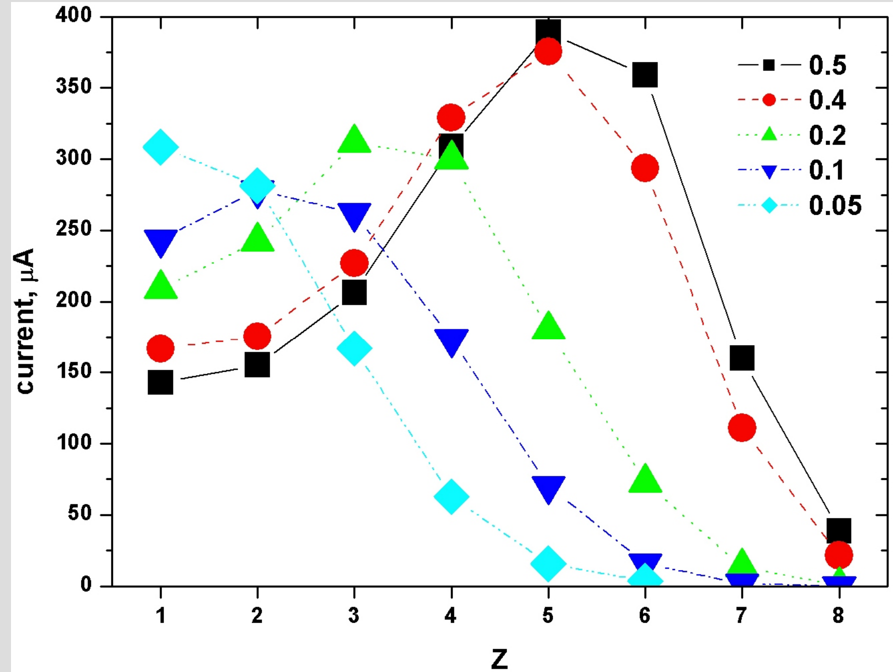
Extracted currents – experiment, different RF powers, fixed gas flow



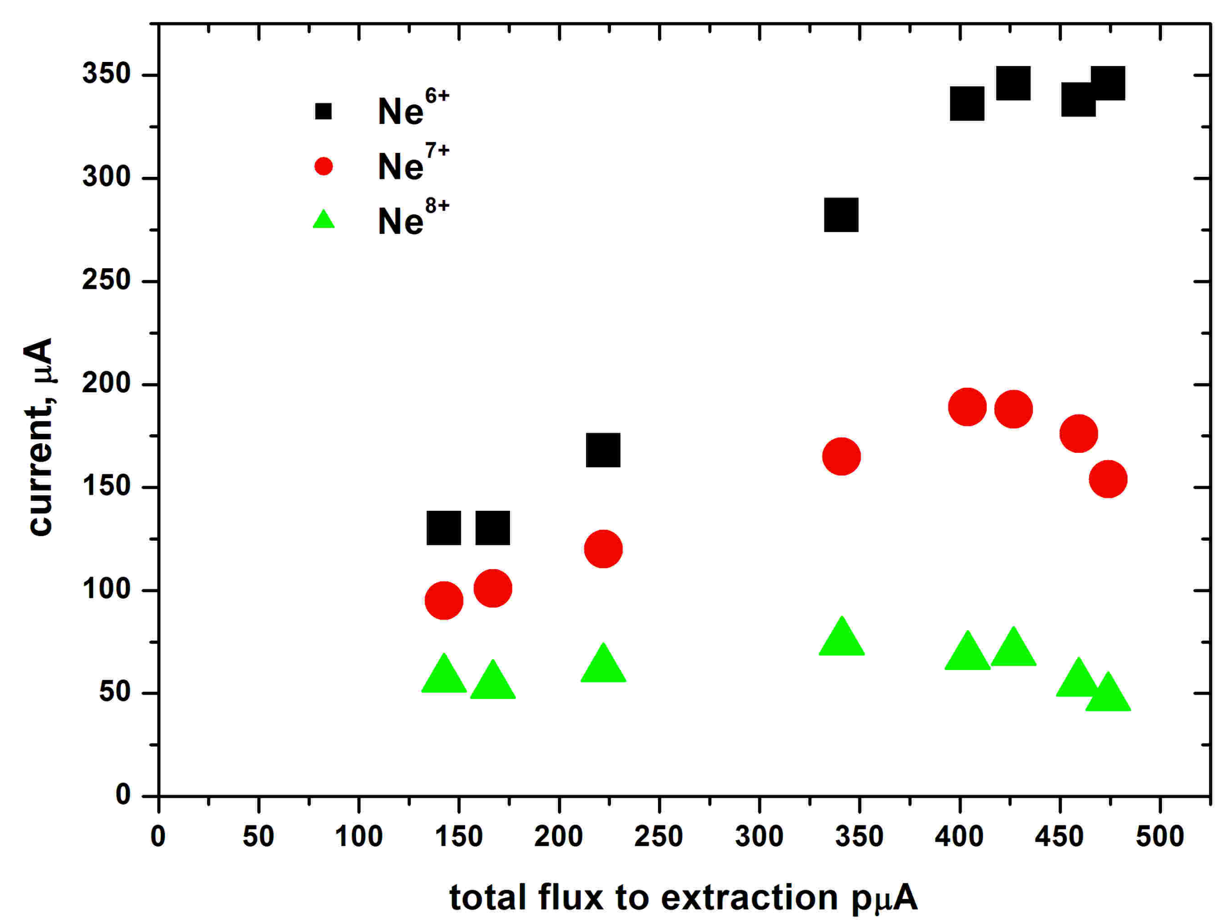
Extracted currents – simulations, different PB height, SW is varied to have the same outflow



