Three-dimensional Simulation of Electrons and Ions in Electron Cyclotron Resonance Ion Sources

H.J. Andrä

Former member of the

Inst. für Kernphysik, Univ. Münster
Wilhelm Klemm Str. 9, D-48149 Münster, Germany

Microwave does heat only electrons

Close to all energy of the plasma is electronic energy

Energy transfer to ions via collisions or ionization is negligible

Electrons thus nearly completely decoupled from ions

except for neutrality and collisions

The spatial and energy distributions of the electrons

do produce and host the neutralizing ions

Actually the ions follow the electrons with inertia

These distributions thus determine the behavior of an ECRIS

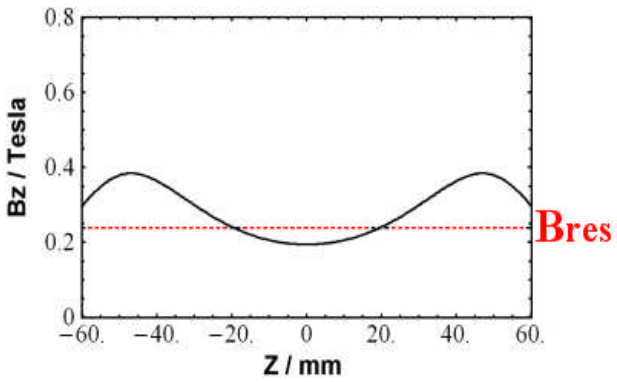
As examples for the simulations three successive ECRIS are chosen

1) A small Standard ECRIS (**SECRIS I**) with permanet magnets and 6.7 GHz

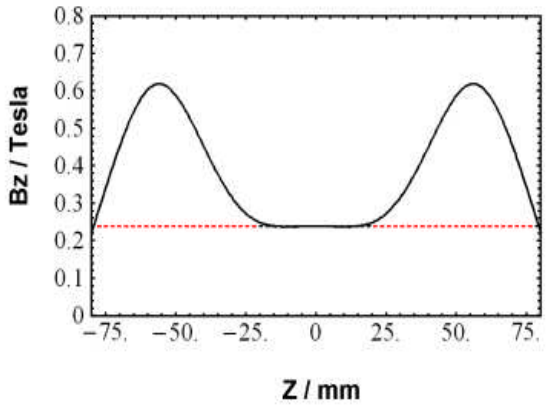
2) A small Plateau ECRIS (**PECRIS III**) with permanet magnets and 6.7 GHz

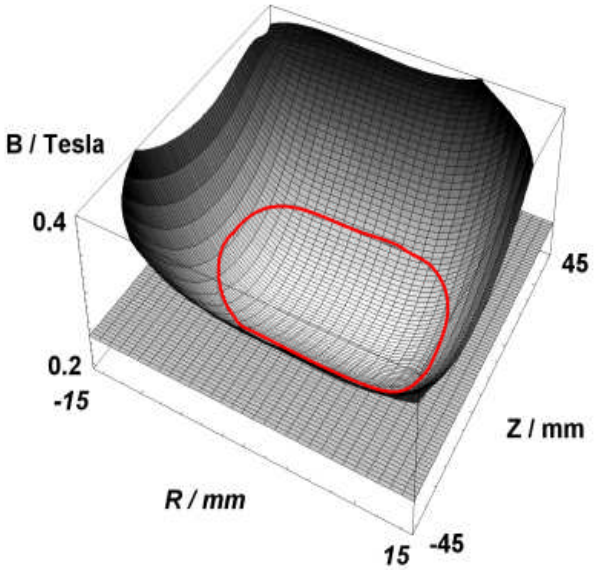
3) A big Plateau ECRIS (**PECRIS V**) with electro-magnets and 16.9 to 18 GHz

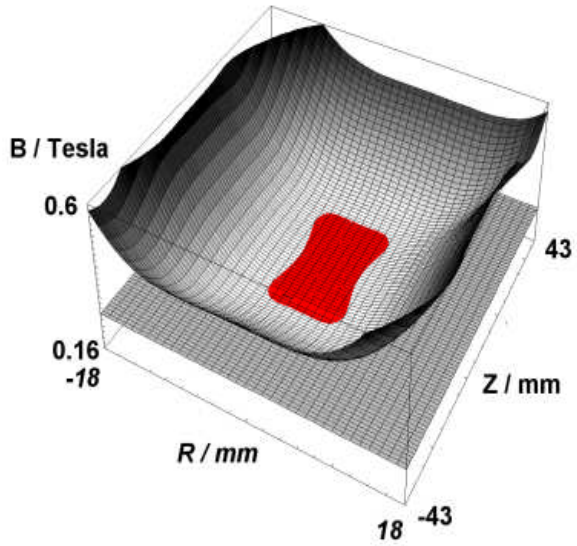
SECRIS I



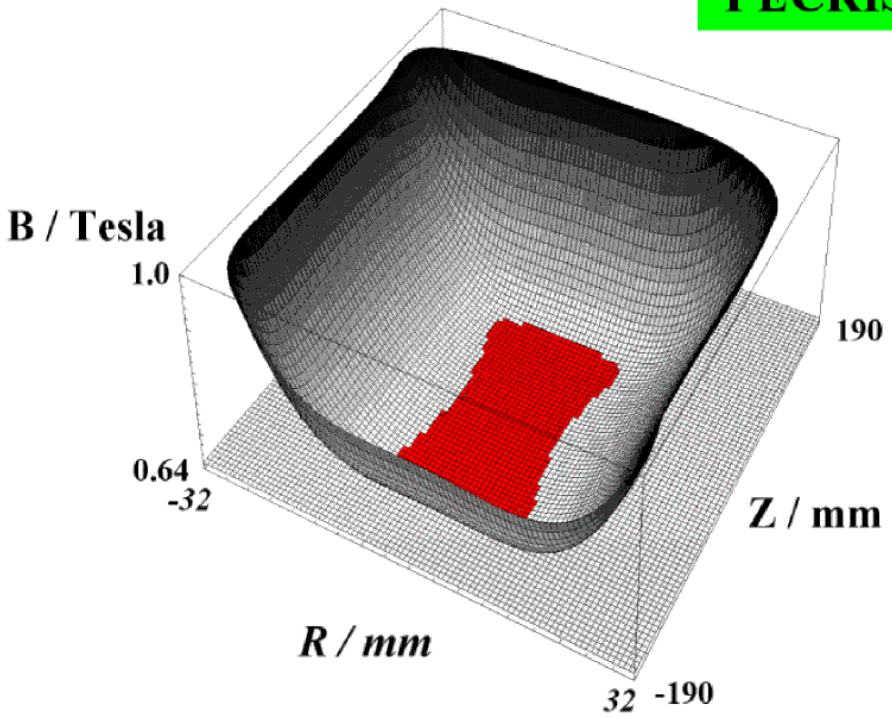
PECRIS III

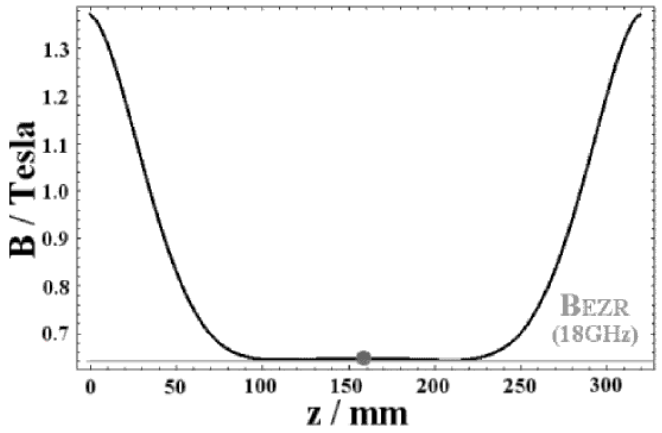






PECRIS V

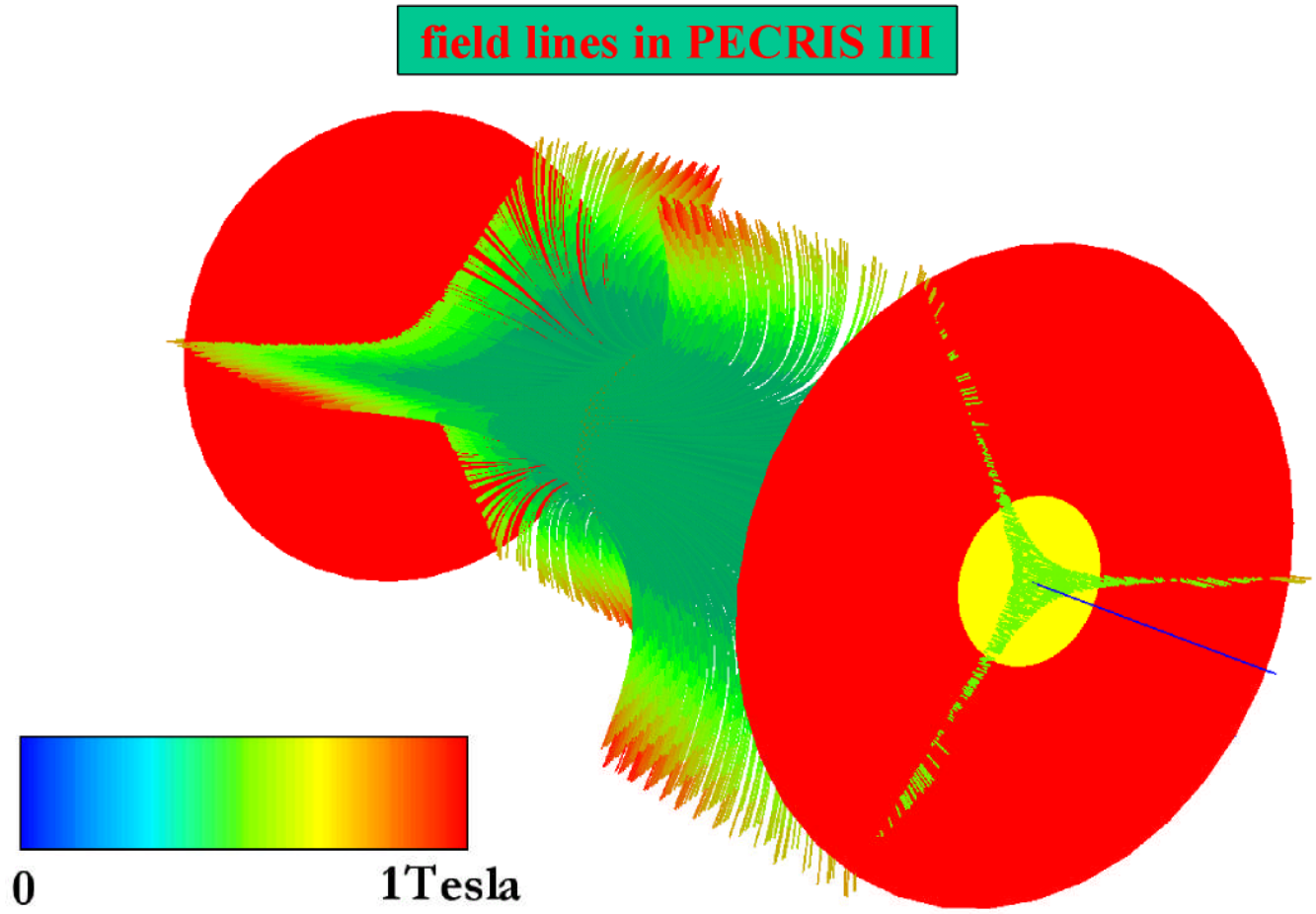




Although the magnetic structure of the troughs is very simple

the real magnetic field vectors are extremely complicated

Magnetic field lines starting from a cylinder in the centre of PECRIS III



A very complex magnetic structure !

Former attempts of descritpion of the plasma:

Early Particle in Cell (PIC) codes limited to azimuthal average

Latest PIC codes still suffering from serious approximations and coarse grid

Focker-Planck code assumes thermal distributions and generalized heating term

They are thus all approximations with

too much attention to electron-ion interaction and collective phenomena

despite the fact that

electrons are decoupled from ions, except for neutralization and collisions

Therefore alternative approximation:

Description of electrons in ECRIS including collisions

Use these results for further refinement like diamagnetism or ion-behavior

Electron trajectory calculations were first used by Jongen

Biri continued with impressive recent results

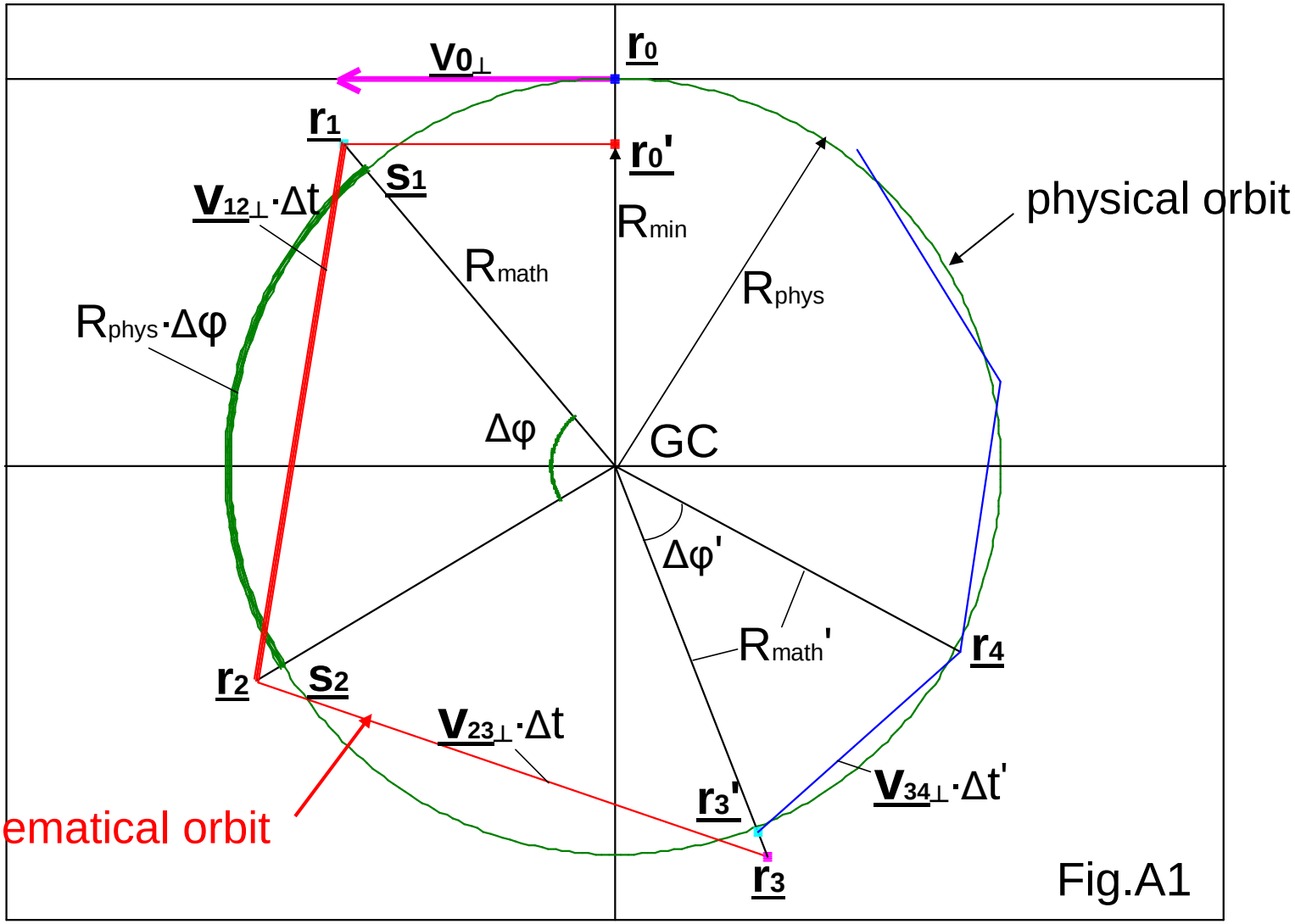
Both use Runge-Kutta - not well adapted to rotational motion

We develop since 1993 a code with the very efficient

Boris-algorithm which takes advantage of rotational motion

With respect to our former results several errors have been eliminated

Boris-algorithm: The circular physical orbit is mathematically represented by a series of red secants. The secant from **r1** to **r2** has equal length as the arc from **s1** to **s2.** At **r2** the new secant is found by rotation by Δφ(**B**(**r2**)) around **B**(**r2**). This algorithm requires precautions for the start (shift from **r0** to **r0'**) and for a change of Δt (shift from **r3** to **r3'**).



For a collision after step from **r2** to **r3**, **r3** has to be shifted to **r0c** on the physical orbit where the collision really takes place. **v23‘** has to calculated which is changed to **v0c** by the collision. The start on the new orbit requires the shift from **r0c** to **r0c‘** And then half a time step on the blue secant from **r0c‘** to **r1c.**

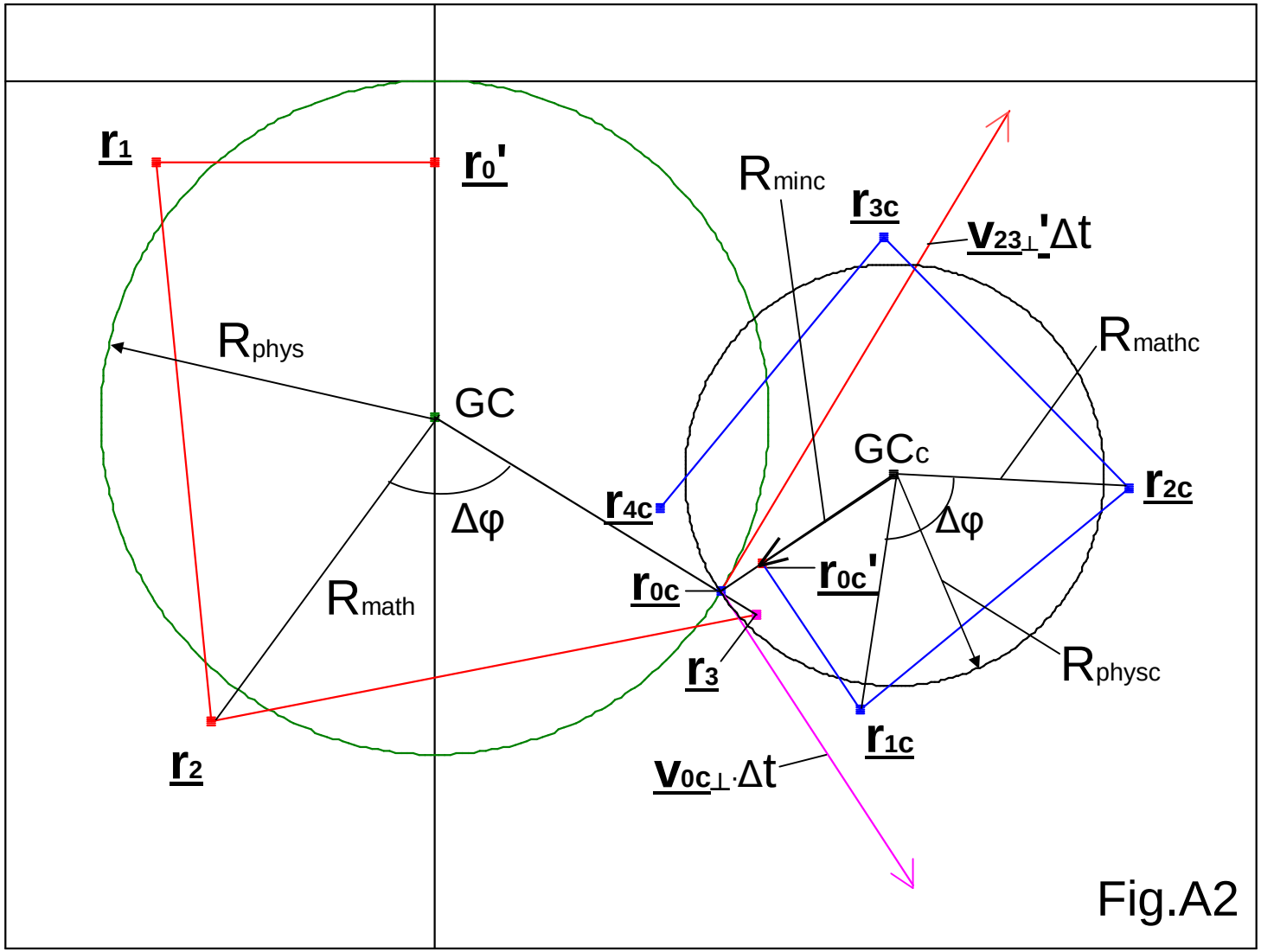


Fig.A2

The advantage of this algorithm is the perfect description of the circular cyclotron orbits in a constant magnetic field when the electric field **E** = 0.

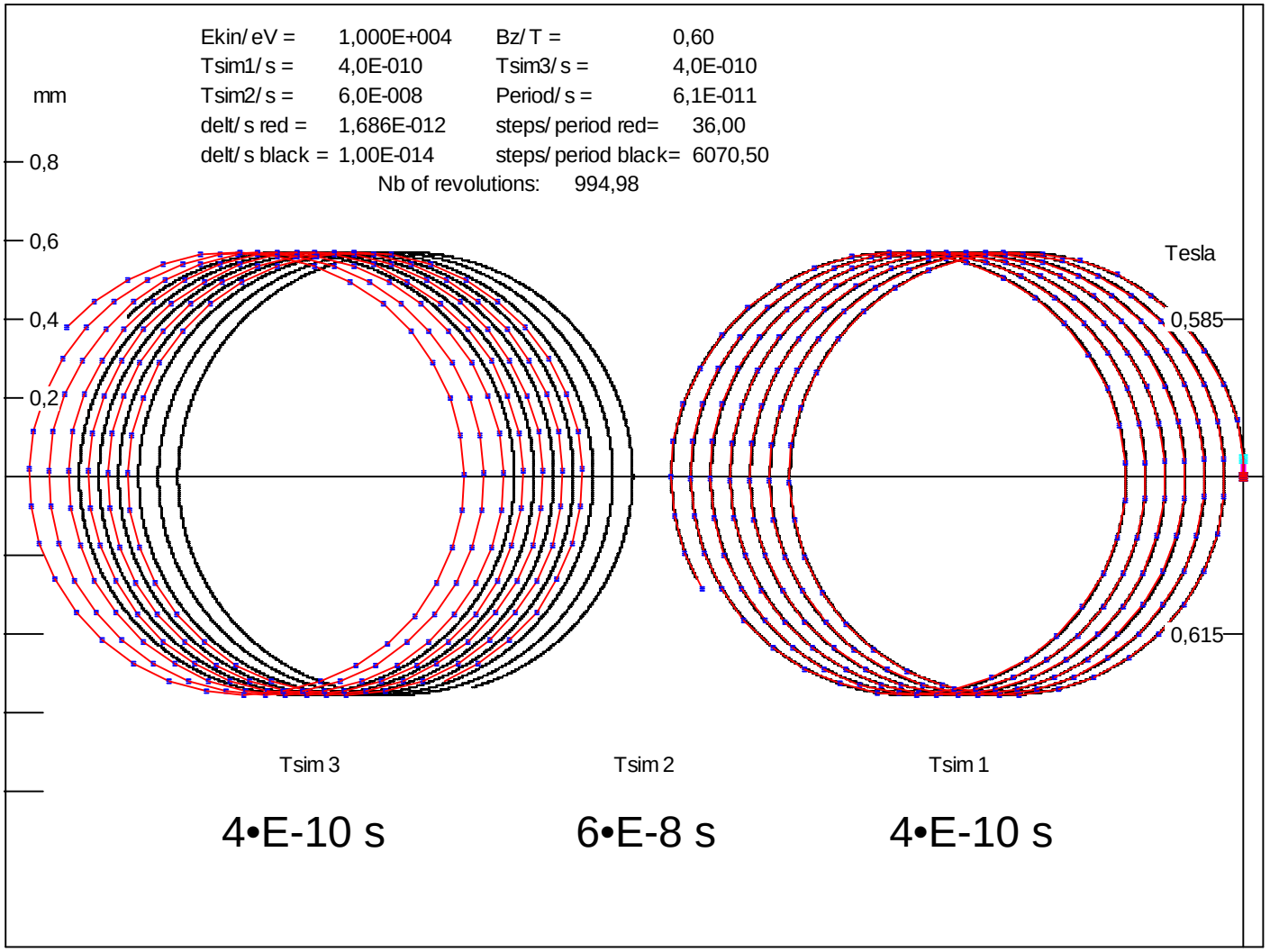
Only three or more time-steps per revolution are required for the correct mathematical reproduction of the orbit.