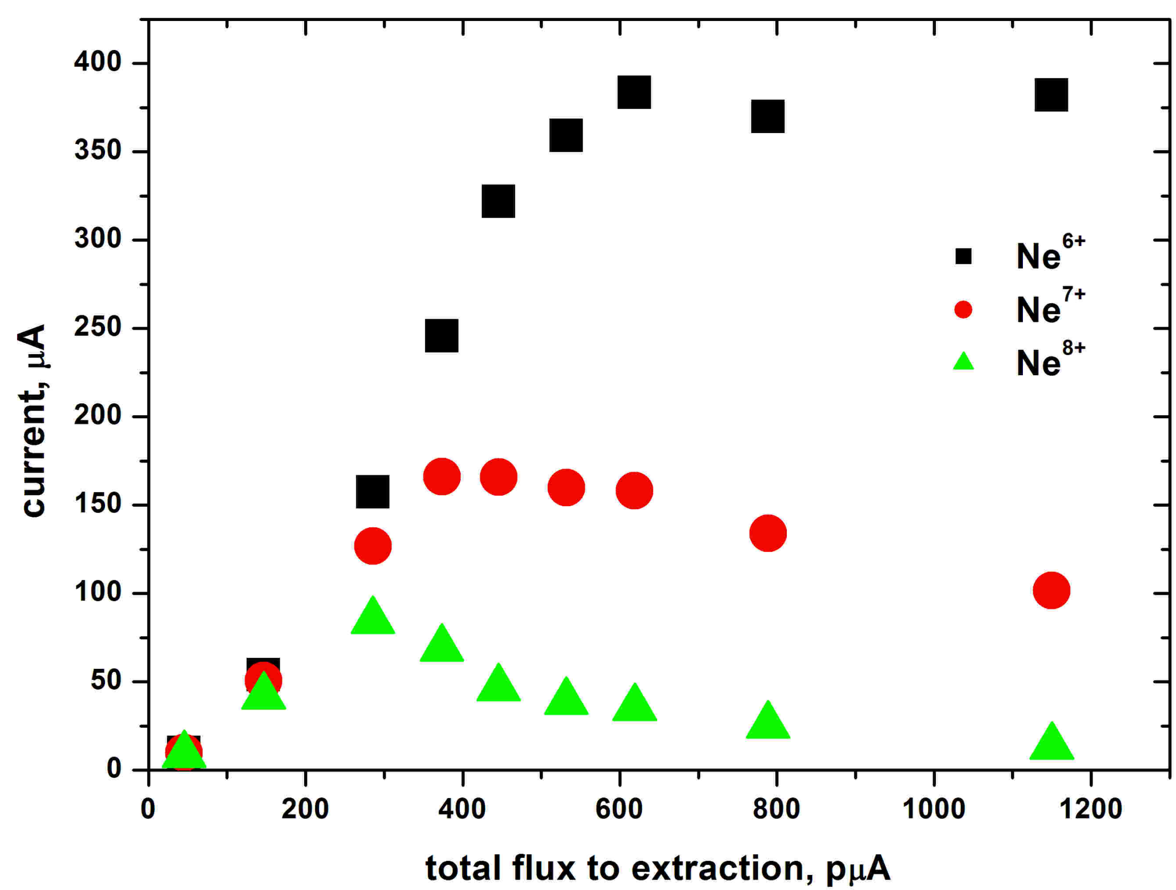

current, μA
Z
800
700
600
500
400
300
200
100


current, μA
Z
0.5
0.4
0.2
0.1
0.05

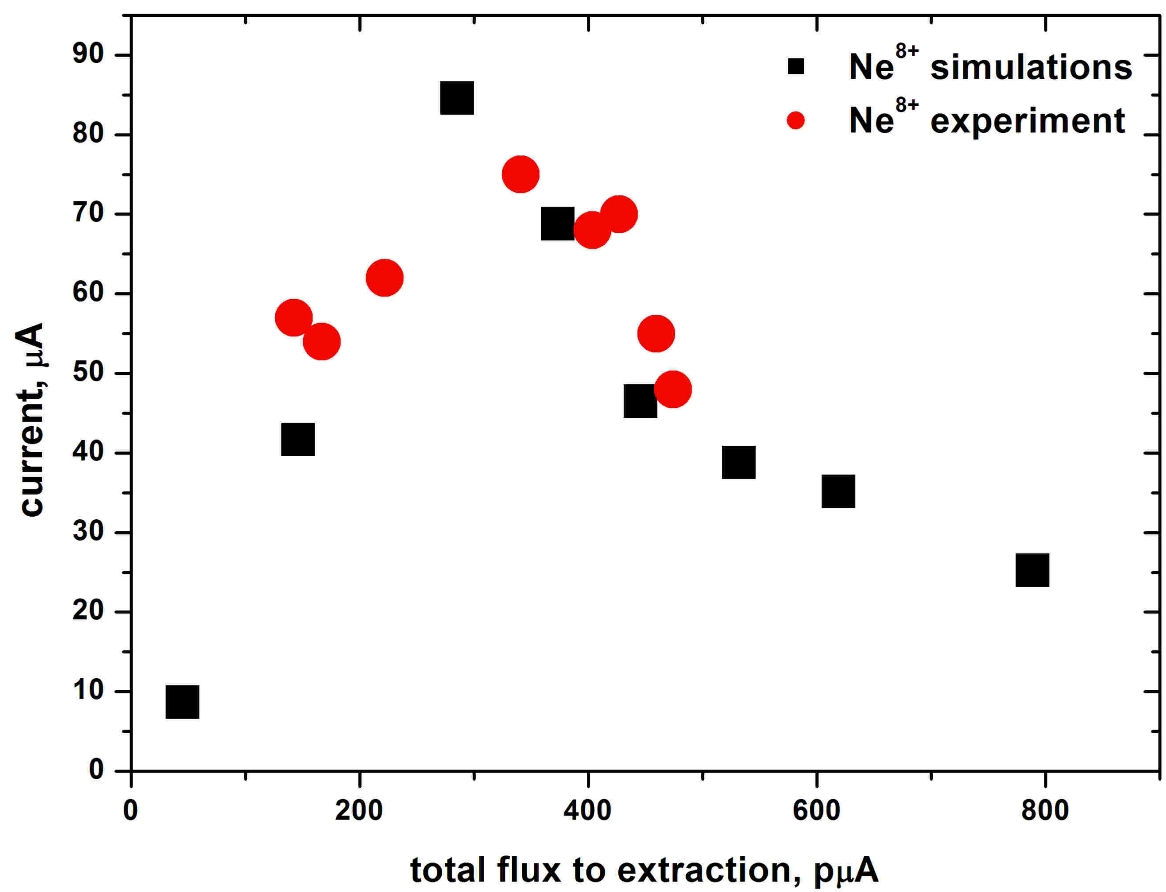
Extracted currents – experiment, different gas flows