This high quality is maintained by the symmetric incorporation of static or time dependent electric fields and of electric or magnetic field gradients.

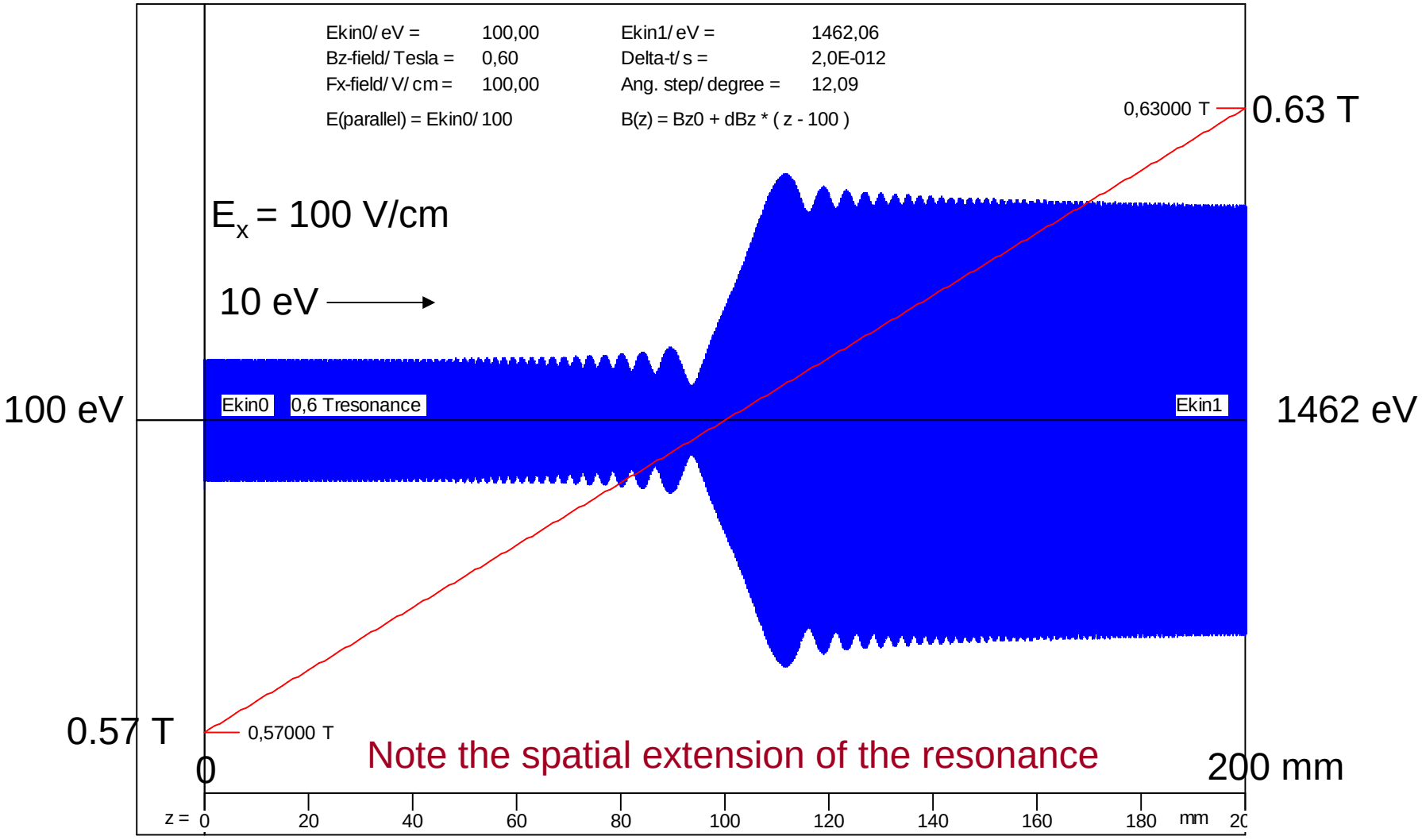
The number of time-steps per revolution is then determined by the correct description of these fields along the orbit of one revolution.

The algorithm thus fully takes into account all drift motions and the ECR-interaction

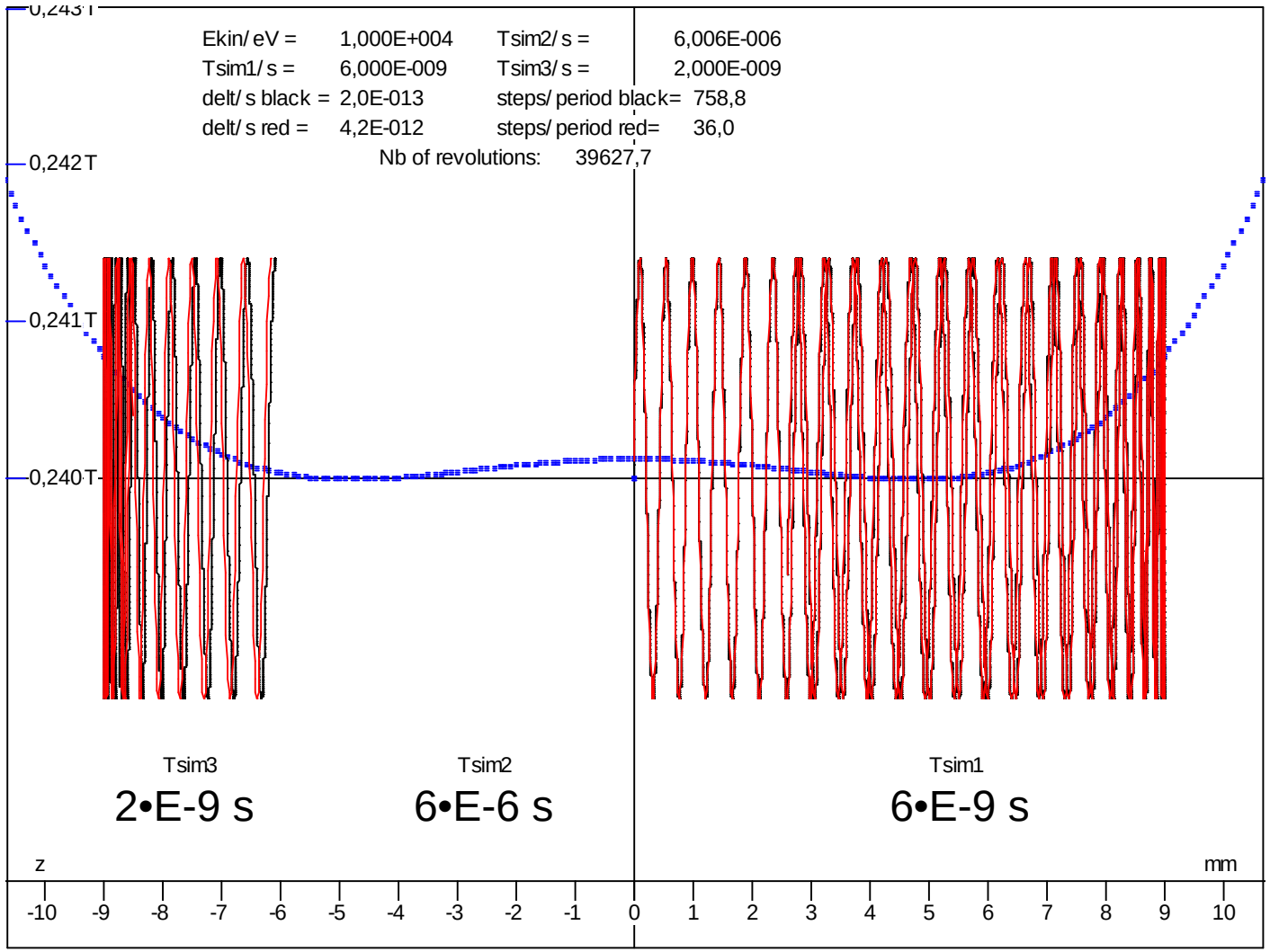
A magnetic field gradient of 0.04 T across an orbit
at 10 keV at 0.6 T requires 36 time-steps.
An orbital shift of only 10% of its diameter occurs after
1000 revolutions with respect to an “exact” calculation
with 6070 time-steps per revolution.



Depending on the phase, the description of acceleration or deceleration of the electrons is well described. Here an electron passes through a spatial region with resonance condition with 30 time steps per revolution. The gain of energy to 1462 eV would only be increased to 1492 eV with more than 600 time-steps per revolution.



An electron with 10 keV bouncing back and forth on axis in the magnetic mirror field of PECRIS III exhibits with 36 time-steps per revolution a near perfect reproduction of the trajectory after 39600 revolutions or 940 bounces compared to an “exact” calculation.



Collisions

For realistic results, elastic collisions have to be included

since they are the most important perturbations of the trajectories.

The presence of electrons, and ions with different

masses and charges as collision partners requires drastic

approximations in order to make the calculations feasible.

All collision partners can be treated on the same footing

if a **policy of the worst case** is adopted.

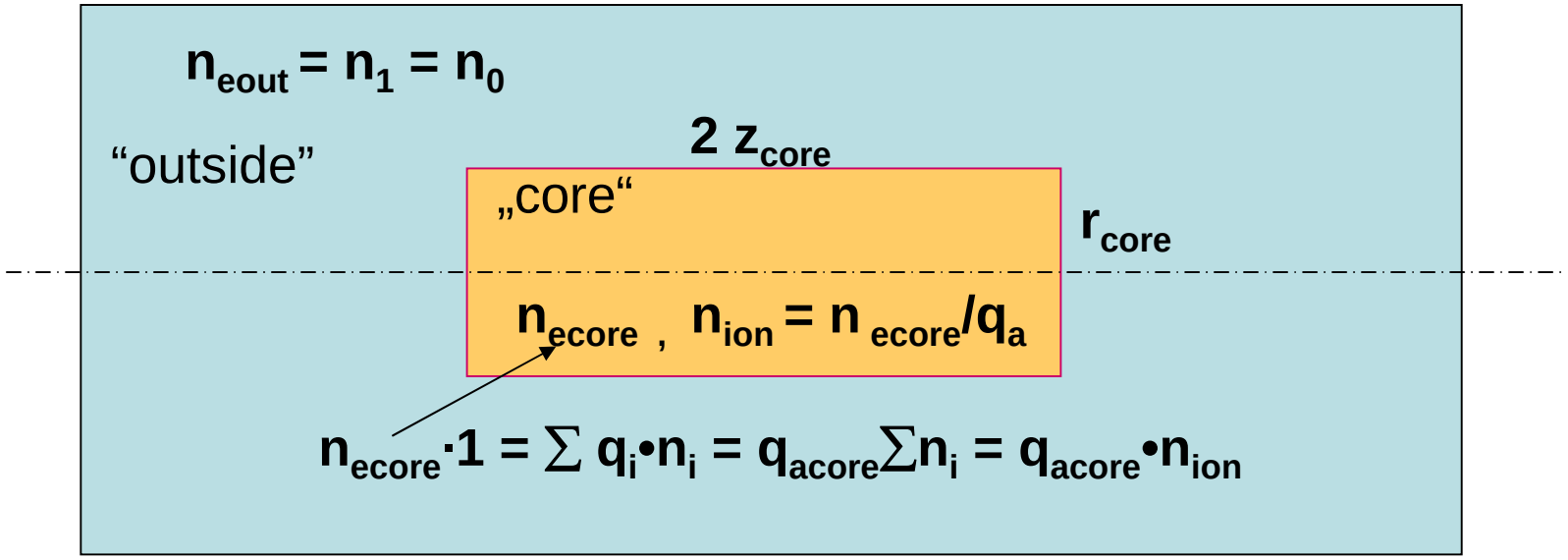
For the simplification, the plasma chamber is divided into a plasma core with r_{core} and $\pm z_{core}$ and the rest “outside” the core.

An electron density

of $\mathbf{n_{ecore} < n_{crit}}$ exists in the core and of $\mathbf{n_{eout} \approx n_{ecore}/\alpha}$ outside.

$\mathbf{n_{ecore}}$ is compensated by positive multi charged ions

with average charge $\mathbf{q_{acore}}$ in the core and by singly charged ions outside.



n_i = density of charge state q_i

Scattering off other electrons with equal mass tranfers energy and momentum to the targets. For the ensemble, however, energy and momentum are conserved.

Approximation : electrons are scattered off infinitely heavy targets at rest.

It produces zero energy loss and twice the scattering angle in the laboratory frame compared to a collision off an electron with equal mass.

It is this approximation of the worst case which is retained

Ions are “infinitely” heavy targets for electron-ion collisions

Electrons and ions can thus be treated on the same footing if

$$\langle q_{cion} \rangle = \sqrt{\left[\sum n_i q_i^2 / \sum n_i \right]}$$

Since σ(Rutherford) ~ q^2

In the core :

Density of targets: $n_{ccore} = n_{ecore} \left(1 + 1/q_a \right)$

$$q_{ccore} = \sqrt{\left[(n_{ecore} \cdot 1^2 + (n_{ecore}/q_a) \cdot \langle q_{cion} \rangle^2) / (n_{ecore} + n_{ecore}/q_a) \right]}$$

Outside :

$n_{cout} = 2 \cdot n_{eout}$; $q_{cout} = 1$

The mean free path of an electron before its next collision

depends on the local density and actual energy

$$\lambda(\underline{\mathbf{r}}, E) = 1/\, n_c(\underline{\mathbf{r}}) \bullet \sigma_{tot}(\underline{\mathbf{r}}, E)$$

Beginning of trajectories

Electrons take off with E_{kin0}=20 eV in arbitrary directions

Their trajectories are calculated during 200 cycles of the µW-field

As soon as electron gains 5 eV it is accepted for simulation

and its position is registered as start position

The start positions are thus equivalent to regions of intense ECRH

or to regions of highest Electron Density

All trajectories end up at walls

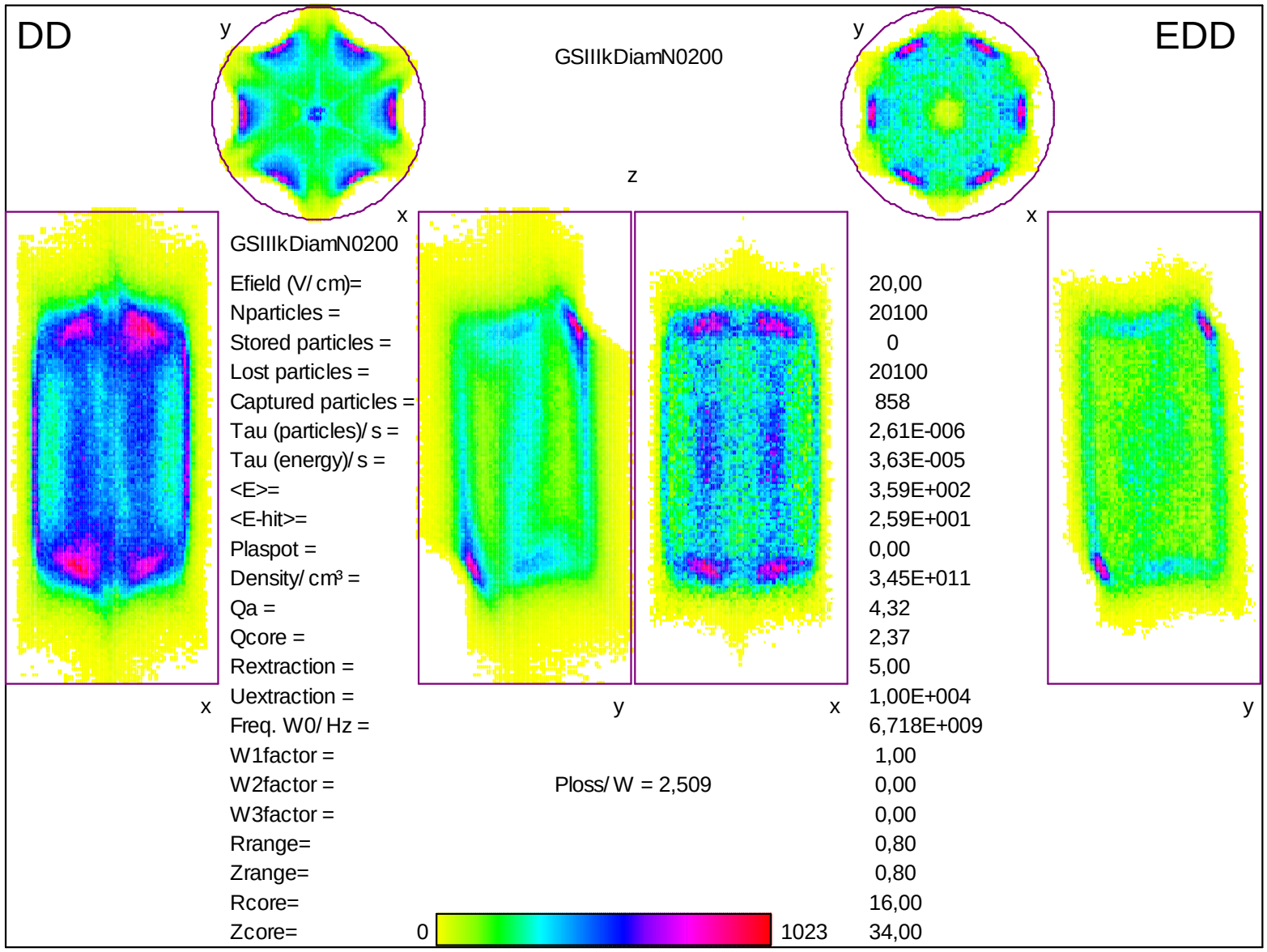
A proper analysis of these trajectories then yields

Electron Density Distribution	DD
Electrons Energy Density Distribution	EDD
Electron Energy Spectrum	ES
Electron Velocity Distribution	VS

First application in SECRIS I with about 30 W of µW

High density 3.45E11 cm^{-3} reduces <tau> = 2.6 µs and <E> = 359 eV

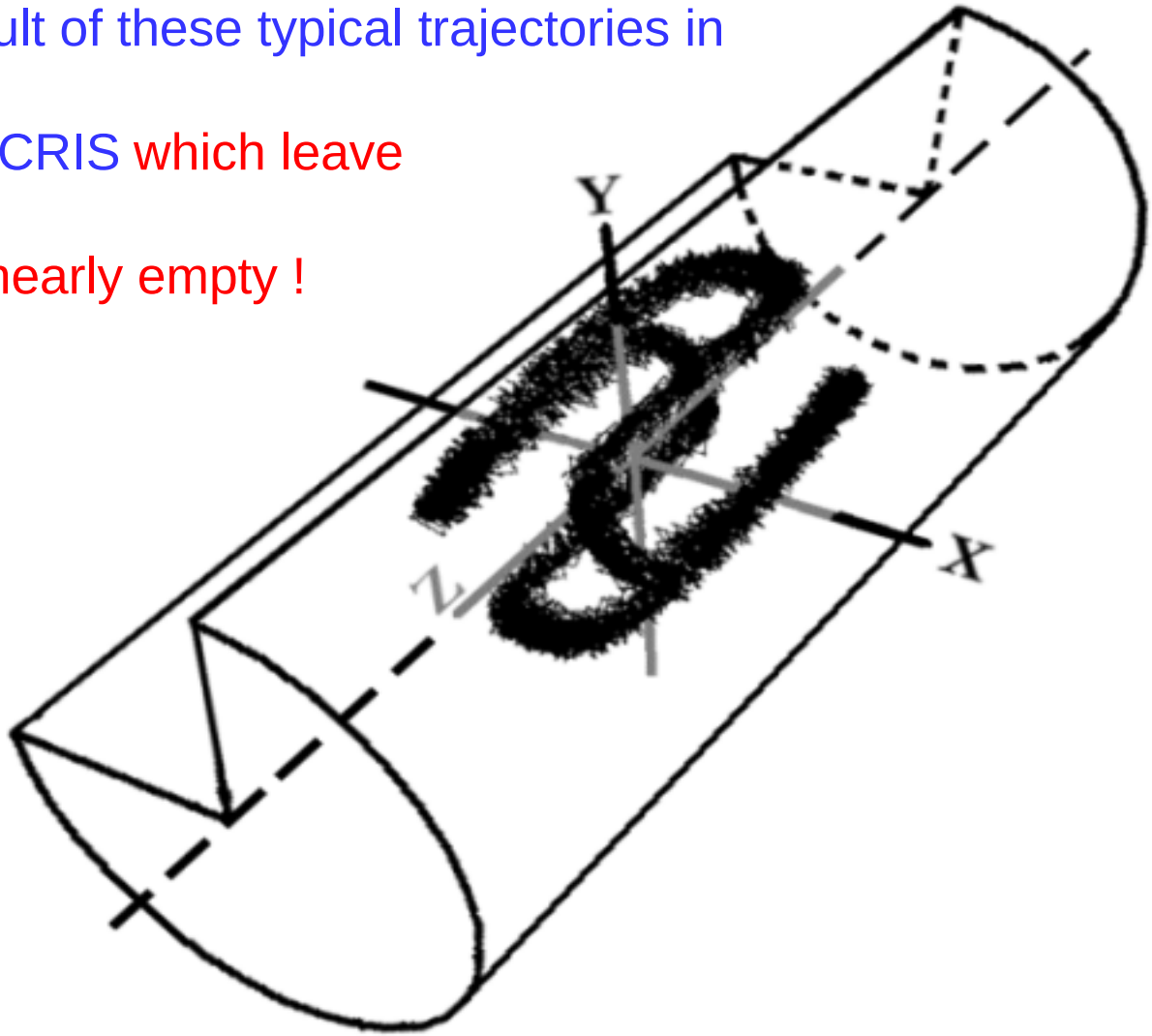
Bad performance !



It is the result of these typical trajectories in

Standard ECRIS which leave

the centre nearly empty !

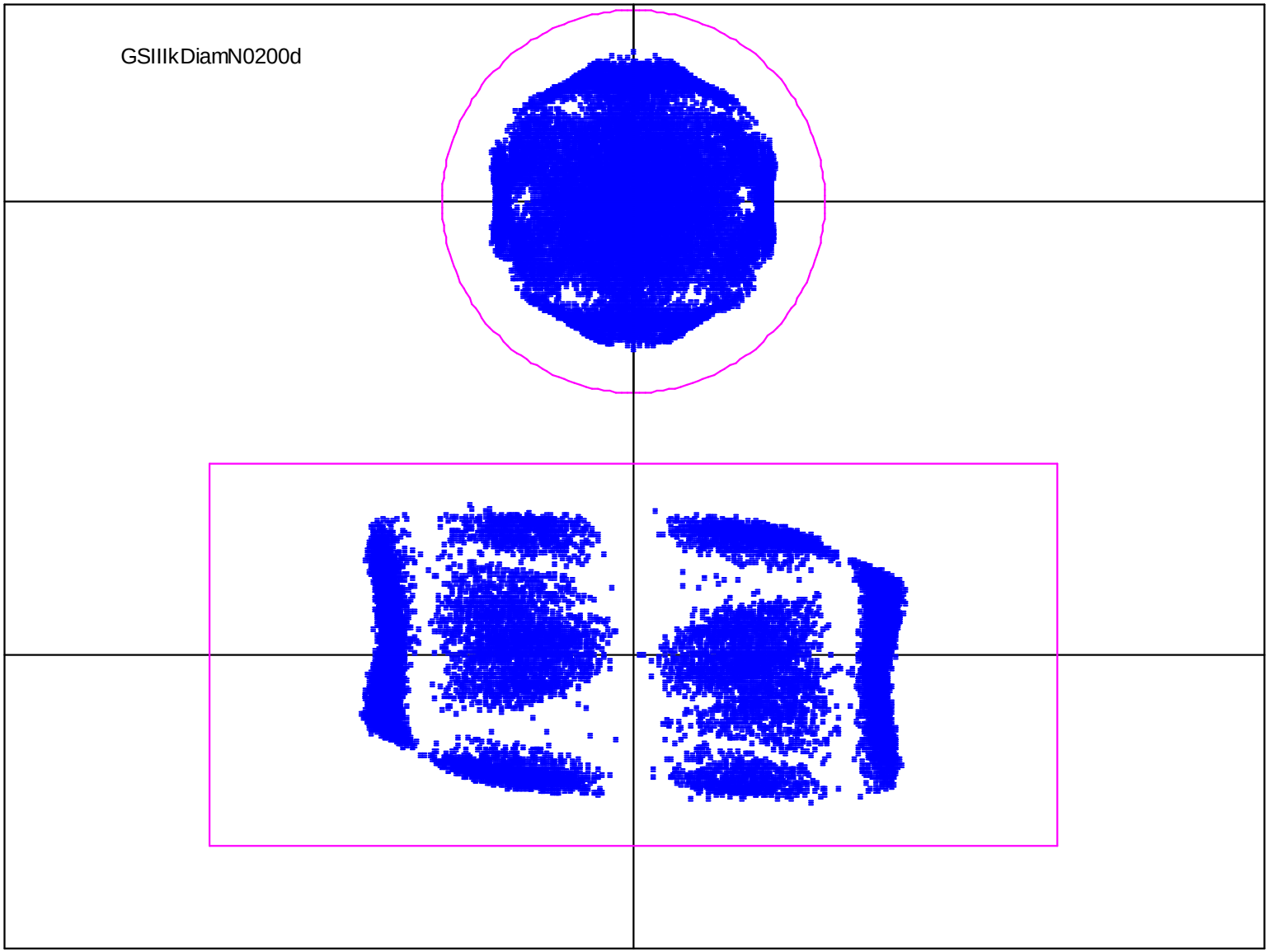


Typical trajectory wound in loops

SECRIS I

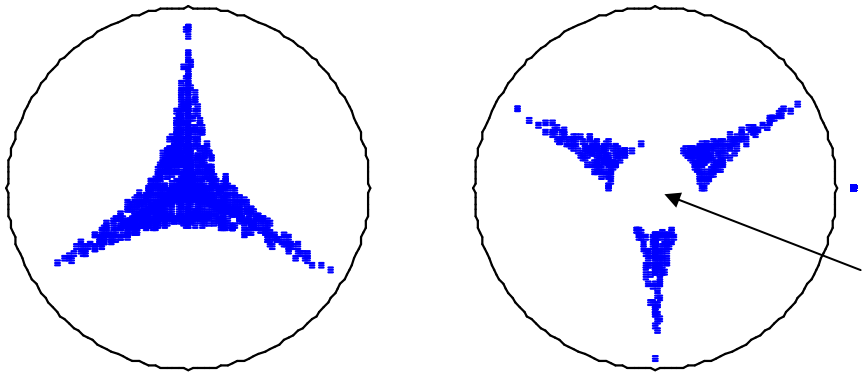
The pattern of start positions of electrons accepted for simulation

reproduces the DD, i.e. where electrons are produced !



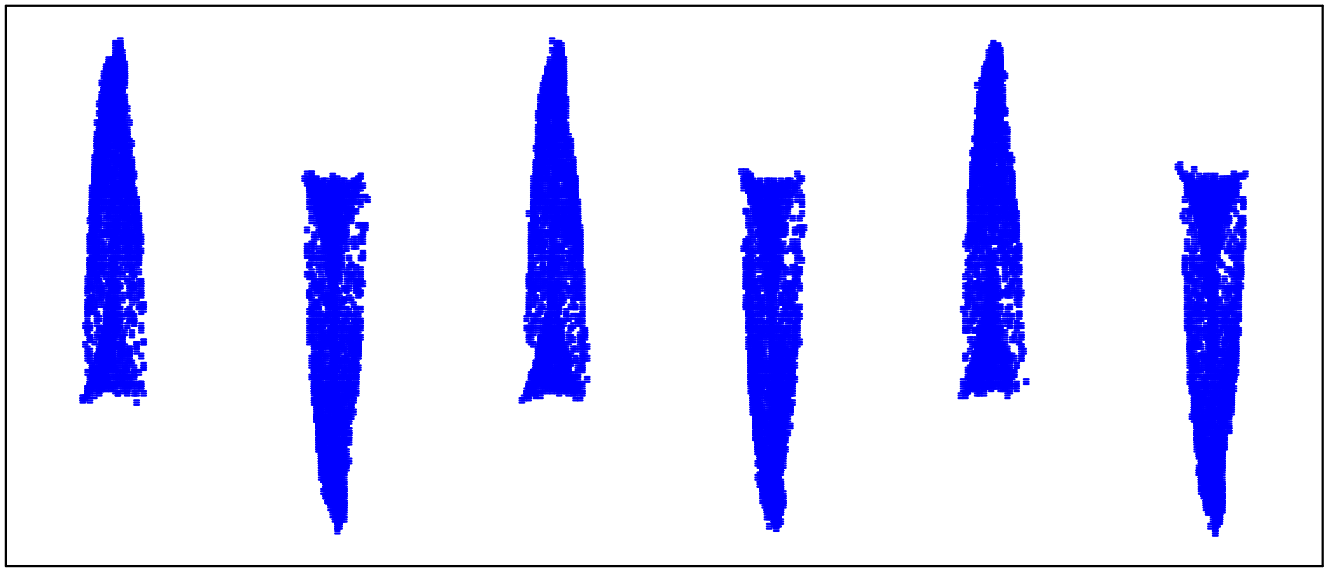
The broad impact patterns are due to the

large radial extend of the DD and EDD



GSIIIkDiamN0200a

reflection of electrons on the potential of the extraction

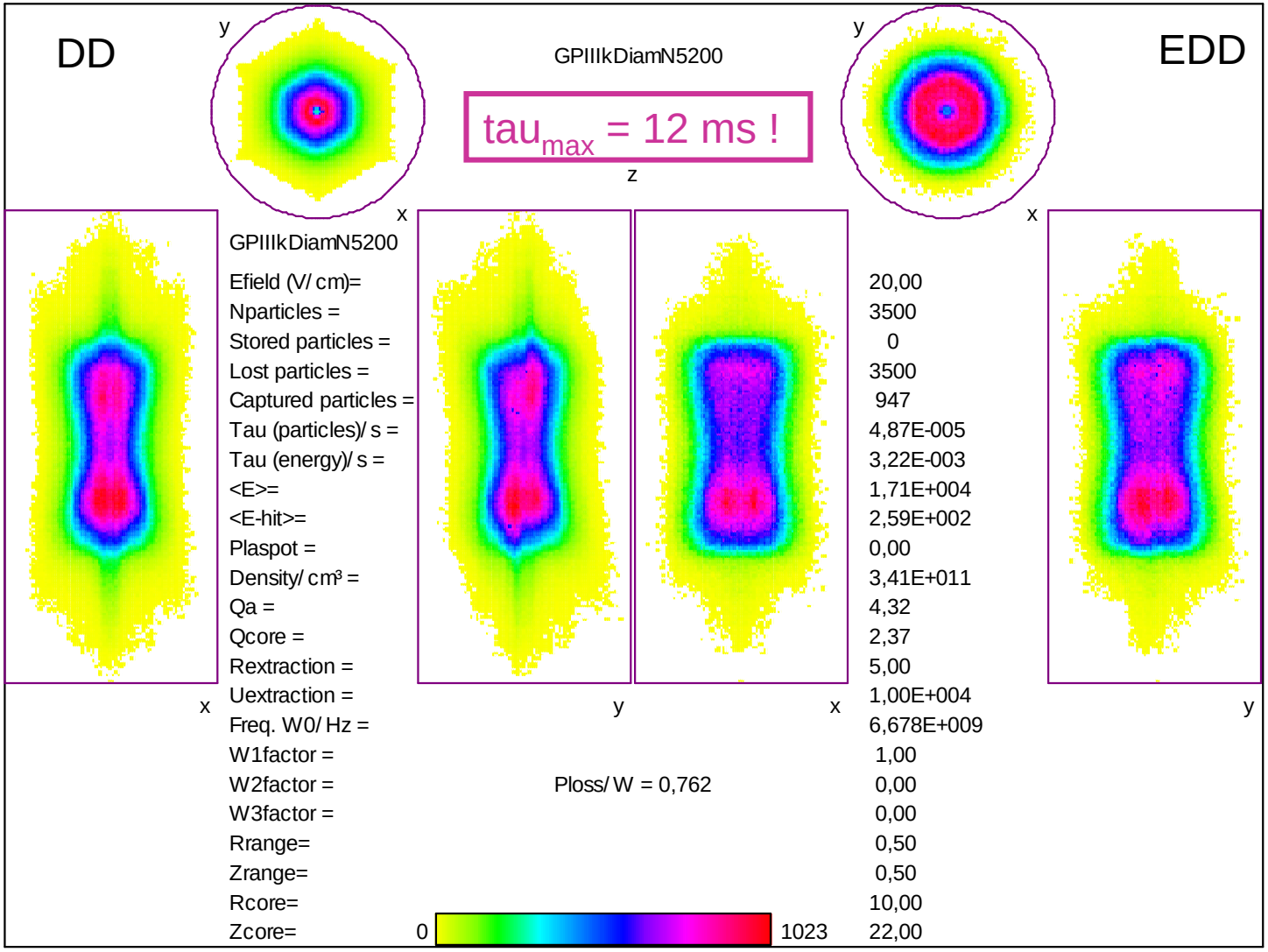


wall of the rolled out cylinder

PECRIS III is much better source. At only 30 W in a mono-mode cavity its heating efficiency is impressive:

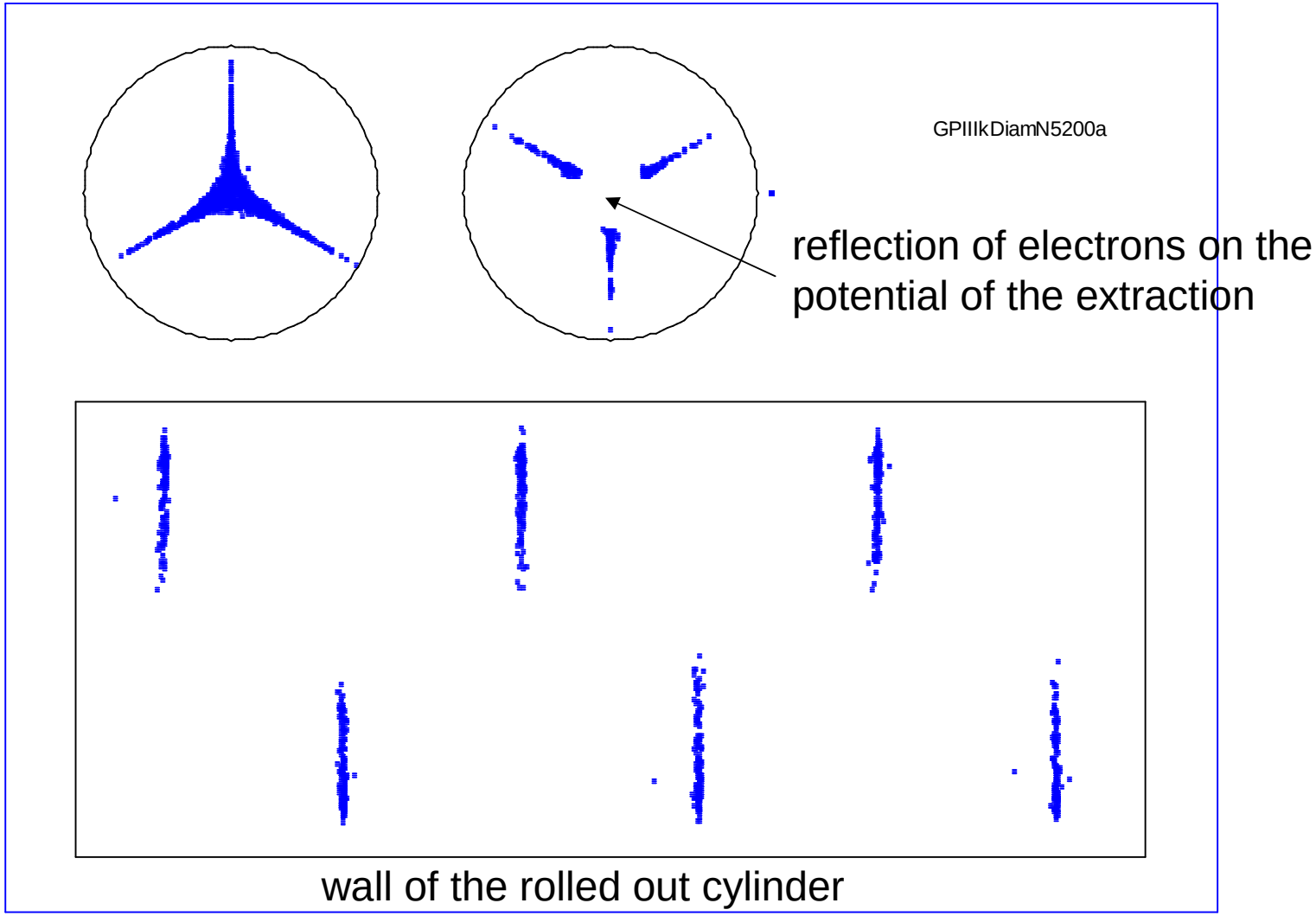
Despte high density 3.45E11 cm^{-3} good <tau> = 48.7 µs and <E> = 17.1 keV !

DD and EDD concentrated on the core in the centre

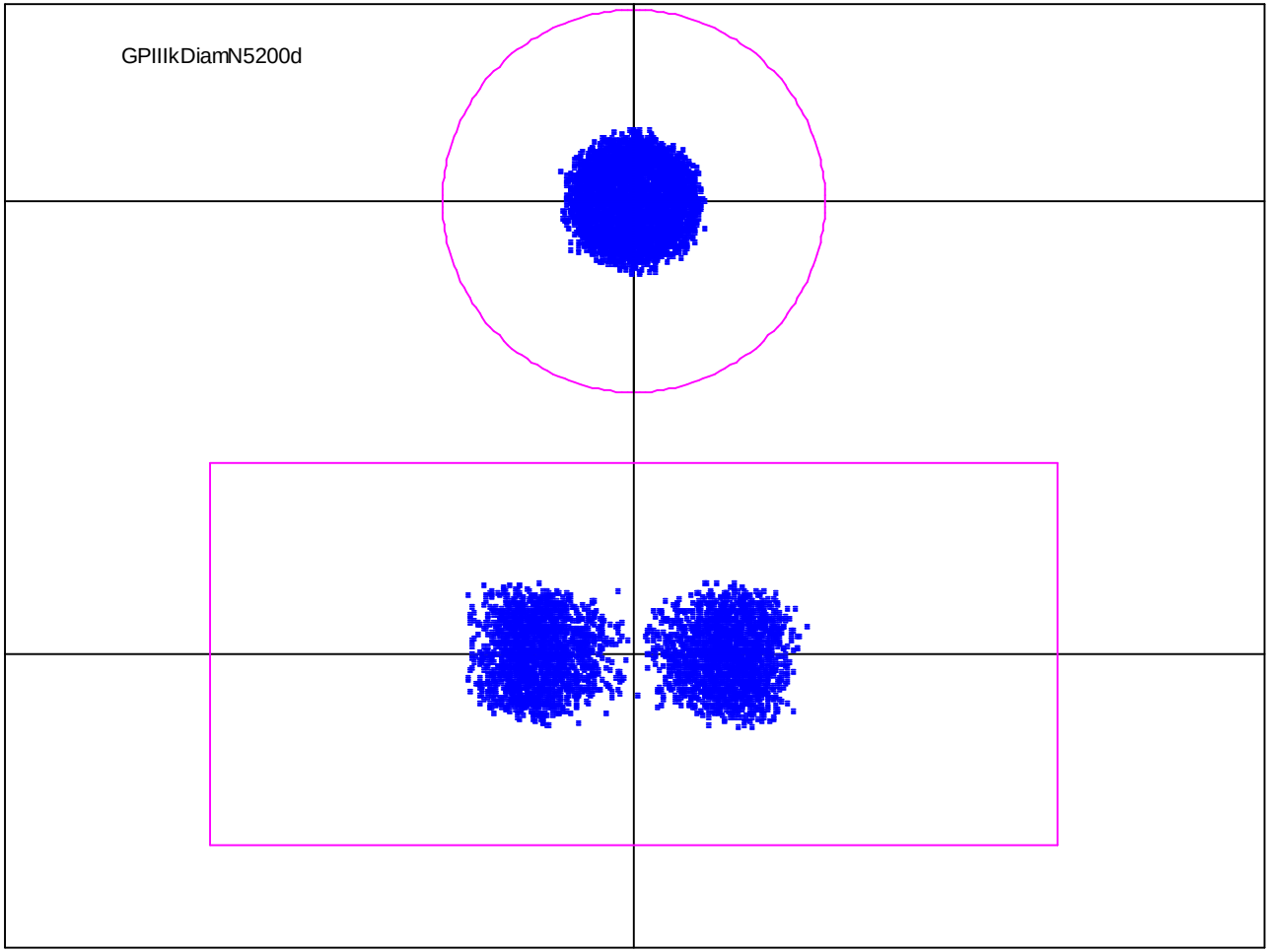


Since the DD and EDD form a well defined plasma core in the centre

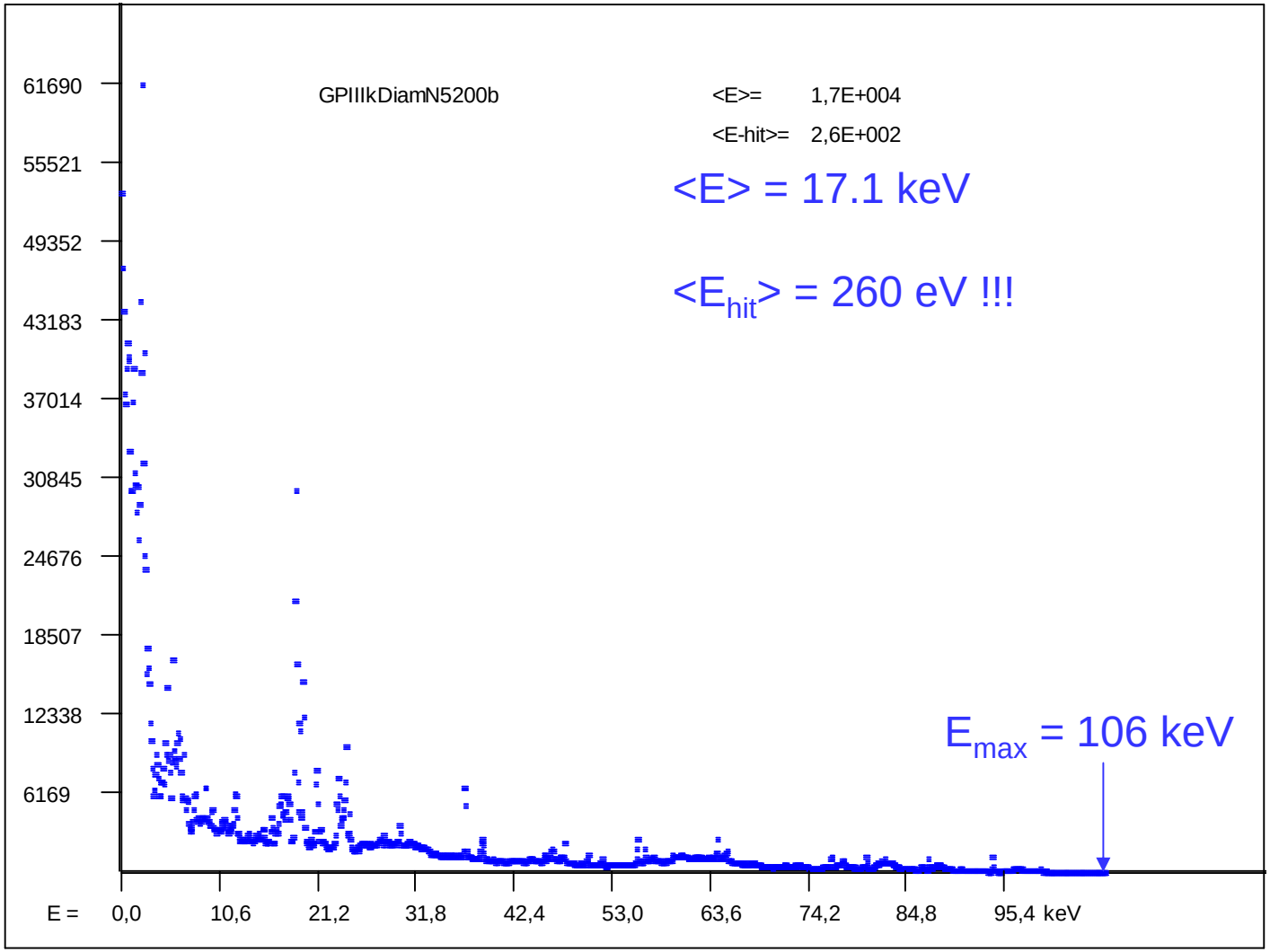
Escaping electrons and ions form a very sharp impact pattern



The electrons are concentrated on the core with further concentration near the ends of the dumb-bell shaped DD.
This is the region with strongest ECR-interaction.
It shows up in the starting positions of the electrons for simulation



The electron energy density (EDD) extends to a slightly greater diameter than the density (DD).
This is due to high energy electrons in the spectrum (ES) which relativistically climb up the magnetic walls.



$B_{res} = B_{res0} \bullet (1+E_{kin}/m_0c^2)$

It is often argued that these high energies are useless for the ionization towards higher q .
But there are about as many electrons from 0 to 4 keV for highly efficient ionization as there are in the high energy tail. The latter form a very stable negative cloud as host for ions.

A high rate of highly charged ion (HCI)-production can therefore be

assumed in this dumb-bell-shaped volume

It ends, however, at a distance of about 23 mm from the extraction hole.