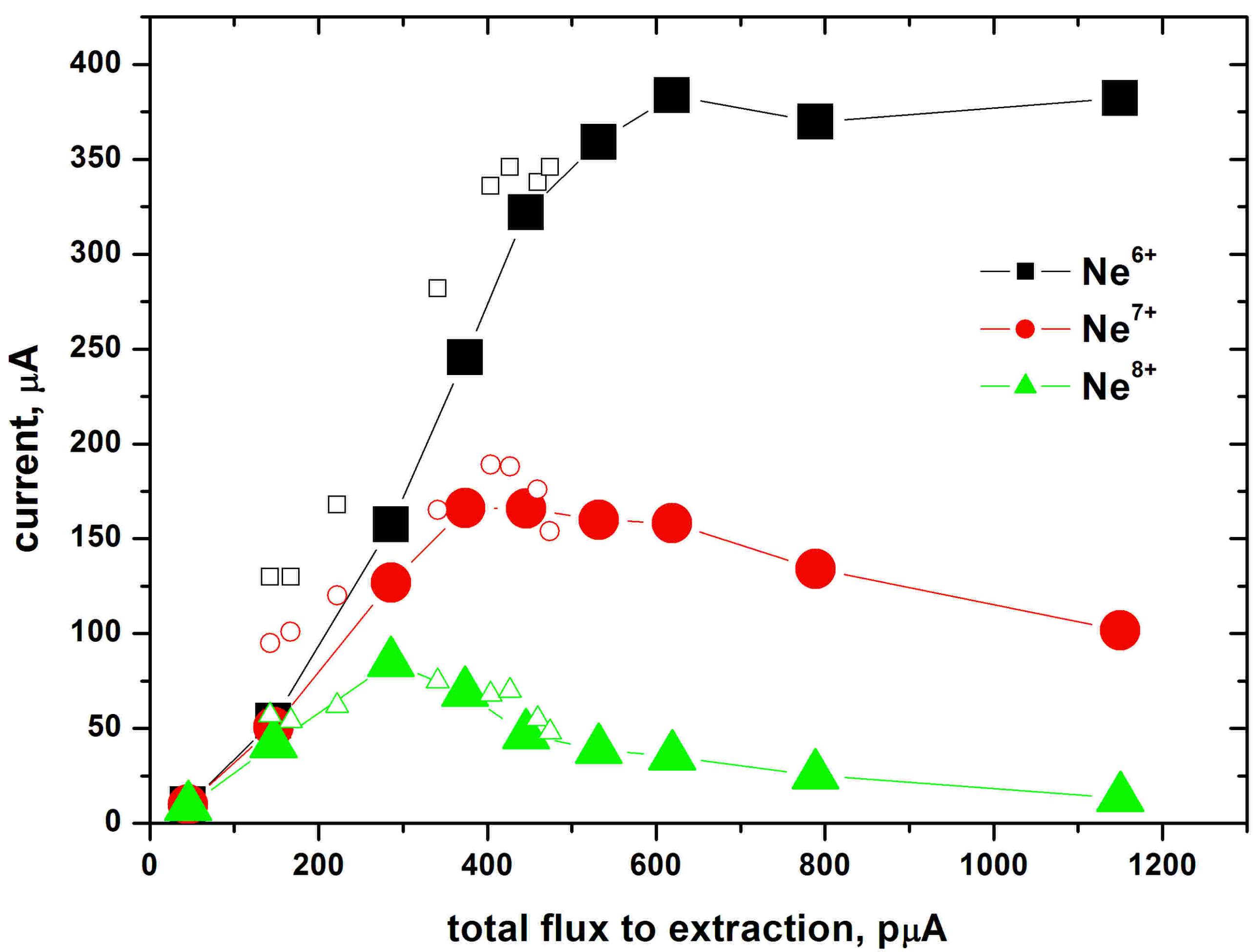
Extracted currents – simulations, different statistical weights of macro-particles