The HCI, although probably abundantly existing in the dumb-bell,

may thus be difficult to extract from PECRIS III

Actually it was necessary to shift the whole magnetic structure and

consequently also the whole DD by 10 mm towards the extraction hole

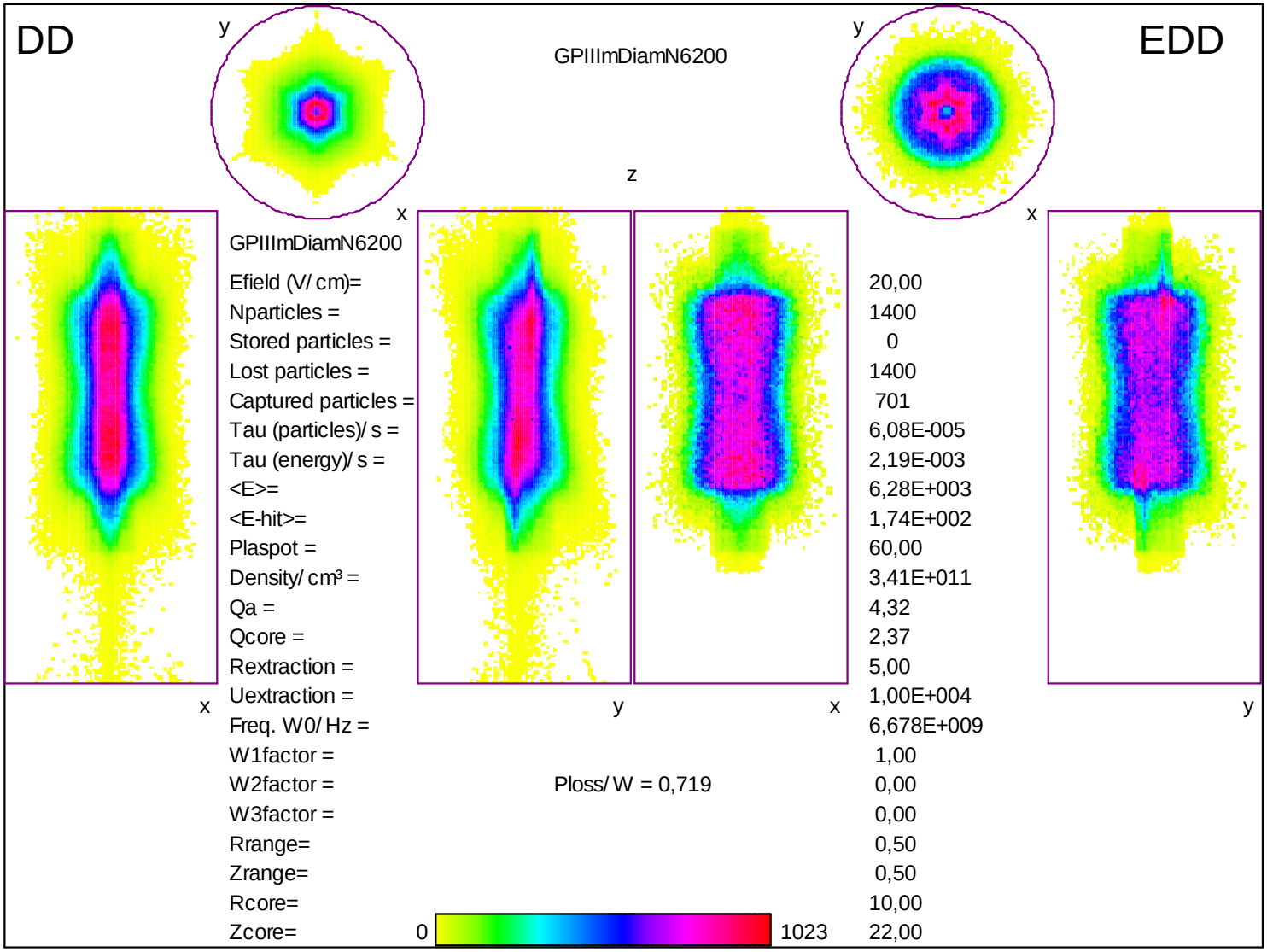
in order to obtain the very satisfactory results of HCI-currents

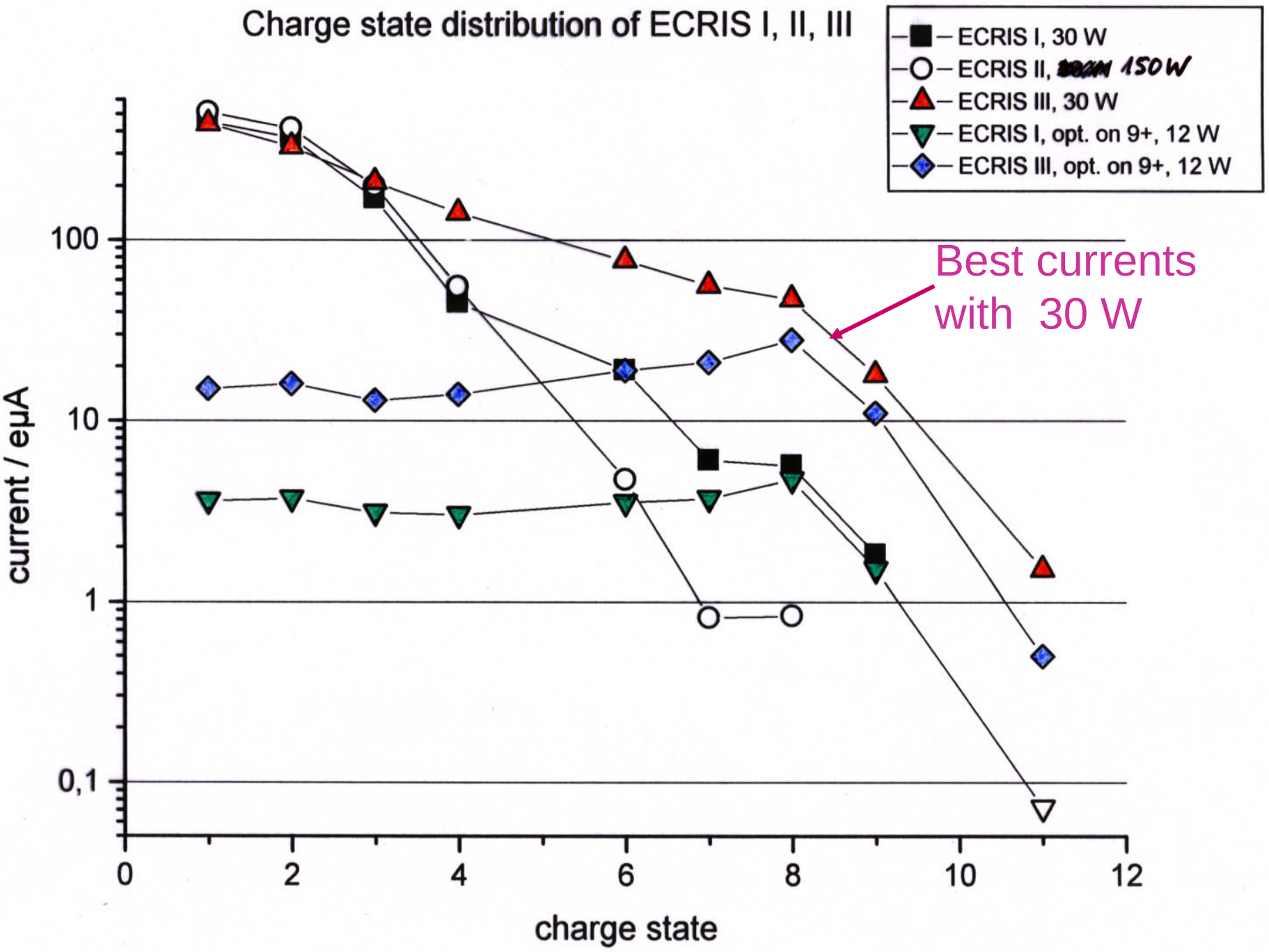
These HCI are extracted with an energy dispersion of about 1eV per charge.

PECRIS III shifted by 10 mm

Still good <tau> = 60.8 µs and <E> = 6.3 keV !

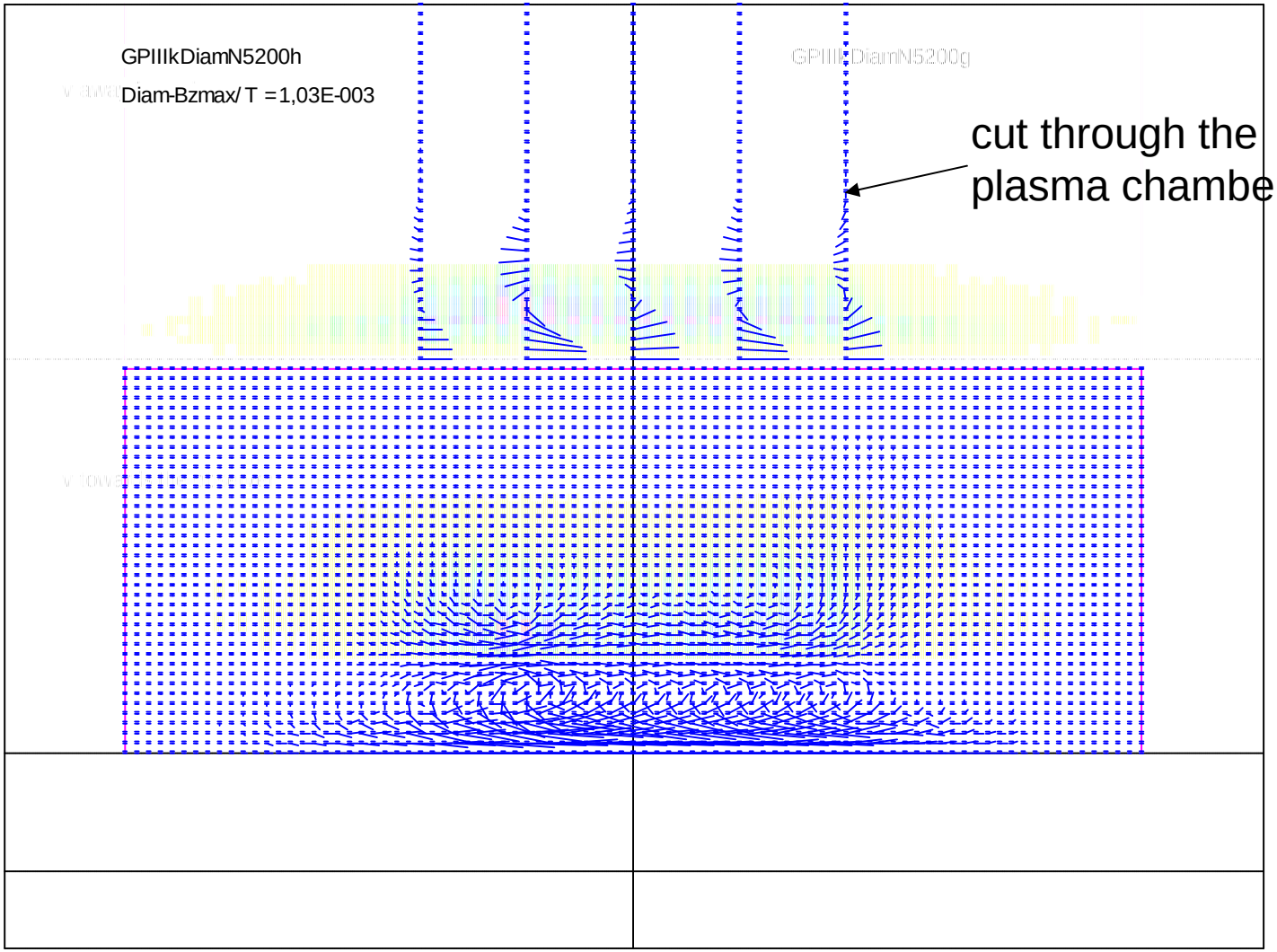
DD and EDD concentrated on the shifted core in the centre




Charge state distribution of ECRIS I, II, III
ECRIS I, 30 W
ECRIS II, 150 W
ECRIS III, 30 W
ECRIS I, opt. on 9+, 12 W
ECRIS III, opt. on 9+, 12 W
Best currents with 30 W
current / eμA
100
10
1
0,1
0
2
4
6
8
10
12
charge state

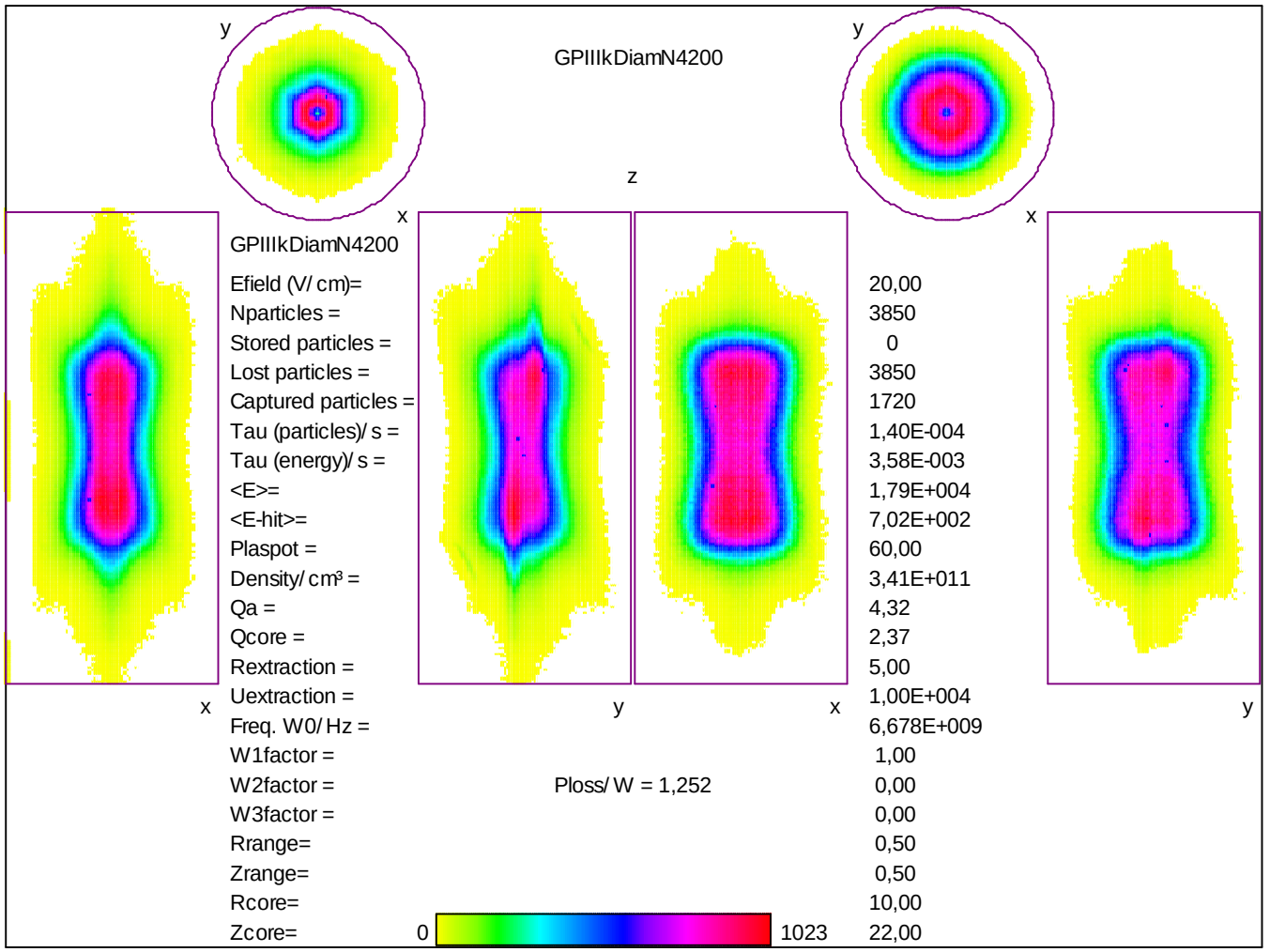
At these high energies one would expect important diamagnetic fields created by rotating electrons

The maximum diamagnetic field is only 1mT ≈ 0.4 % of B_{res}

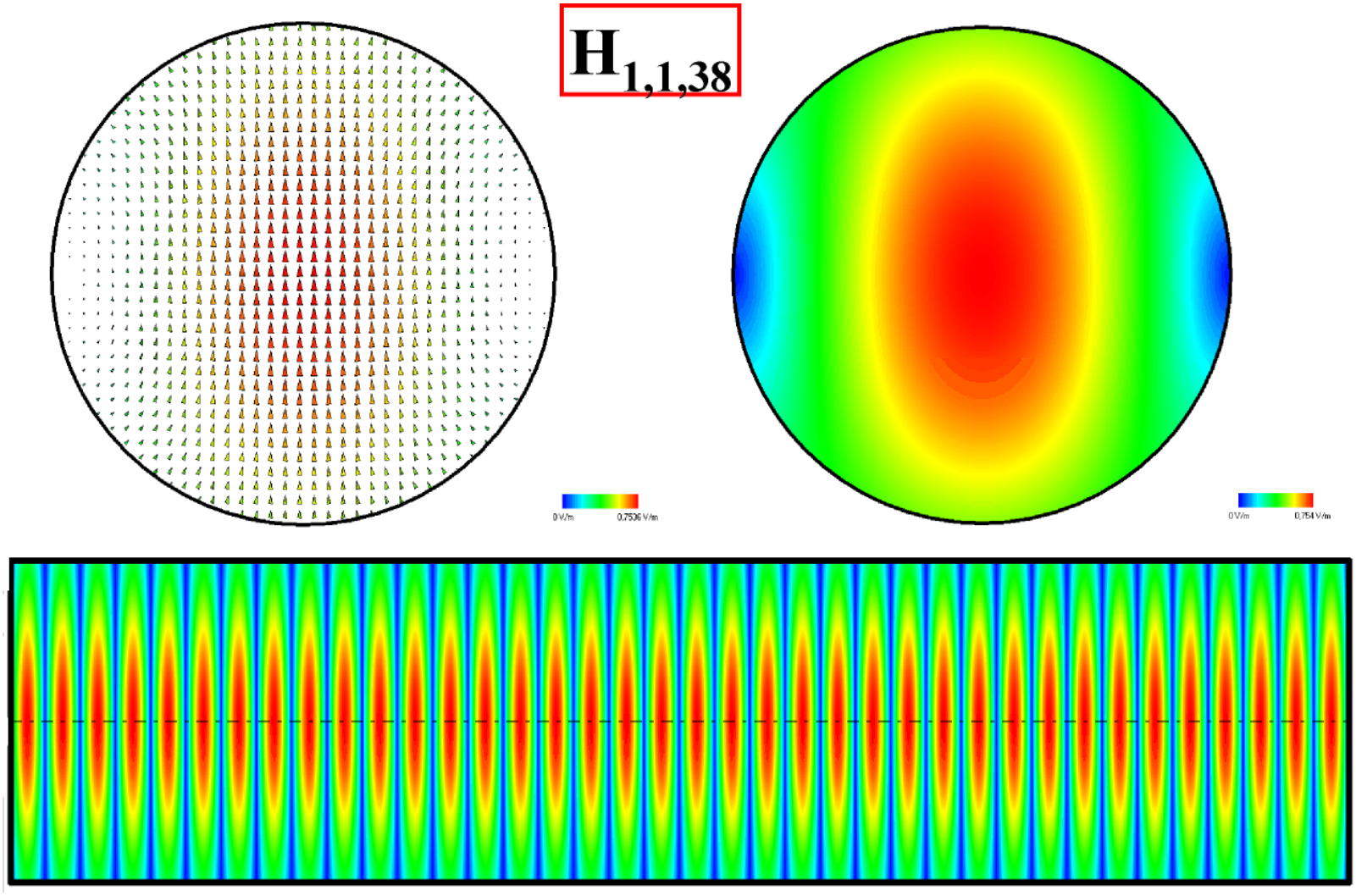


If one introduces Al_2O_3-layers on the end caps
they may charge up to -60 V like the biased disk
Electrons with „perpendicular energy“ < 60 eV are thus reflected :

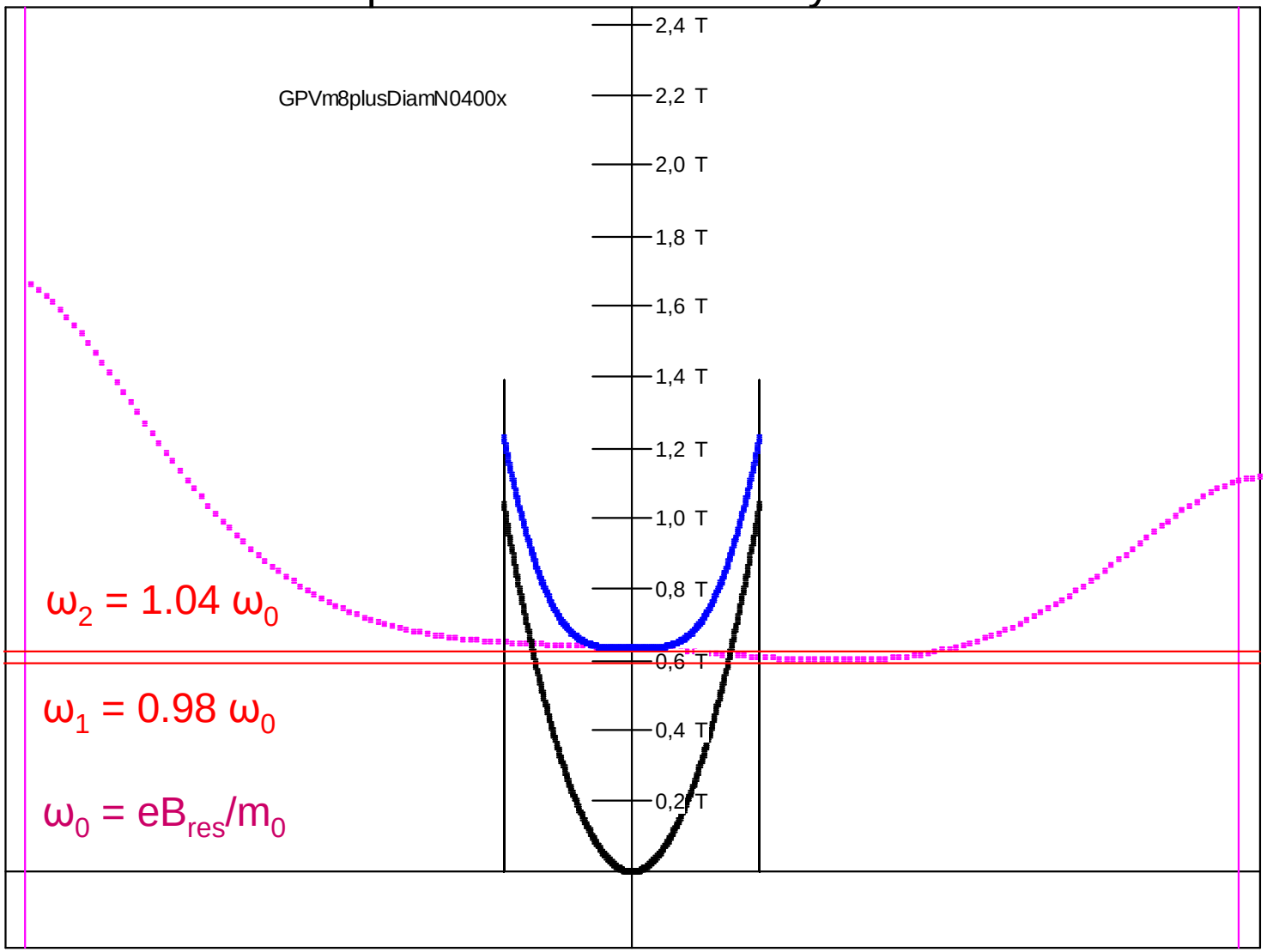
<tau> = increases from 48.7 to 140 µs !



The simulation in PECRIS V : As approximation a single H1,1,38-single mode is used the amplitudes of which drop from their centre values to 25 % at the walls of the cylinder without azimuthal dependence



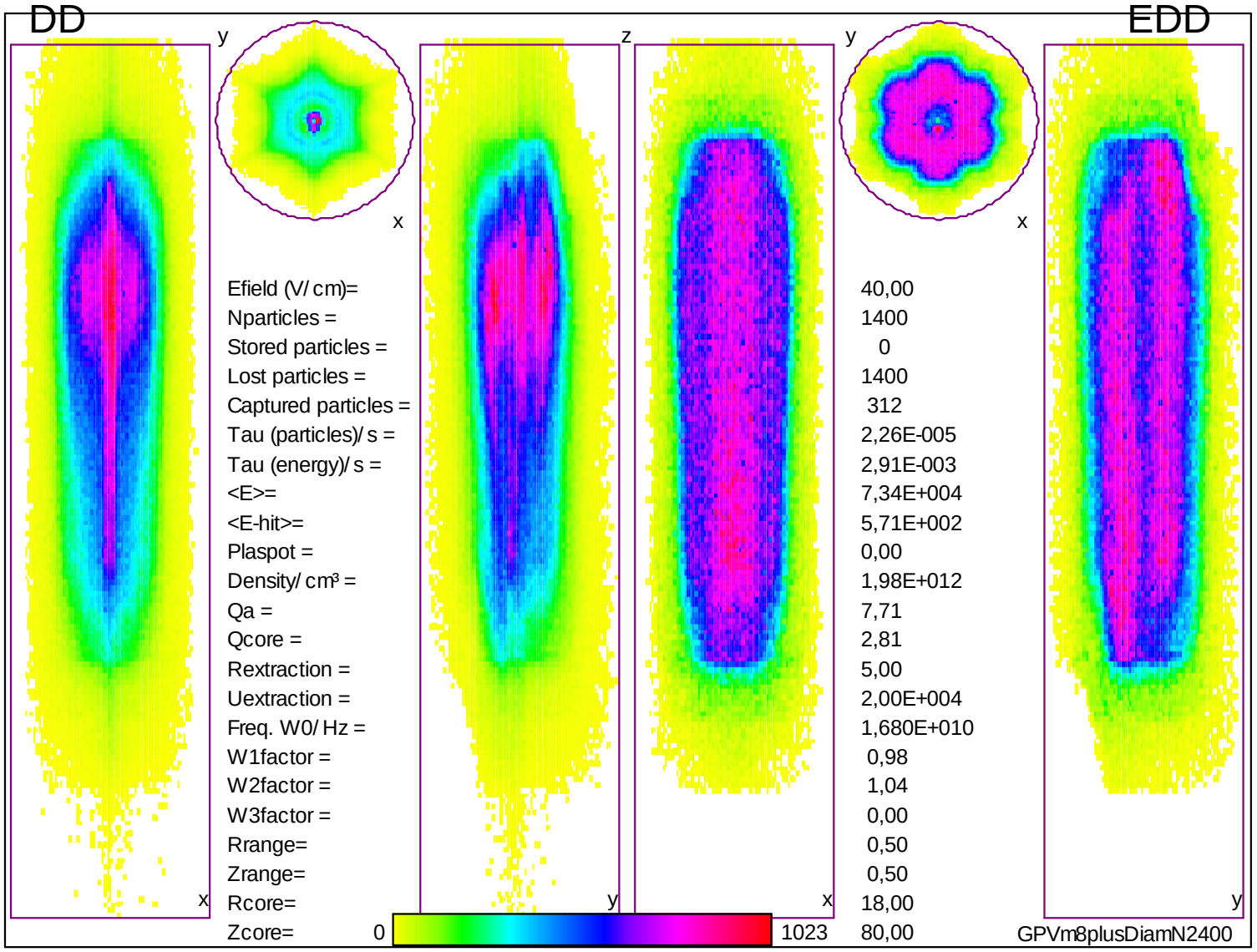
Two frequencies with 40 V/cm each are adapted
to the magnetic field for **optimization of Ar8+**
The extraction voltage is 20 kV
For the collisions $q_a = 7.71$ and $q_c = 2.81$
as derived from experiments corrected by the PUMAEX-factors.



From pressure readings: $n_{ecore} = n_c/2 = 1.75E12\ cm^{-3}$; $n_{eout} = n_c/10 = 3.5E11\ cm^{-3}$

in a core of 160 mm length and 36 mm diameter

High density and shift reduce <tau> = 22.6 µs ; <E> = 73.4 keV



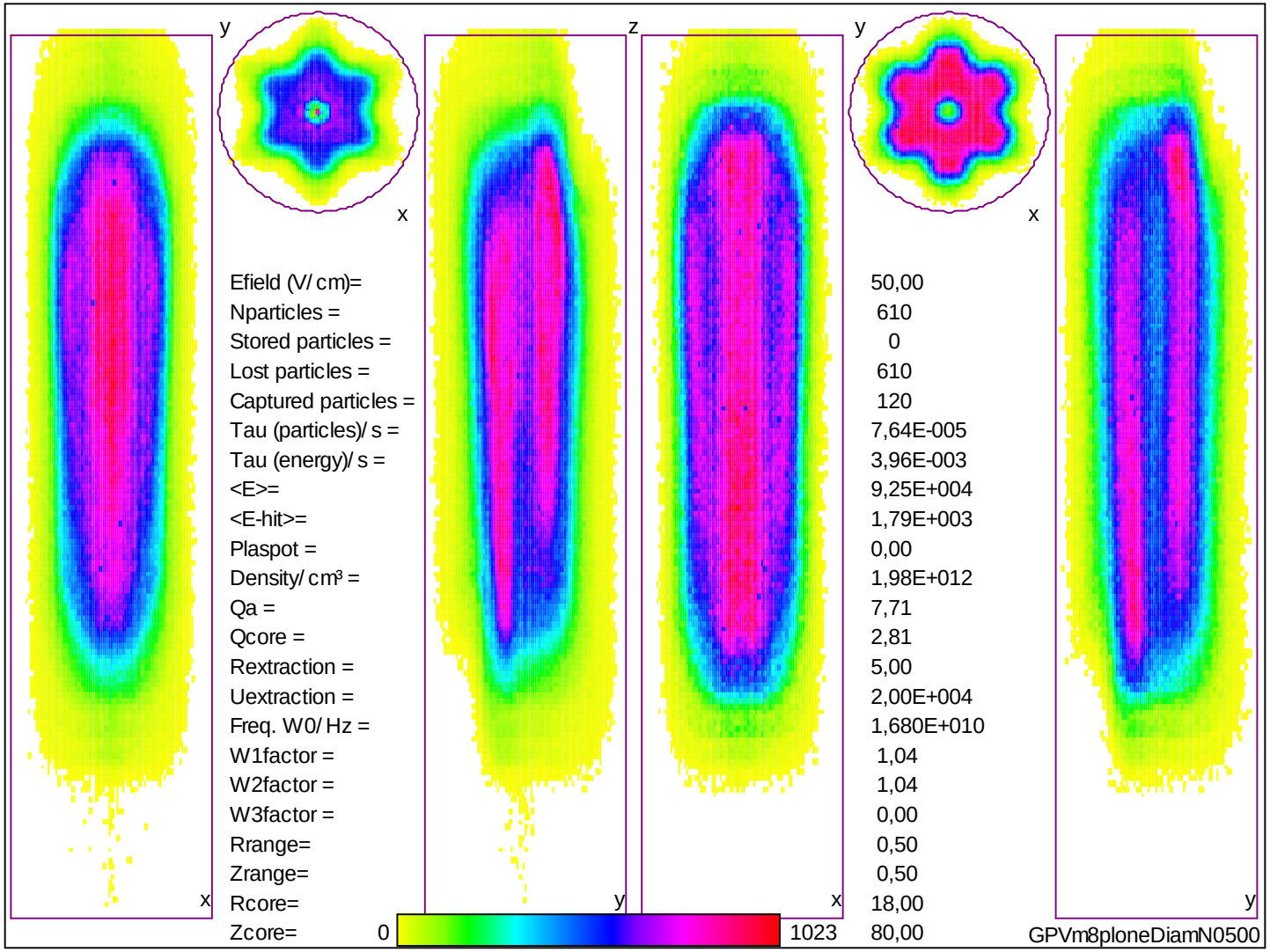
tau_{max}=6.3 ms !

EDD has greater radius than DD due to relativistic effect

The same simulation with only one frequency ω2 = 1.04 ω0

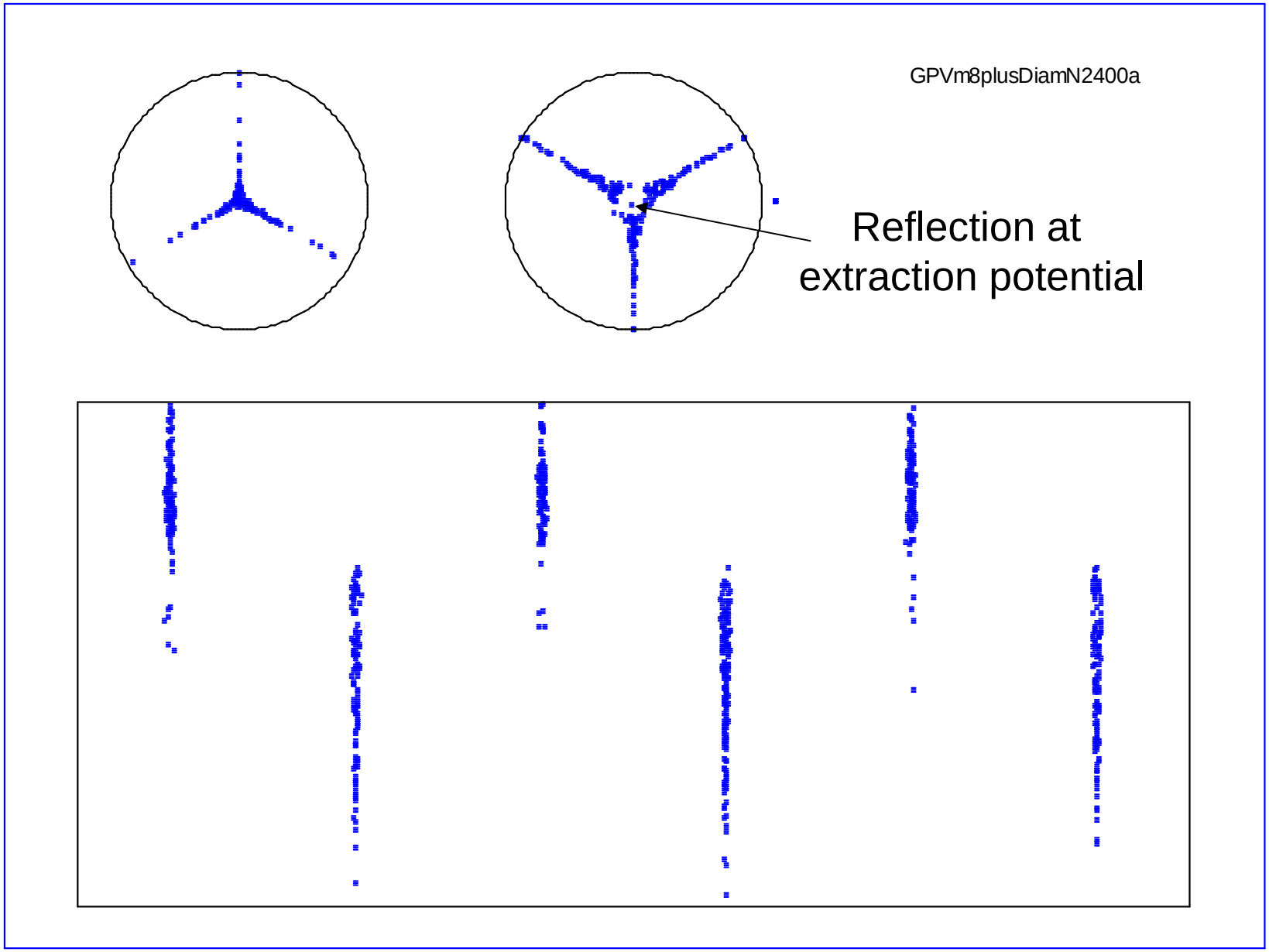
This frequency drives the density away from the axis

<tau> = 76.4 µs ; <E> = 92.5 keV



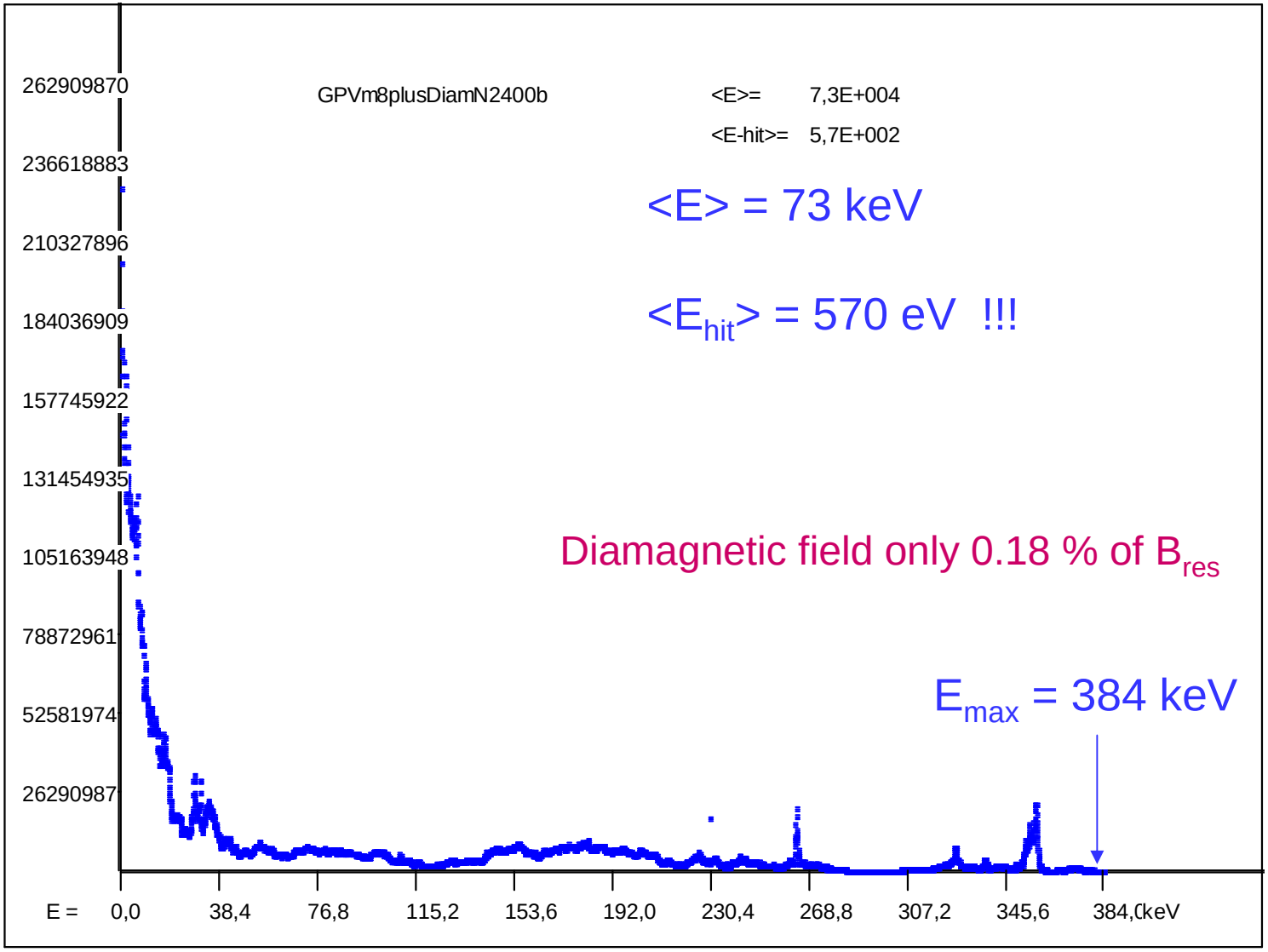
The low energies
Close to the axis
are missing

Due to shift of magnetic structure impact pattern also shifted



The concentration of the µW-power limits the highest energy

PECRIS V would allow up to 1.1 MeV with power in the corner with greatest B

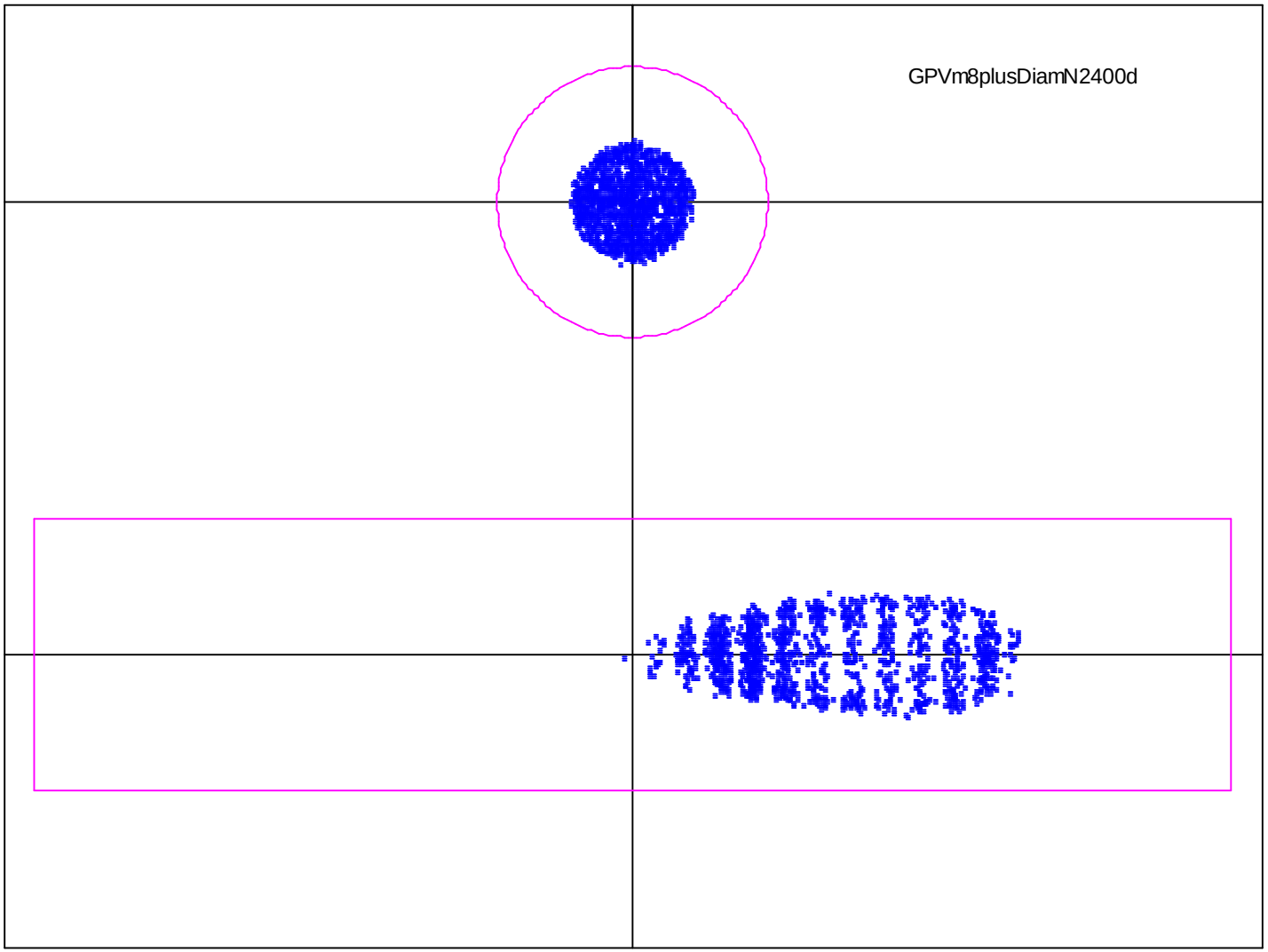


The core with strongest ECR-interaction

is region of starting positions of the electrons for simulation

The maxima and minima of the cavity mode clearly show up

They represent successions of fast spatial change of phase

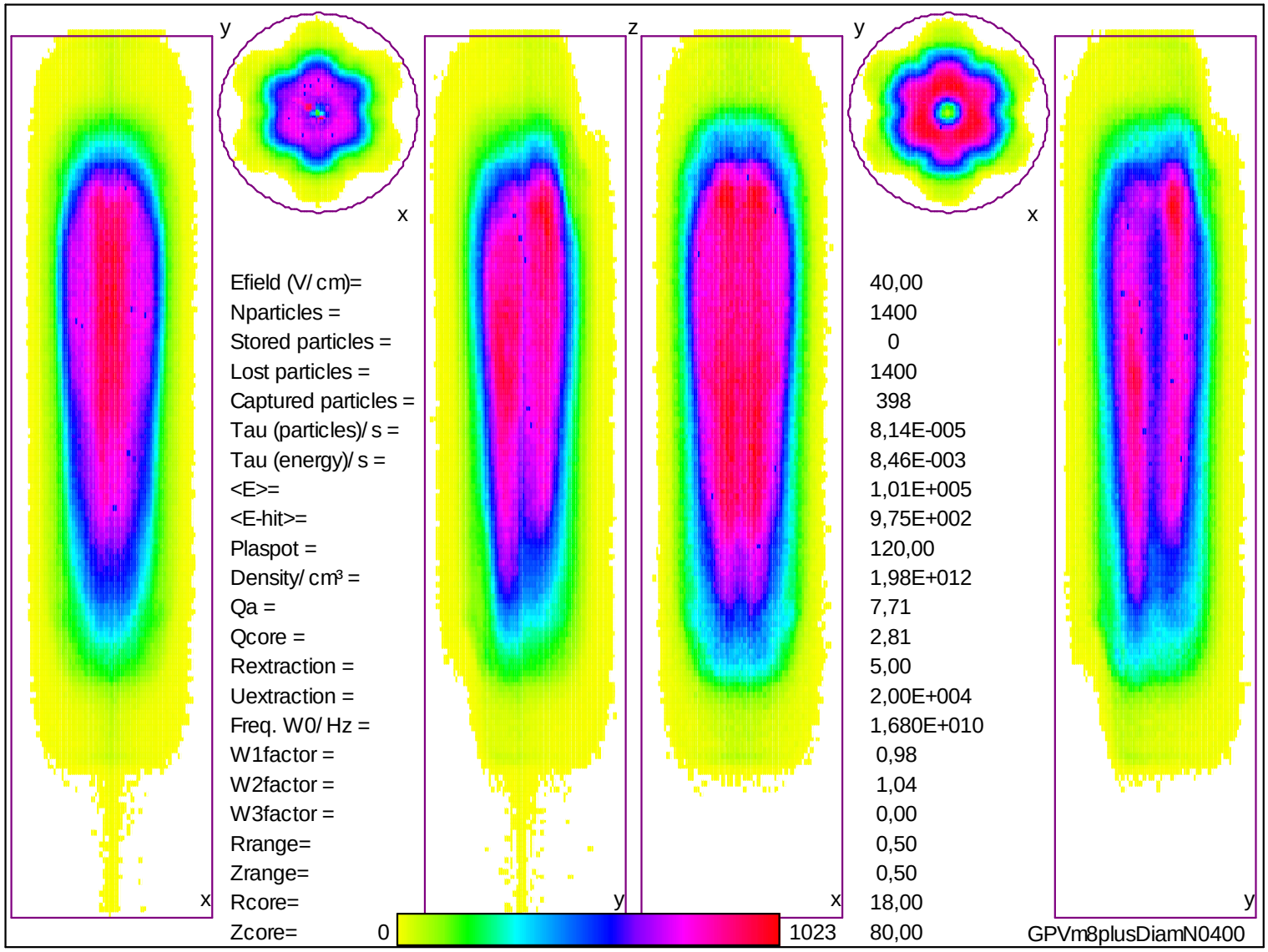


If one introduces Al_2O_3-layers on the end caps

they may charge up to -120 V like the biased disk

Electrons with „perpendicular energy“ < 120 eV are thus reflected :

<tau> = increases from 22.6 to 81.4 µs !