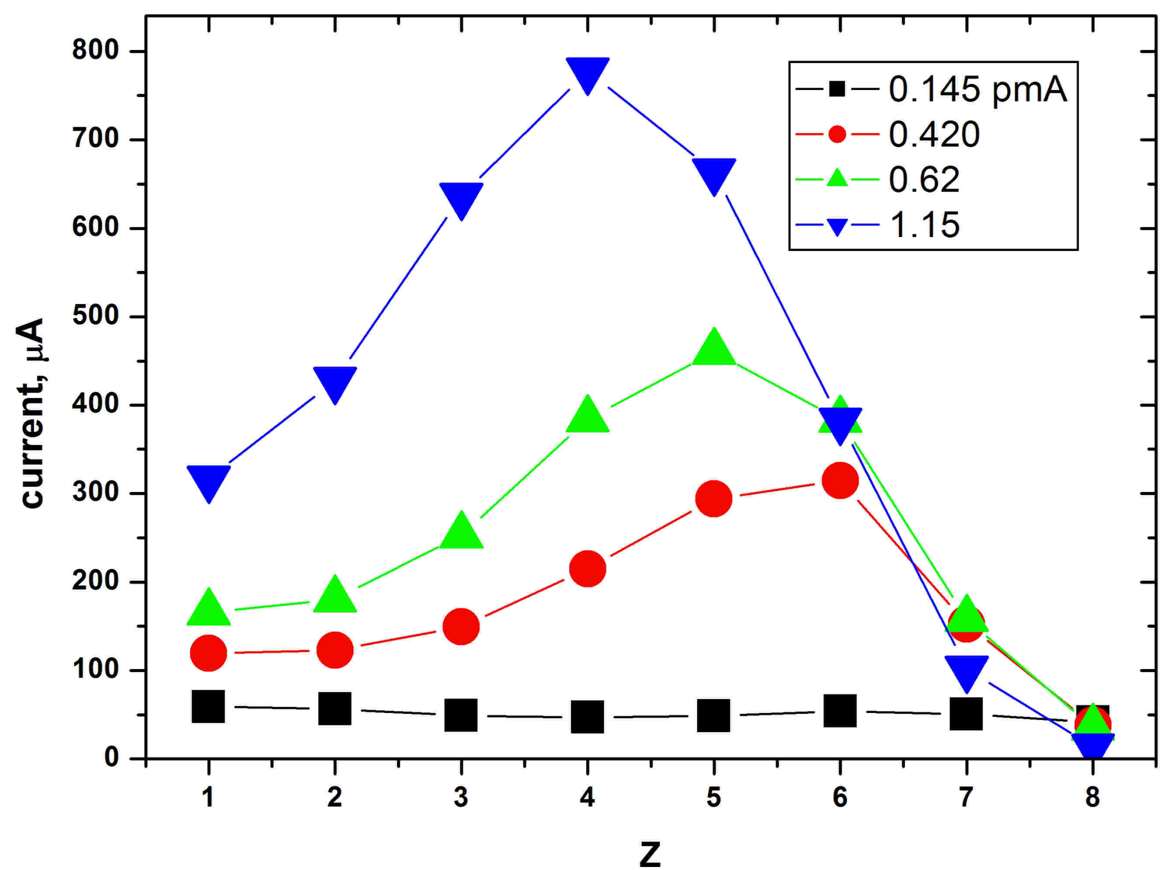
Extracted Ne^{8+} current – experiment and simulations