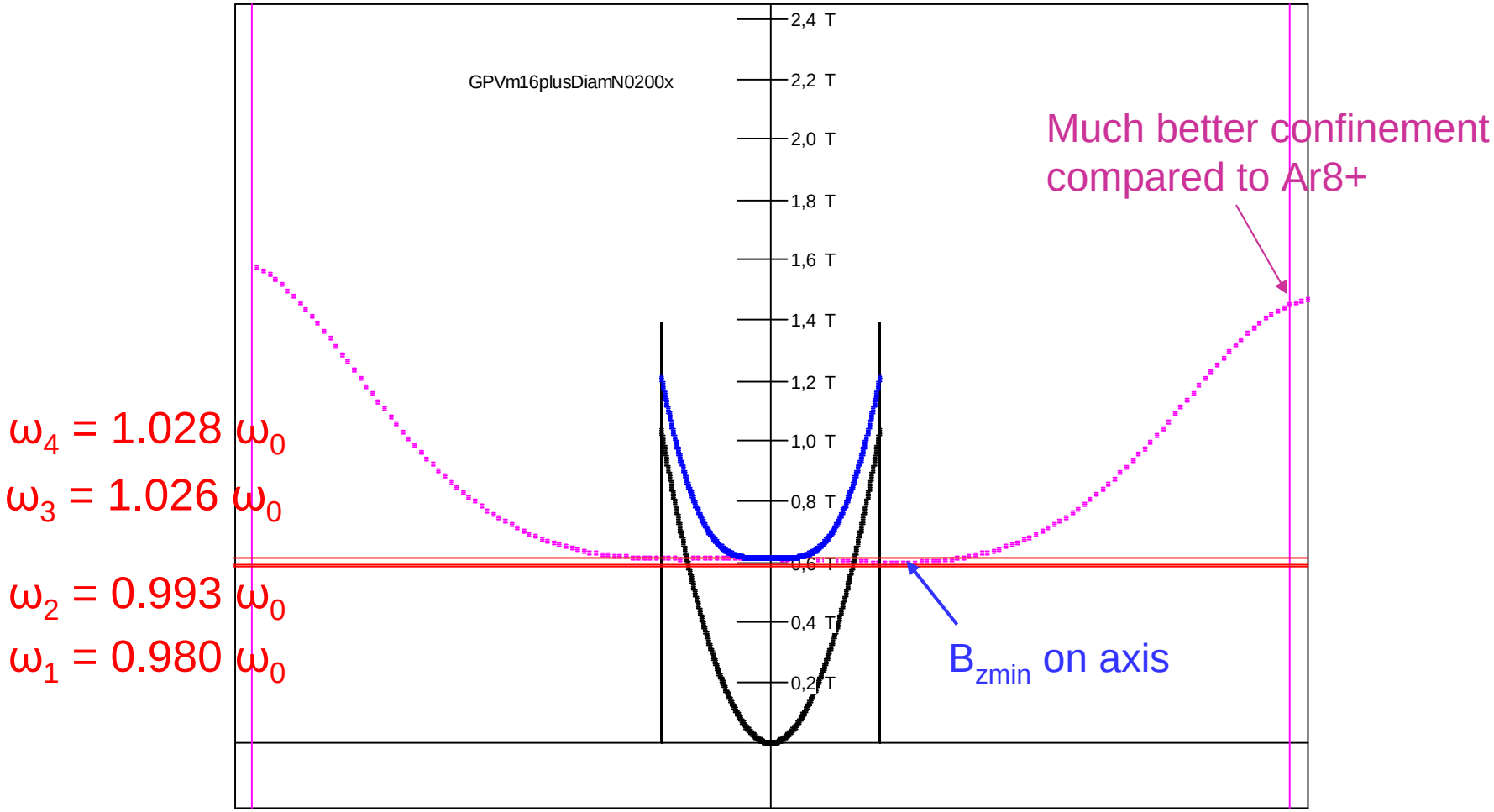
Four frequencies with 20 V/cm each are adapted

to the magnetic field for **optimization of Ar16+**

The extraction voltage is 20 kV

For the collisions $q_a = 8.28$ and $q_c = 3.18$

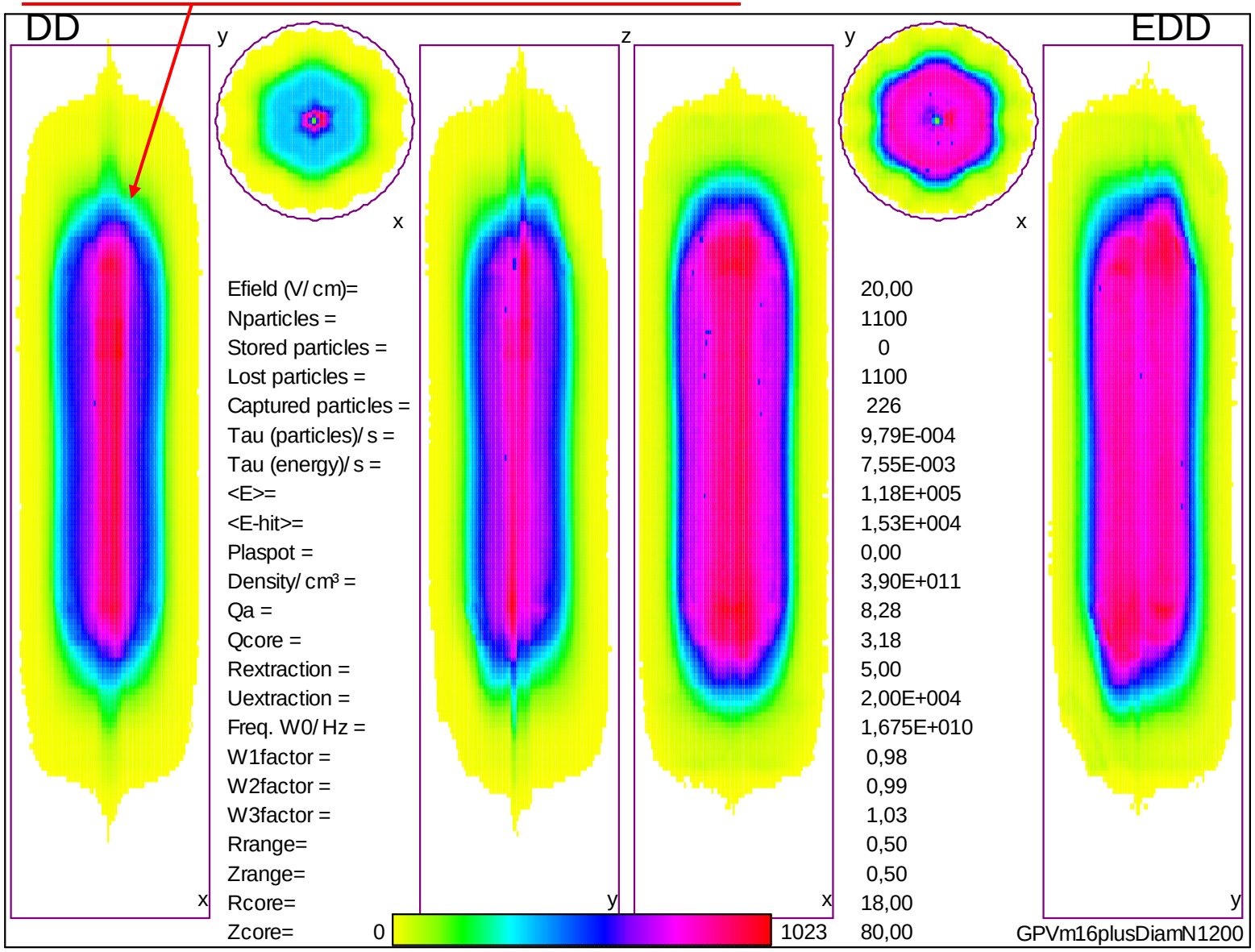
as derived from experiments corrected by the PUMAEX-factors.



From pressure readings: $n_{ecore} = n_c/10 = 3.5E11\ cm^{-3}$; $n_{eout} = n_c/50 = 7E10\ cm^{-3}$
in a core of 160 mm length and 36 mm diameter

Low density and reduced shift increase <tau> = 0.98 ms ; <E> = 118 keV

! Ideal concentration of DD near axis !



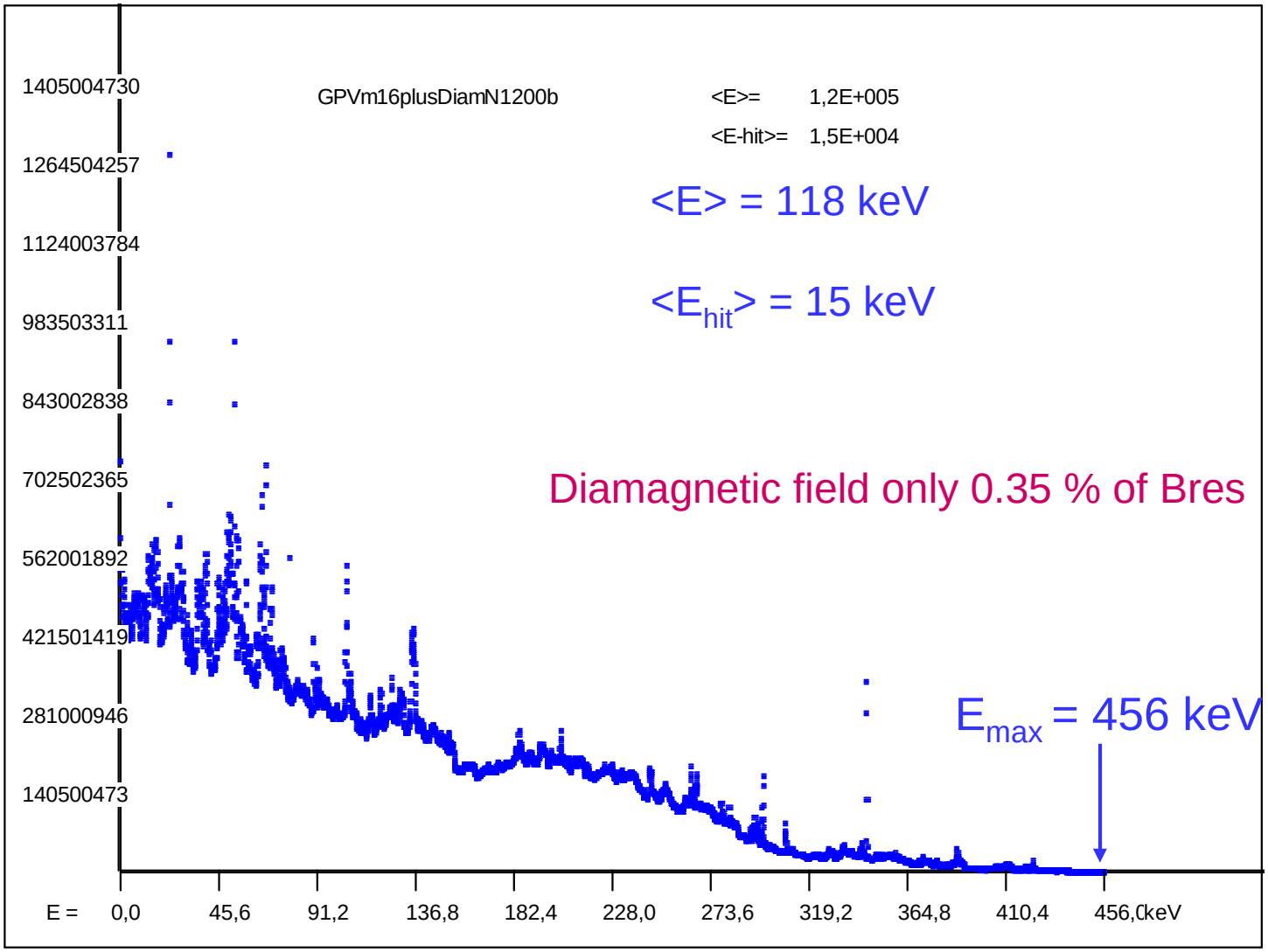
tau_{max}=70 ms !

EDD has greater radius than DD due to relativistic effect

The concentration of the µW-power limits the highest energy

PECRIS V would allow up to 1.1 MeV with power in the corner with greatest B

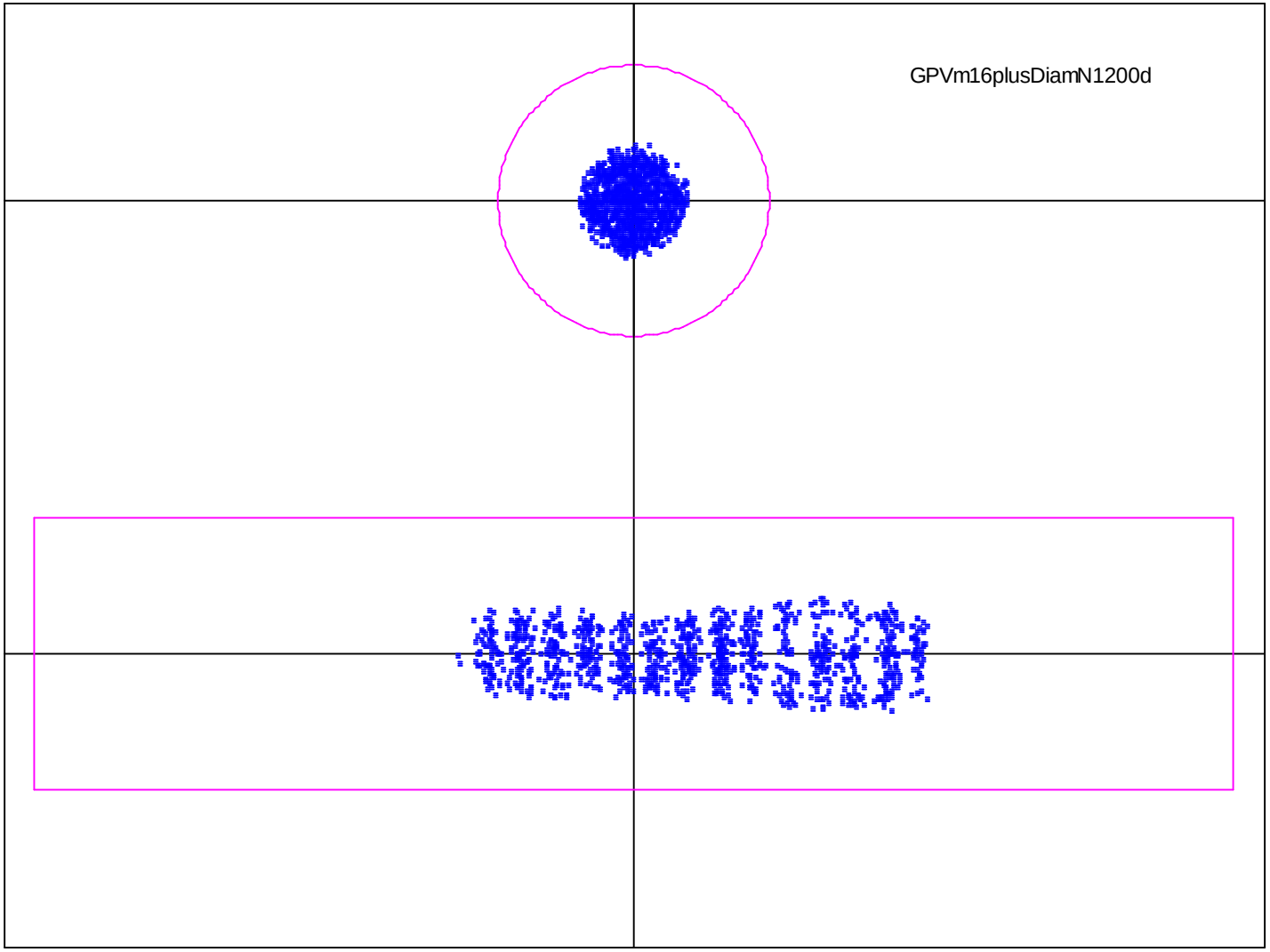
Spectrum has changed : Good confinement allows longer ECRH



The core with strongest ECR-interaction

is region of starting positions of the electrons for simulation

The centre of strongest ECR-interaction is at B_{zmin}

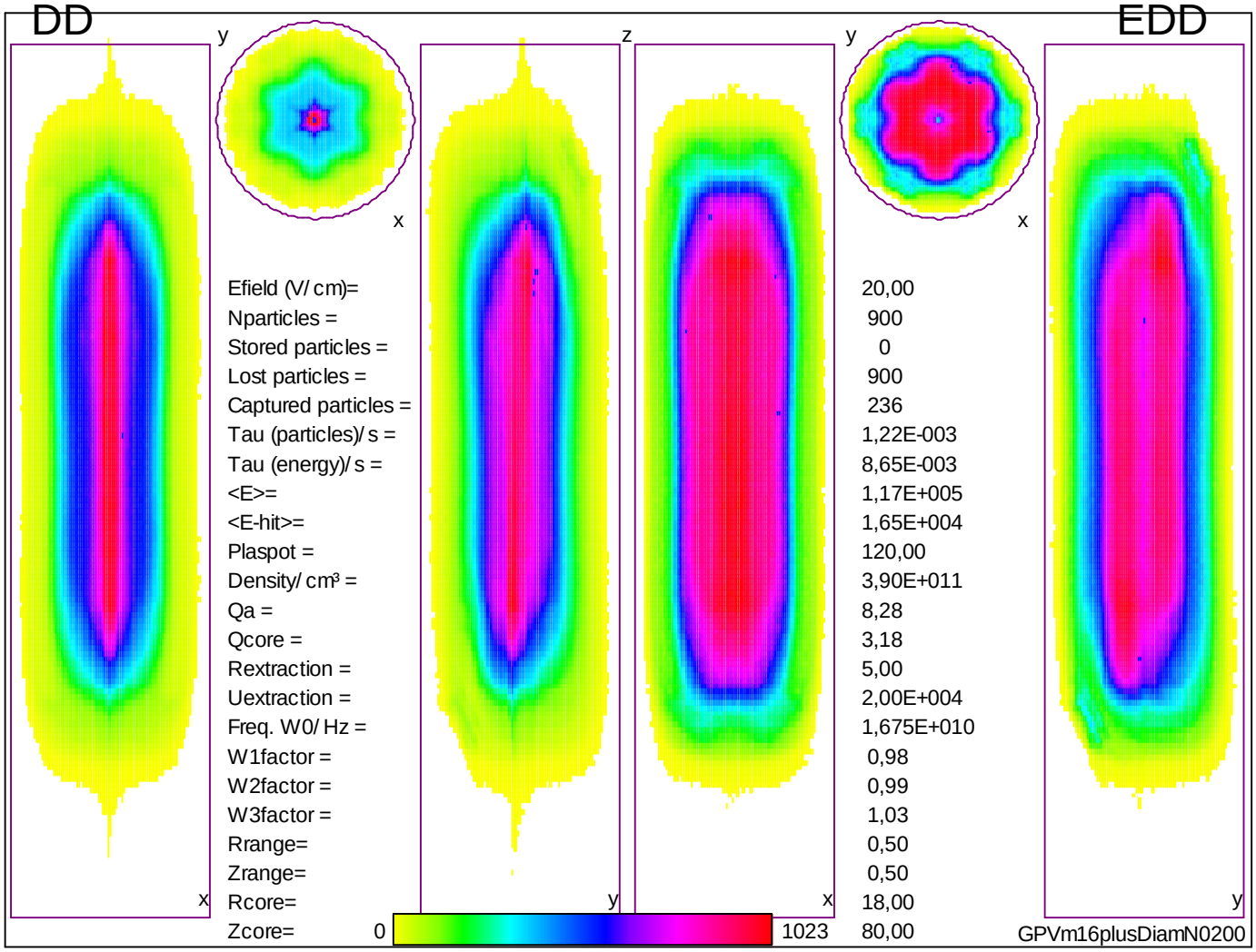


If one introduces Al_2O_3-layers on the end caps

they may charge up to -120 V like the biased disk

Electrons with „perpendicular energy“ < 120 eV are thus reflected :

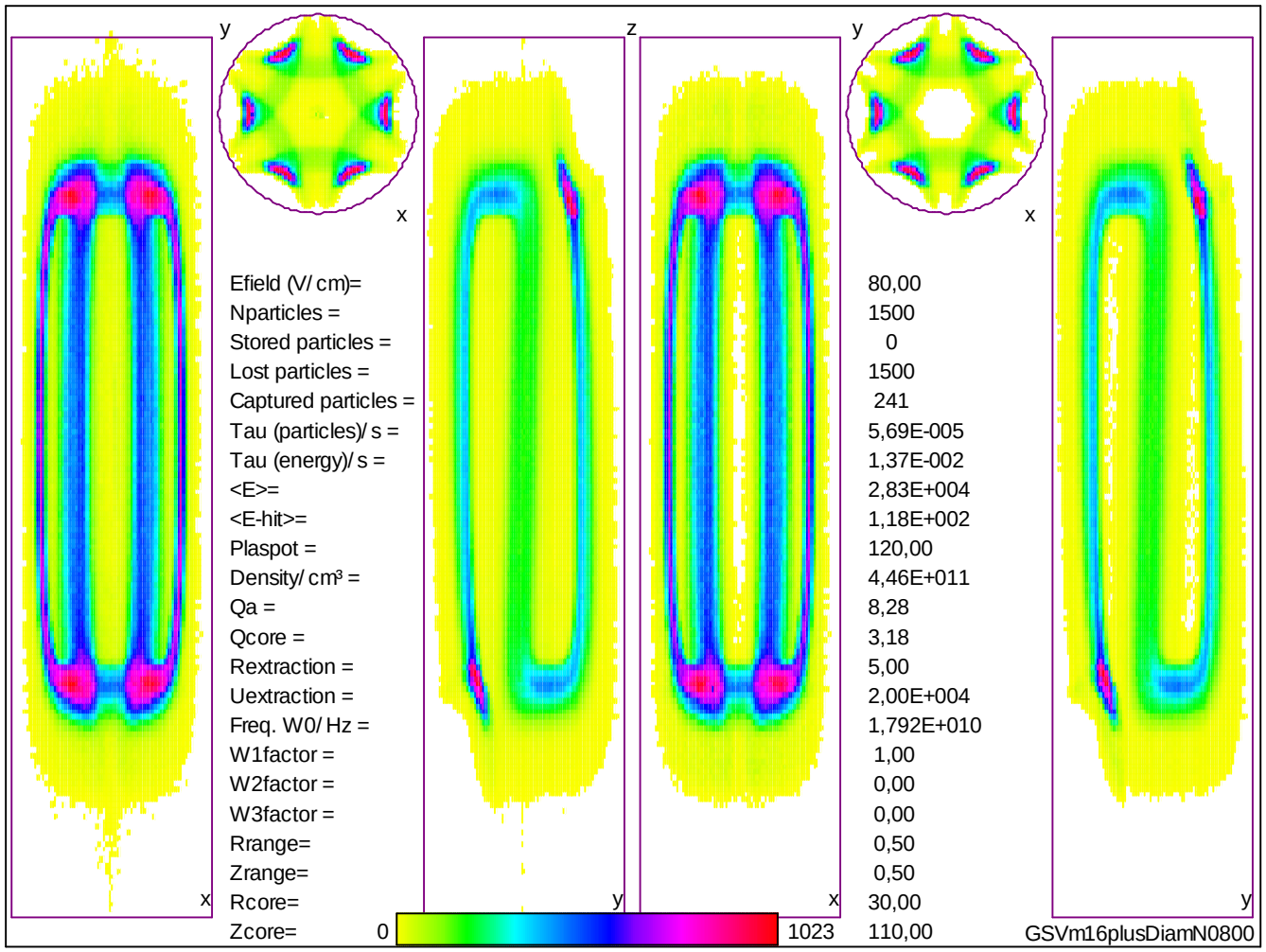
<tau> = only increases from 0.98 to 1.22 ms due to good confinement



tau_{max}=72 ms !

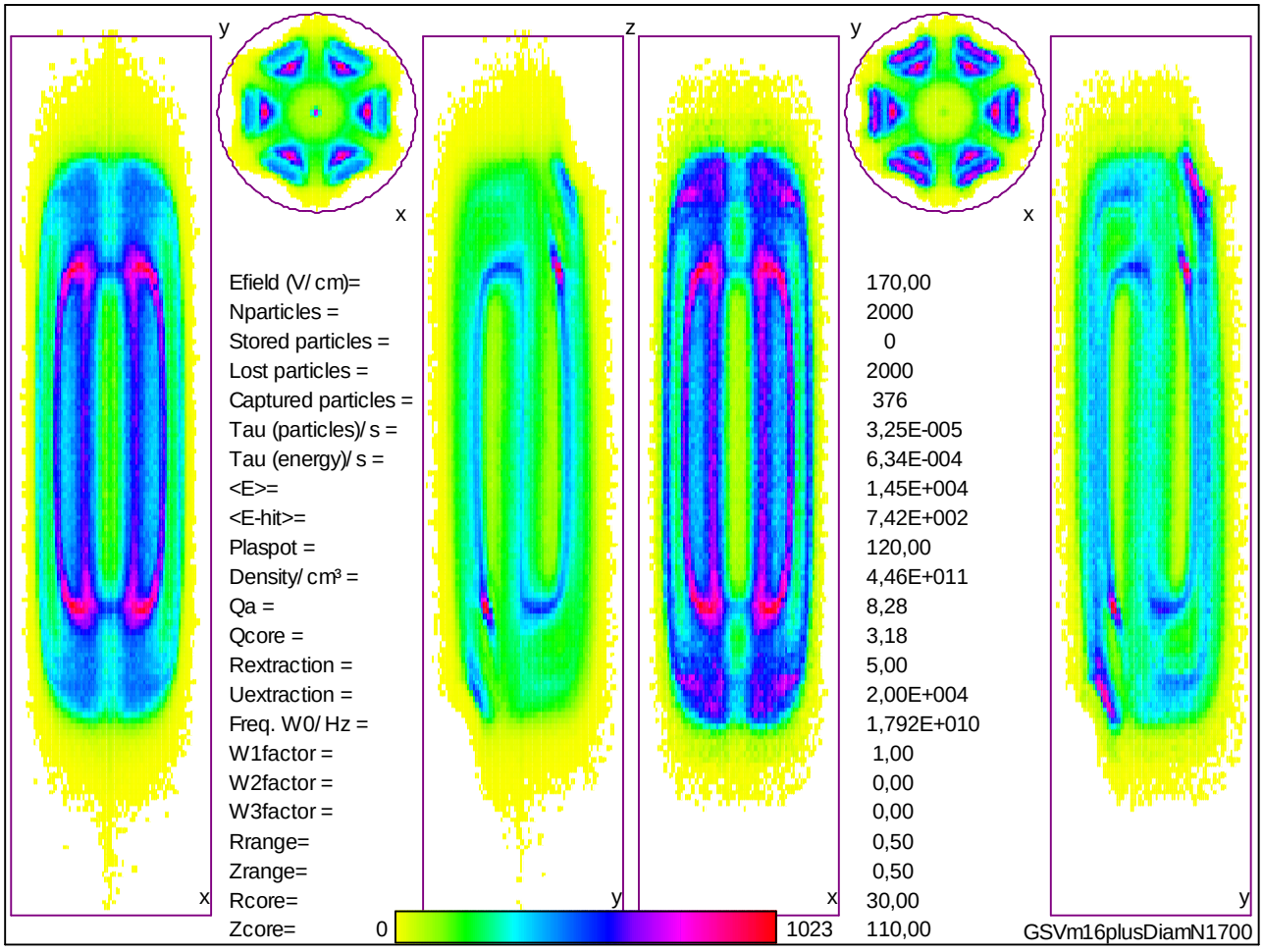
If we had used a parabolic minimum istead of the plateau :

parabolic		plateau
1.25 kW	µW-power	500 W
<E> = 28.3 keV		<E> = 117 keV
<tau> = 56.9 µs		<tau> = 1.12 ms



If we had used a parabolic minimum istead of the plateau :

parabolic		plateau
10 kW	µW-power	500 W
<E> = 14.5 keV		<E> = 117 keV
<tau> = 32.5 µs		<tau> = 1.12 ms



For the simulation of ions with rotational energy

created by **Ion-Cyclotron-Resonance-Heating (ICRH)**

the same, but non-relativistic code can be used.

The main difference :

amount and nature of the targets of collisions

Since the collisions with electrons are negligible,

only the ionic targets are left

They can be treated as the electron-ion collisions before:

In the core :

Density of targets: $n_{ccore} = n_{ecore}/q_a$

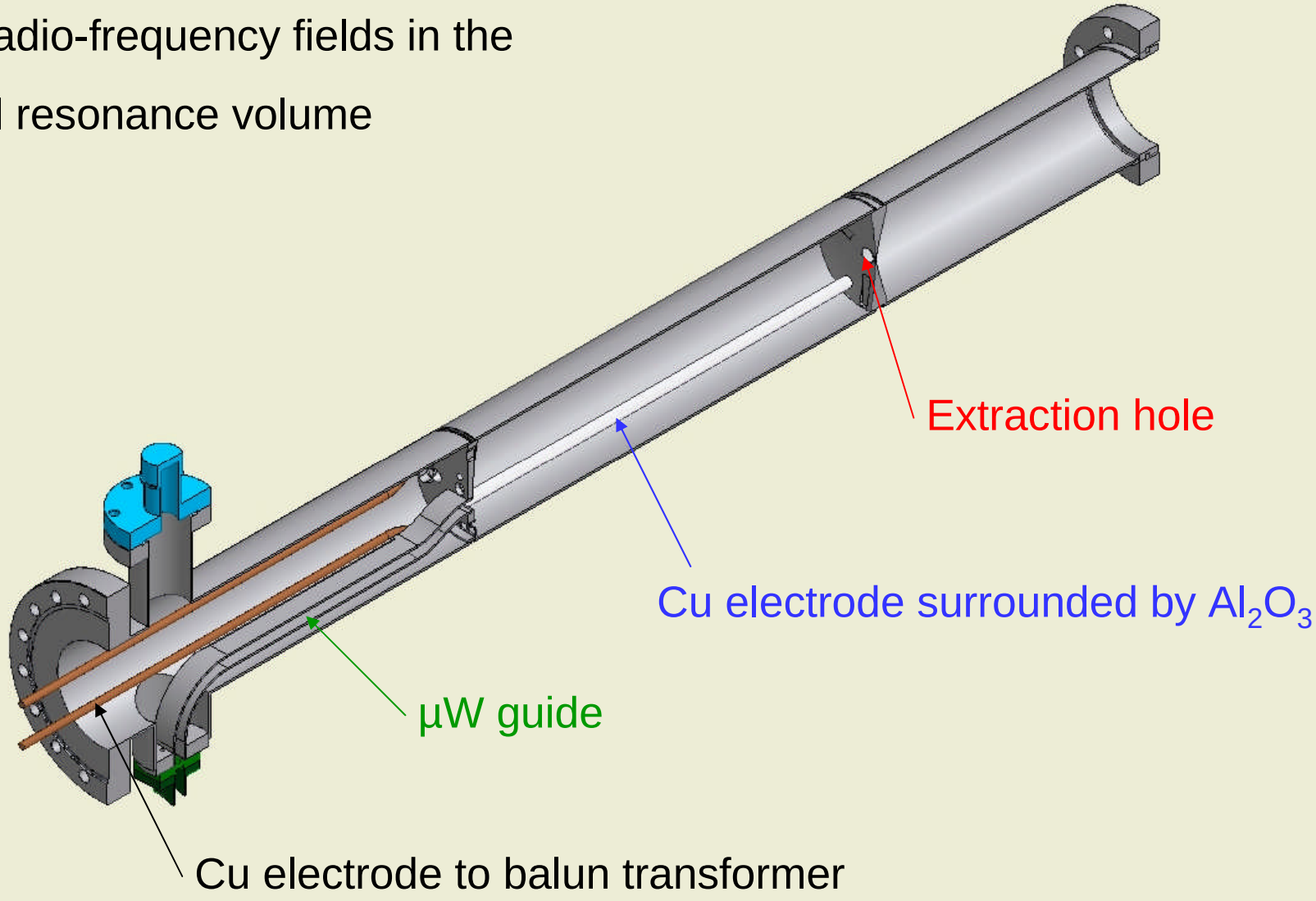
Average charge of target : $q_{ccore} = \langle q_{ion} \rangle = \sqrt{[\sum n_i q_i^2 / \sum n_i]}$

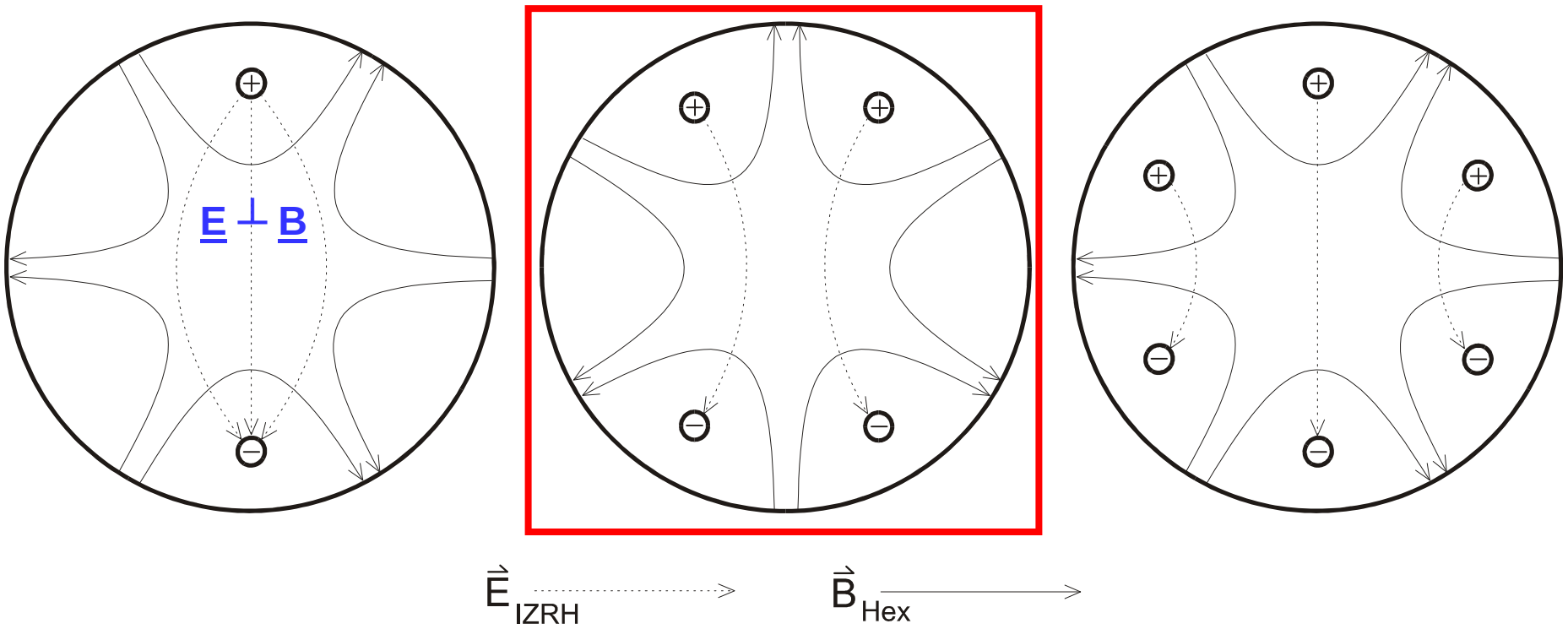
Outside the core:

Density of targets: $n_{cout} = n_{eout}$

Average charge of target : $q_{cout} = 1$

Electrodes in PECRIS V for production of MHz-radio-frequency fields in the central resonance volume





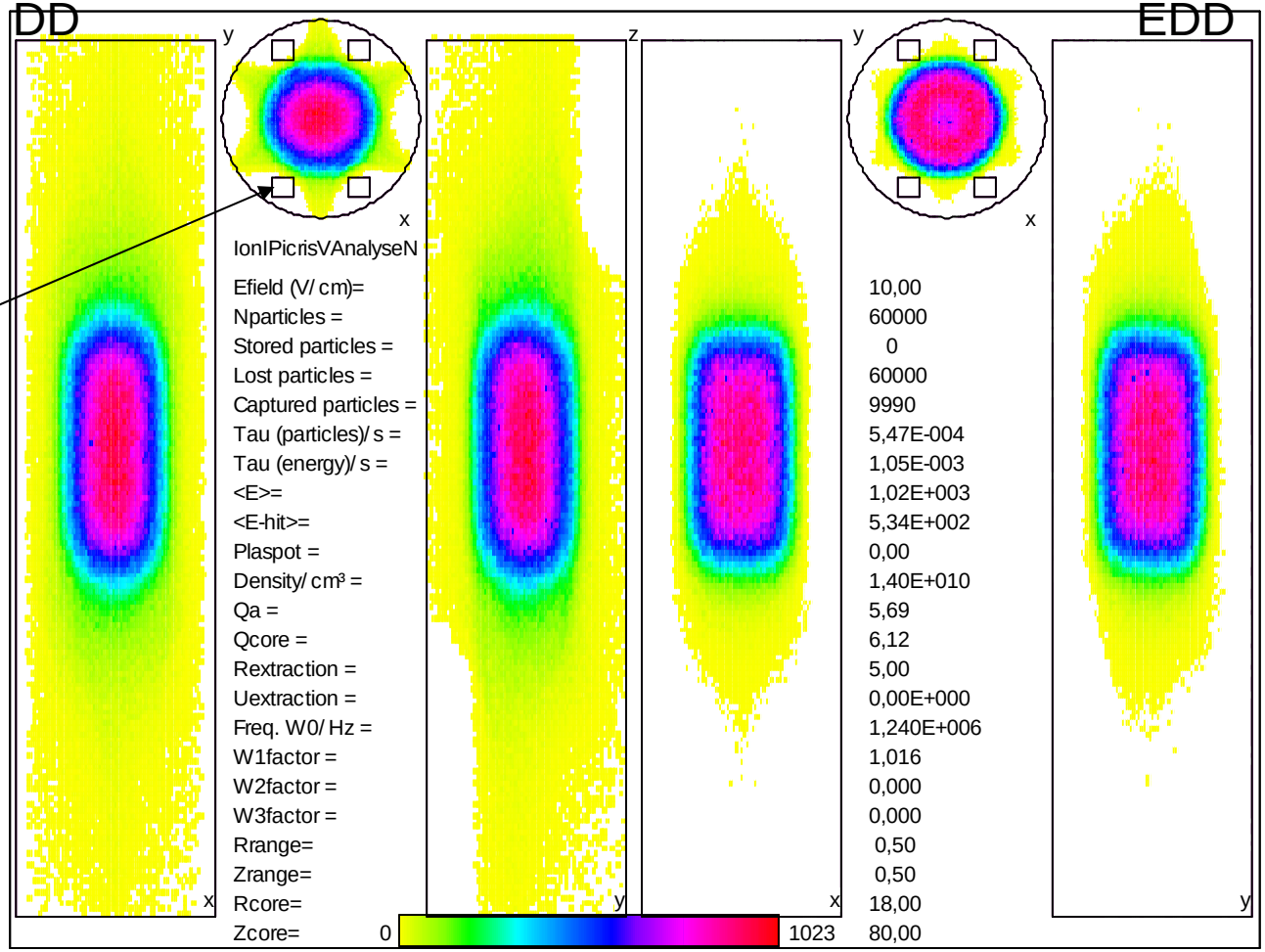
Our choice with smallest electric field between electrodes and wall

The great advantage of ICRH : RF has everywhere the same phase

It is very efficient, the RF-amplitudes can be small, at start E_{kin0} = 0.025 to 1 eV

With 10 V/cm (as in the experiments to be described)

ICRH of **Ar5+** yields <E> = 1.05 keV and <tau> = 0.55 ms



IonIPVfNAr54100

Approxi-mation for electrodes

E_{max} = 4.5 keV

tau_{max} = 40 ms

In the core:

target density = 1.4E10 cm-3

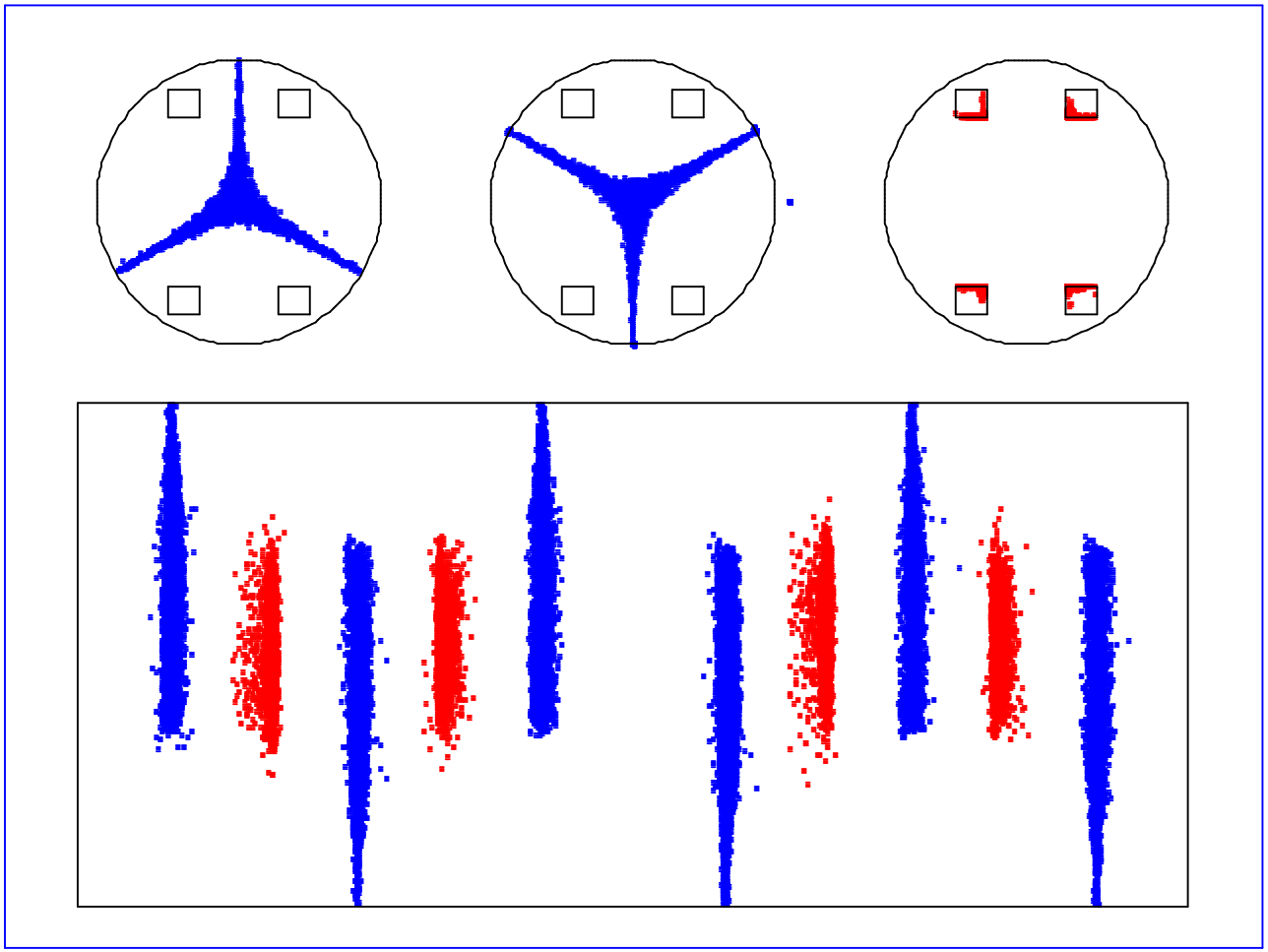
q_a = 5.69

q_c = 6.12

The relatively short <tau> = 0.55 ms is due to the

strong perturbations by the electrodes and due to the

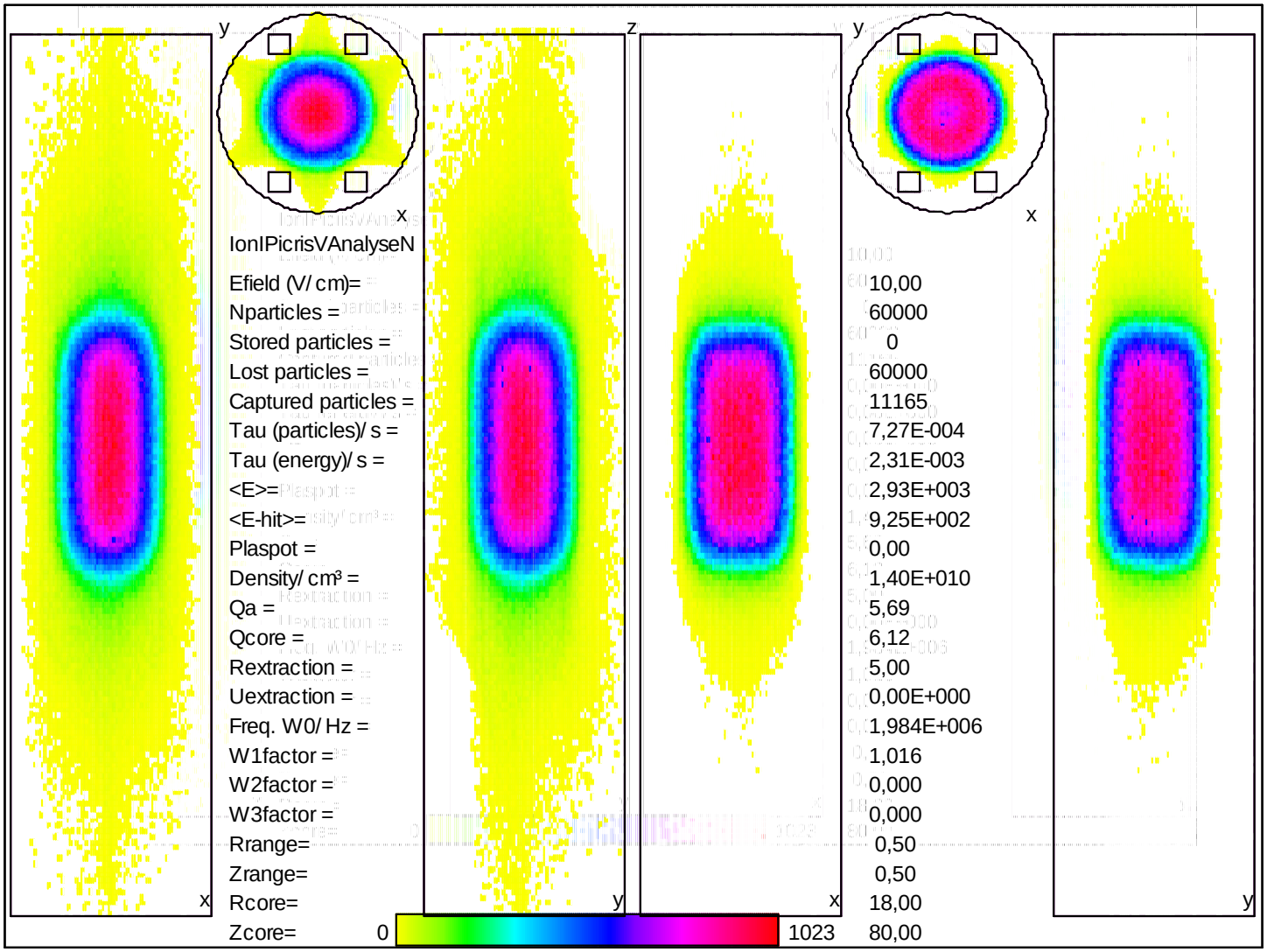
rapid expulsions to the walls of a chamber too small in diameter