Extracted currents – experiment and simulations

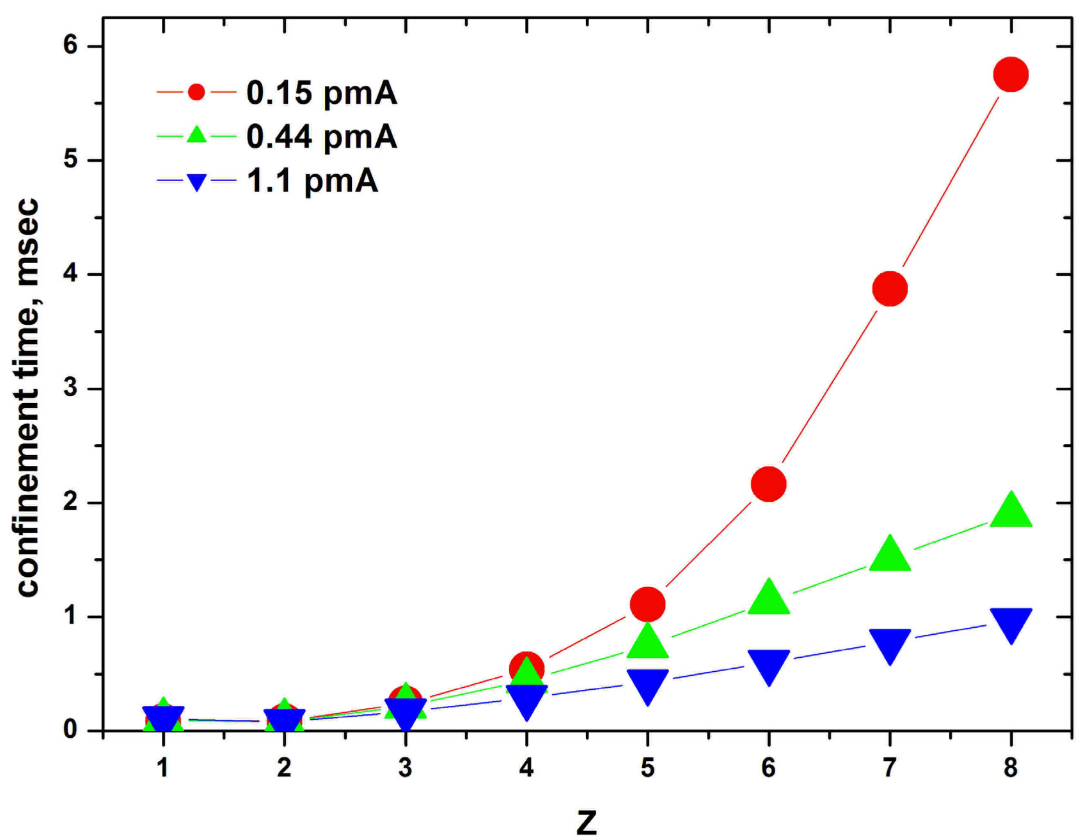


Extracted currents – simulations, different statistical weights of macro-particles