IonIPVfNAr54100a

Ar8+ couples stronger to the RF-fields and yields

<E> = 2.93 keV, E_{max} = 11.2 keV, <tau> = 0.73 ms, and tau_{max} = 43 ms

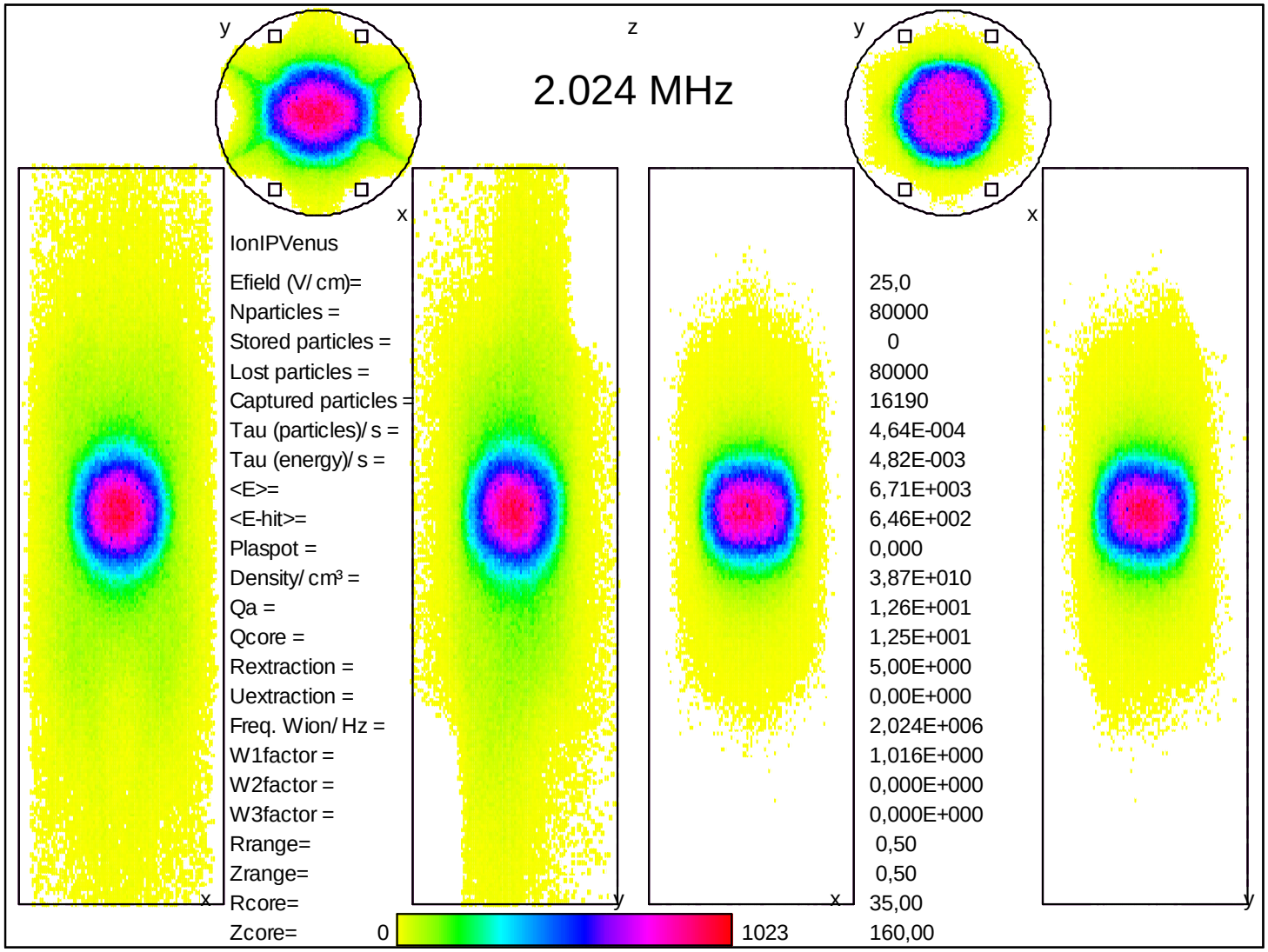


IonIPVfNAr84100

ICRH of **Ar8+** at 1.6 % above the central B_{min} of **VENUS**

Assumption of Ar8+ being present in the centre of VENUS

<E> = 6.7 keV, E_{max} = 31.2 keV, <tau> = 4.8 ms, and tau_{max} = 31 ms



25 V/cm

<u>In the core:</u>

target density =

3.9E10 cm-3

q_a = 12.6 !

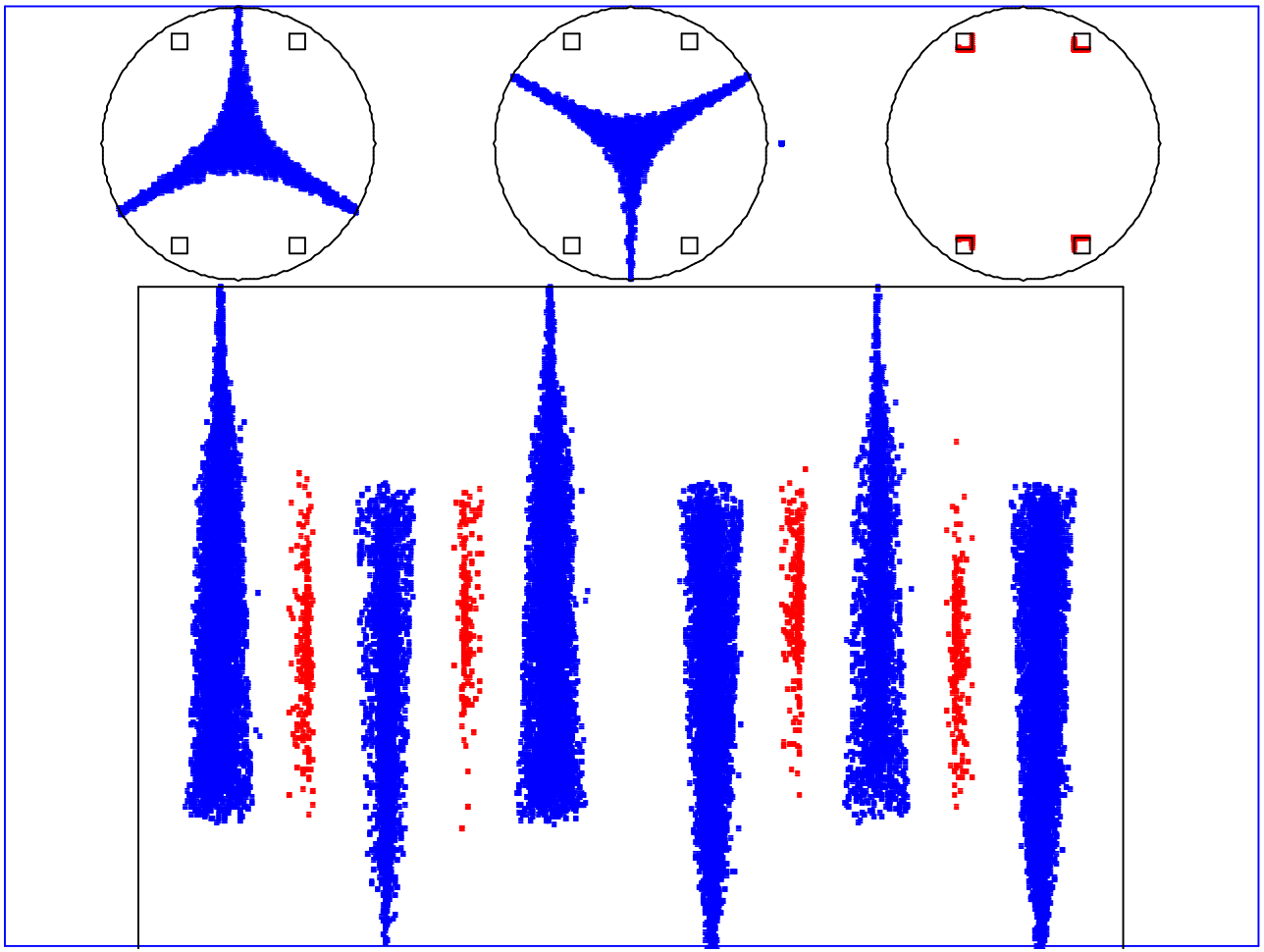
q_c = 12.5 !

IonIPhVenusNar8b1250

Despite bigger chamber still strong deposition of Ar8+ on the walls

But $<E_{hit}>$ = 650 eV only with respect to <E> = 6.7 keV

Perturbation by electrodes relatively reduced

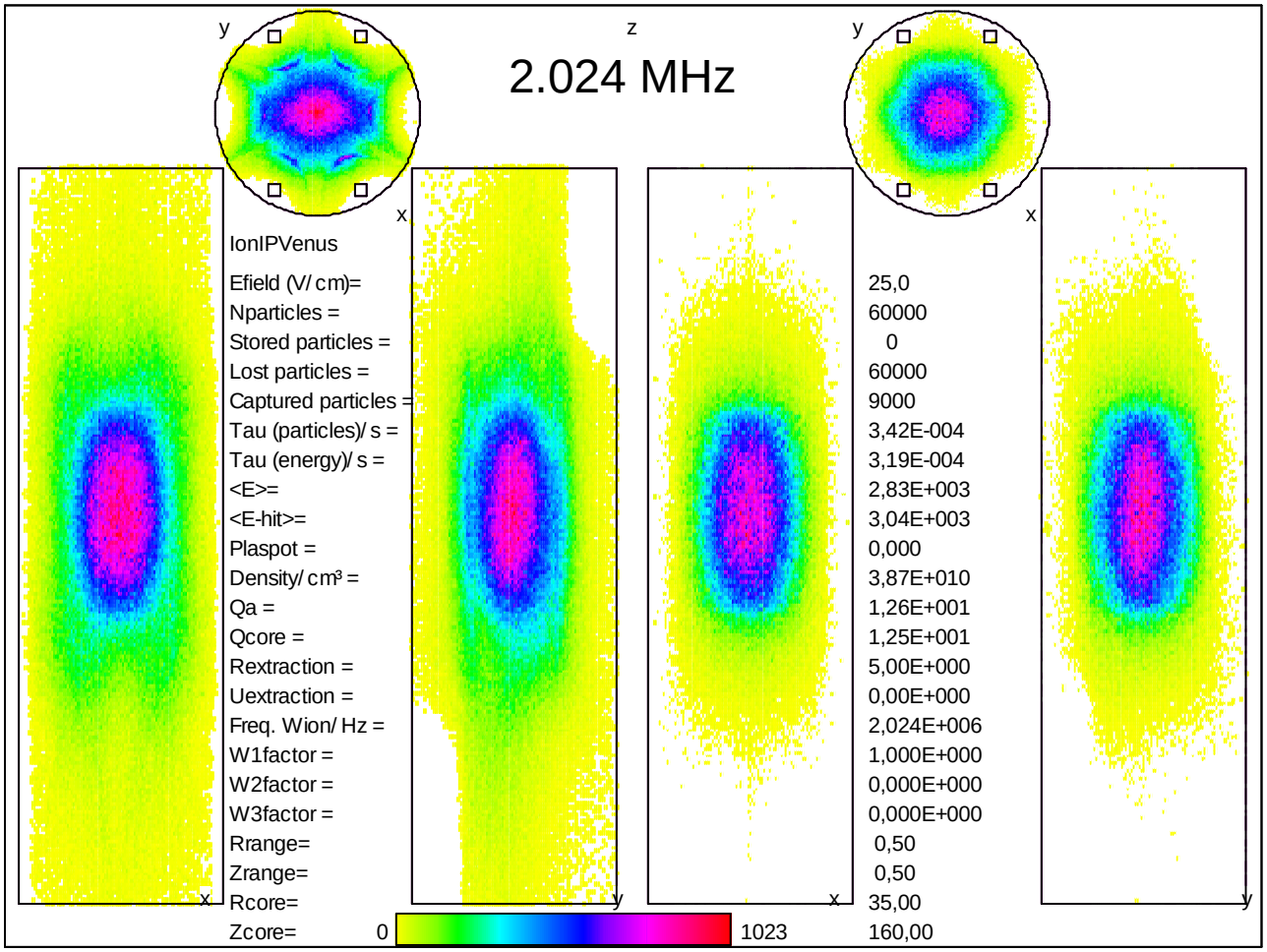


IonIPhVenusNAr8b1250a

ICRH of Ar7+ at 0.7586 T, i.e. 16.2 % above the central B_{min} of VENUS

<E> = 2.8 keV, E_{max} = 34.5 keV, <tau> = 0.34 ms, and tau_{max} = 13 ms

<Ehit> = 3 keV

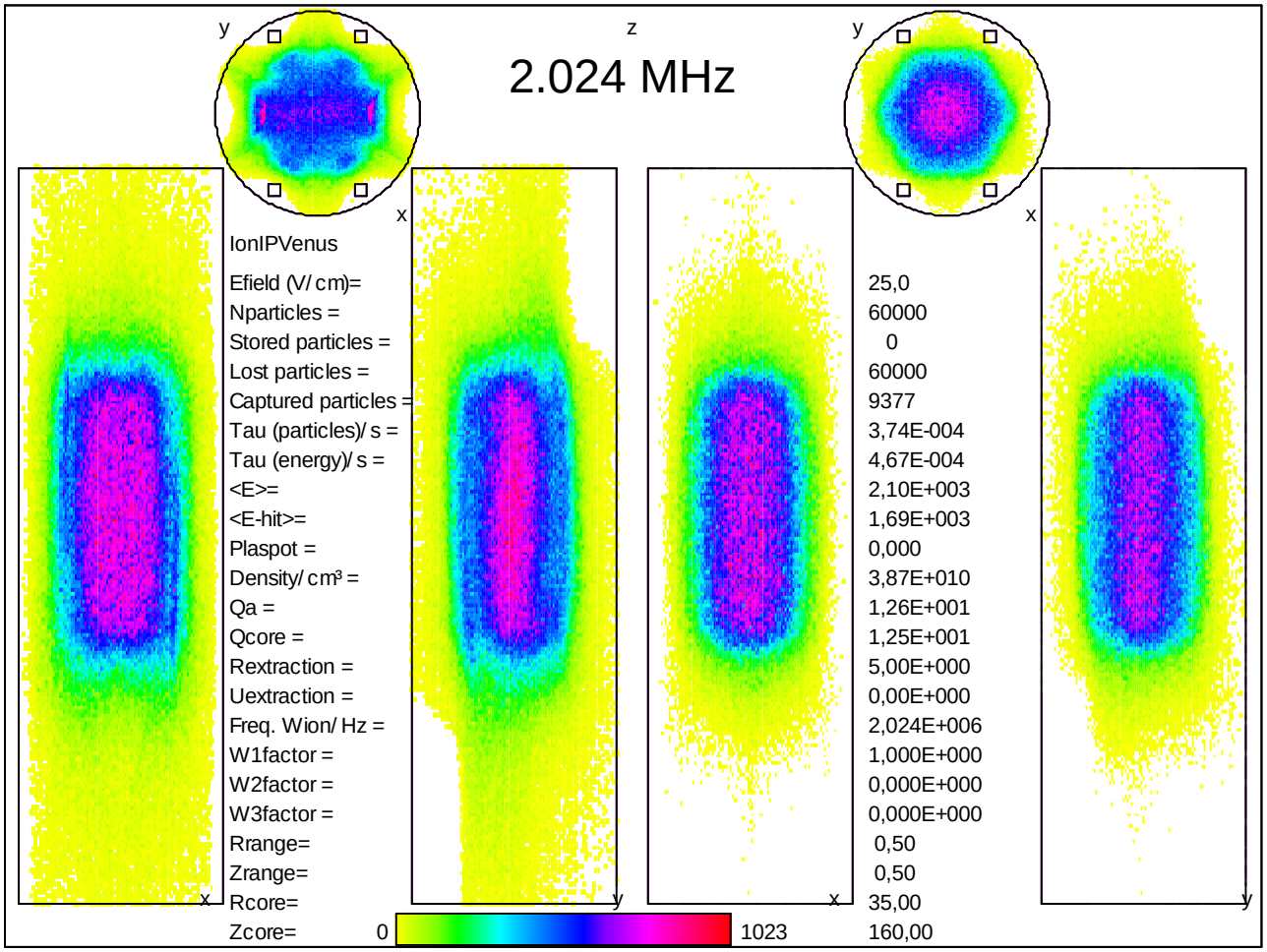


IonIPhVenusNAr7c1250

ICRH of Ar6+ at 0.8851 T, i.e. 35.5 % above the central B_{min} of VENUS

<E> = 2.1 keV, E_{max} = 19.6 keV, <tau> = 0.37 ms, and tau_{max} = 16 ms

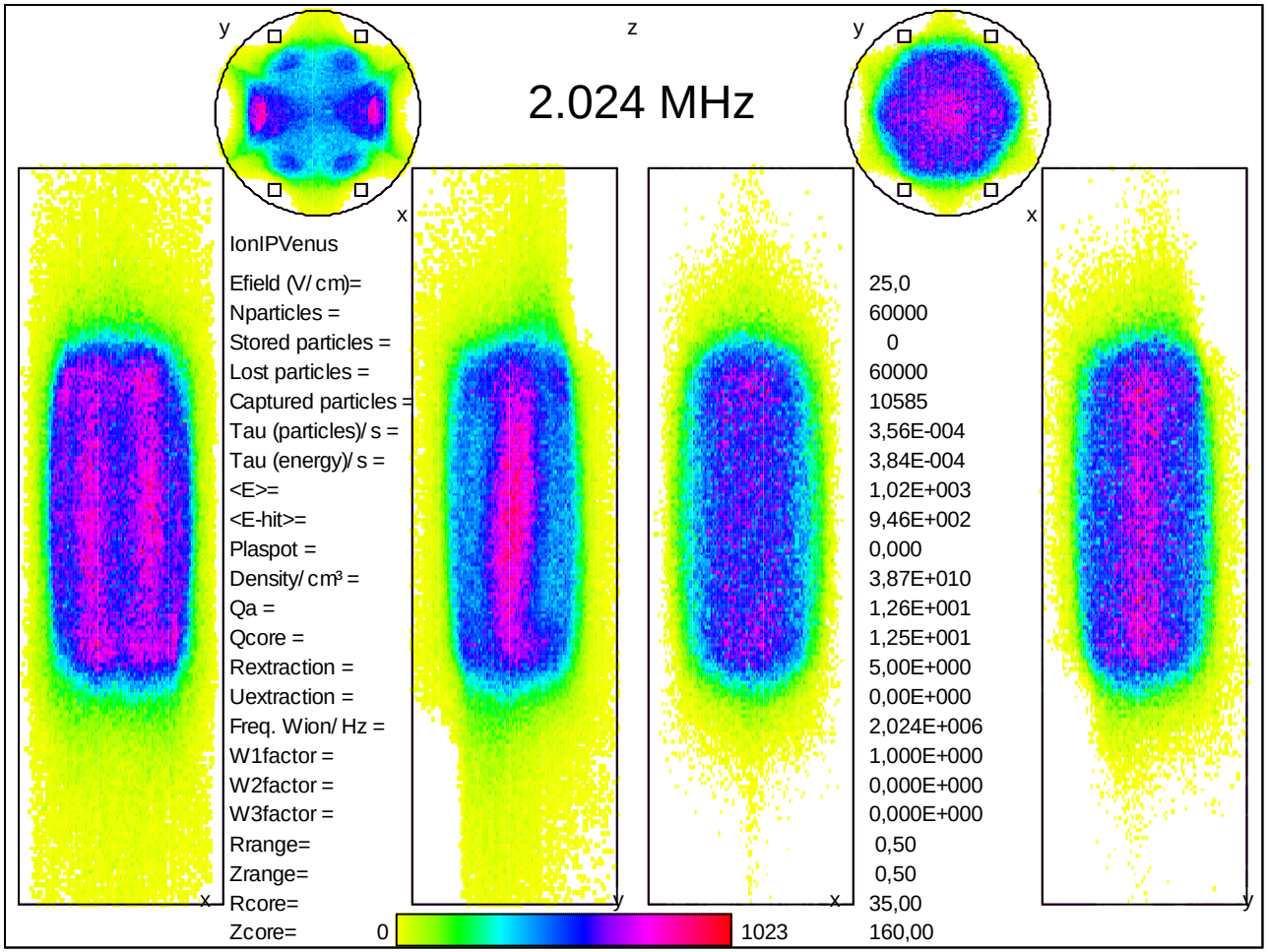
$<E_{hit}>$ = 1.7 keV



ICRH of Ar5+ at 1.062 T, i.e. 62.7 % above the central B_{min} of VENUS

<E> = 1 keV, E_{max} = 9.9 keV, <tau> = 0.36 ms, and tau_{max} = 11 ms

$<E_{hit}>$ = 0.95 keV



The mean free path of an electron before its next collision

depends on the local density and actual energy

$$\lambda(\underline{\mathbf{r}}, E) = 1/\, n_c(\underline{\mathbf{r}}) \bullet \sigma_{tot}(\underline{\mathbf{r}}, E)$$

At every time step one has to recalculate $\sigma_{tot}(\underline{\mathbf{r}}, E)$ and $\lambda(\underline{\mathbf{r}}, E)$

A collsion takes place when $\exp(-x/\lambda) = \exp(-1)$,

One has to add up the distances x_i coverd by each step divided by the local λ_i

Collision when $\sum(x_i/\lambda_i) = 1$

How to start the trajectories ?

The spatial starting conditions should reproduce the final
EDD (Electron Density Distribution)
as regions of highest rate of ionization or production of electrons

Since they are regions of intense ECRH, the most rapid energy gain of the electrons is found in these regions

Electrons are thus started with E_{kin0}=20 eV in arbitrary directions

Their trajectories are calculated during 200 cycles of the µW-field

As soon as electron gains 5 eV it is accepted for simulation

All others are either hitting a wall during this time interval (80 %)
or are on orbits without ever crossing an ECR-zone (10 %)
They are considered as lost for the simulation

Analysis of the trajectories with the goal to obtain the spatial

Electron Density Distribution	DD
Electrons Energy Density Distribution	EDD
Electron Energy Spectrum	ES
Electron Velocity Distribution	VS

in the Stationary State (SS) of the plasma.

The SS of N_0 electrons simultaneously present in the plasma

can be probed periodically every $t_{probe} \approx 200$ periods of μW

to get the informations $\underline{\mathbf{r}}$, $E(\underline{\mathbf{r}})$, E, $\underline{\mathbf{v}}(\underline{\mathbf{r}})$ for the above distributions

Independent of its lifetime each of the N_0 electrons

is thus probed periodically until it hits a wall

This is equivalent to periodically probing every single electron started at time zero during its whole time of existence before it hits a wall

The SS is thus reproduced by calculating the trajectories of each of the N_0 electrons and probing its properties periodically until it hits a wall

The informations **r**, E(**r**), E, **v**(**r**) are stored at every probe in the corresponding cubic or rectangular volumes the plasma chamber has been divided in to yield the distributions wanted