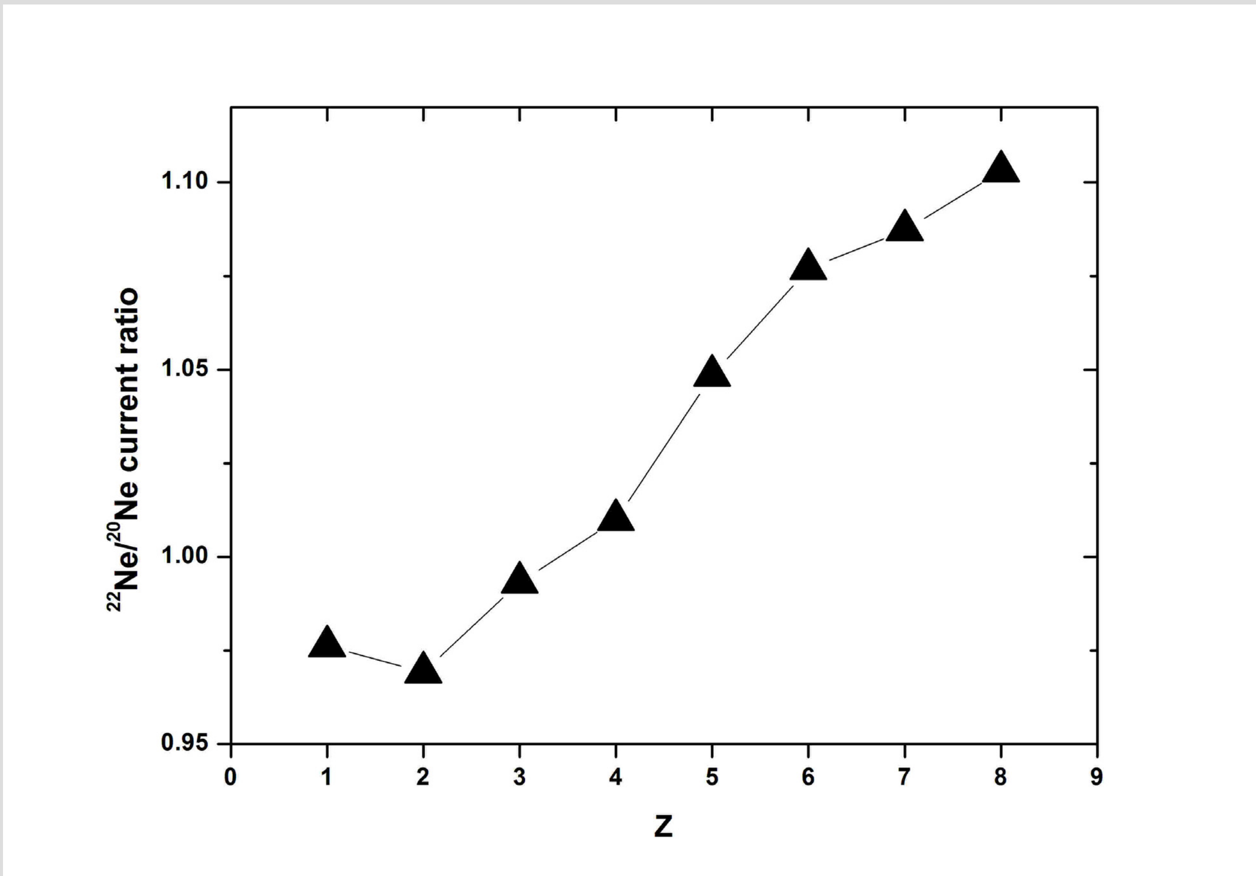
Confinement times of ions

(0→1+); (1+→2+);→….Z+ is extracted
t=0→…………………t=t_c(Z) (confinement time after averaging)



Isotope Anomaly

Mixing ^{20}Ne + ^{22}Ne and demanding that the gas flows of isotopes are the same



Conclusions

-With our 3D PIC-MCC code, we are able to reproduce the main features of ECRIS performance

-Reasons for various effects can be investigated and clarified

-Wall coating

-Afterglow

-Gas mixing

-Isotope anomaly

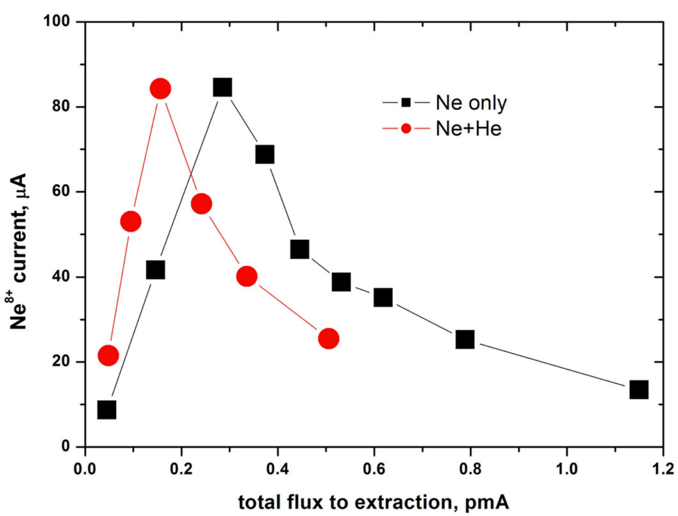
-HCI concentration on axis

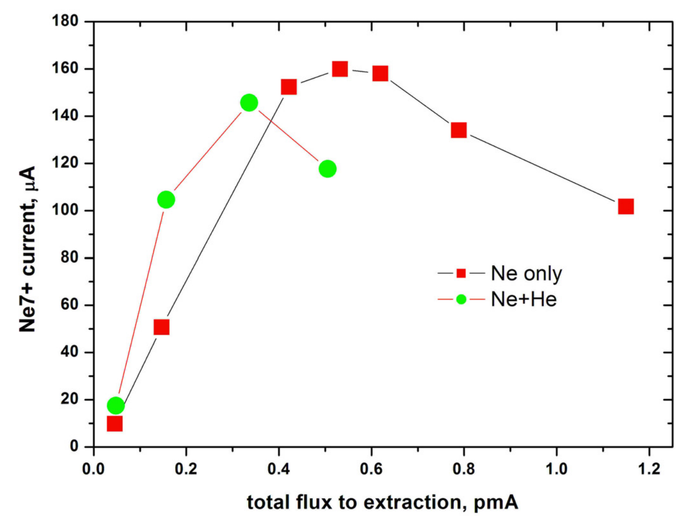
-Frequency tuning and scaling

Thanks!

Gas-Mixing

Mixing He and Ne (1:1) does not result in the increased currents of the highest charge states





Switching the Ne-He ion collisions off