# Atomic-physics approach for determination of charge-state fractions and mean charges for heavy and superheavy ions in the dilute gases

J. Khuyagbaatar*, **V.P. Shevelko****

* HIM, Mainz and GSI, Darmstadt
** Lebedev Physical Institute, Moscow,
GSI, Darmstadt and HIM Fellowship
from 01.06 – 31.10, 2017

**TASCA-2017, GSI**
**September 1, 2017**

Mean charges <q> ($\langle q \rangle = \Sigma q F_q$, $F_q$ is the charge-state fraction) are key values in detection of heavy and superheavy elements with the help of the gas-filled separators. To estimate mean charges <q>, empirical and semiempirical formulae are often used (e.g., Bohr, Schiwietz, Nikolaev and others). However, these formulae do not include dependencies on the atomic structure of colliding particles, the density effect (gas-pressure dependence) and other characterictics.

Here, an atomic treatment for determination of <q> values is considered, based on atomic physics calculations, i.e., on finding the loss and capture cross sections and solving the balance rate equations for the charge-state fractions. The results, presented here, demonstrate an example of how atomic and nuclear physics are related with each other.

# Contents:

1. Atomic physics approach for determination of the charge-state fractions $F_q$ and mean charges <q>.

2. Determination of charge-changing cross sections for electron-loss EL and electron-capture EC processes.

3. Equilibrium mean charges and comparison with experimental data obtained at TASCA/GSI.

4. Dynamics of charge-state fractions and mean charges as a function of the target thickness. A newly created BREIT code as an affective tool to solve this problem.

5. Numerical calculations and prediction of the optimal conditions of the future TASCA experiments with heavy and superheavy ions.

Conclusion

# 1. Atomic approach

## Balance rate equations for change-state fractions $F_q(x)$:

(H.D. Betz: Rev. Mod. Phys. 1972)

$$\frac{dF_q}{dx} = \sum_{q' \neq q} F_{q'}(x)\,\sigma_{q'q} - F_q(x) \sum_{q' \neq q} \sigma_{qq'}$$

$$\sum_q F_q(x) = 1$$

**Mean charge:** $$< q > (x) = \sum_q q F_q(x)$$

*x*: target thickness or areal density

$\sigma_{qq'}$ : single- and multiple-electron charge-changing cross sections of loss and capture processes

Atomic approach: determination of the charge-state fractions on the basis of the balance rate equations using loss and capture cross sections which should account for two components:

1. the influence of the **target-density** (gas-solid) effect, i.e. gas-pressure effect,
2. **multiple-electron** loss and capture processes.

These conclusions follow from atomic calculations and experimental data obtained recently at GSI in the works:


J. Khuyagbaatar, V.P. Shevelko, et al. Phys. Rev. A 88, 042703 (2013)

Barth, W., Adonin, A., Düllmann, Ch. E., et al. Phys. Rev. Special Topics - Acce;erators and Beams 18, 040101 (2015)

Scharrer , P., D¨ullmann, Ch. E.,et al PR Acce and beams 20, 043503 (2017)

# 2. Charge-changing cross section calculations

The main charge-changing processes are :

1. multi-electron *loss* (projectile ionization):

$$X^{q+} + A \rightarrow X^{(q+m)+} + \Sigma A + m e^{-},\ m \geq 1$$

2. multi-electron *capture*:

$$X^{q+} + A \rightarrow X^{(q-k)+} + A^{k+},\ k \geq 1$$

**Multiple-electron cross sections in $U^{q+}$ + Ar collisions at 3.5 MeV/u**

(exp. by R.Watson et al., NIMB **227**, 251 , 2005) (in $10^{-18}$ $cm^2$)

| q | EC single | EC total | EL single | EL total |
|---|---|---|---|---|
| **28** | **12.6** | **12.6** | **13.4** | **40.6** |
| **31** | **19.7** | **20.8** | **12.5** | **34.7** |
| **33** | **25.0** | **27.0** | **8.7** | **26.3** |
| **39** | **52.3** | **60.7** | **8.0** | **19.7** |
| **42** | **61.6** | **79.7** | **6.7** | **13.8** |
| **51** | **82.5** | **130.** | **-** | **-** |

**For calculation of charge-changing cross sections a few main computer codes are used:**

**CAPTURE** code for EC, E > 10 keV/u,

**ARSENY** code for low-energy EC, 10 eV/u < E < 10 keV/u,

**RICODE-M** code for the binding energies and LOSS cross sections (high and relativistic energies),
E = 50 keV/u – 10 GeV/u,

**DEPOSIT** code for one- and multiple-electron loss at low and intermediate energies 50 keV/u < E < 500 keV/u.

(see review paper by I.Tolstikhina, V.Shevelko. Physics – Uspekhi, 56, 213 (2013))

# 3. Equilibrium mean charges for heavy and superheavy ions

## **Equilibrium fractions:** $\mathbf{d}F_q(x)/\mathrm{d}x \rightarrow 0$

$$0 = \sum_{q' \neq q} F_{q'} \sigma_{q'q} - F_q \sum_{q' \neq q} \sigma_{qq'}$$

$$\sum_q F_q = 1$$

System of linear arithmetical equations.

For single-electron loss and capture cross sections, the system has analytical solution, expressed via ratios of loss-to-capture cross sections.
For 4 charge-state model:

$$F_0^\infty = \frac{1}{1 + \frac{\sigma_{01}}{\sigma_{10}}\left(1 + \frac{\sigma_{12}}{\sigma_{21}}\left(1 + \frac{\sigma_{23}}{\sigma_{32}}\right)\right)}$$

$$F_1^\infty = F_0^\infty \frac{\sigma_{01}}{\sigma_{10}}$$

$$F_2^\infty = F_1^\infty \frac{\sigma_{12}}{\sigma_{21}} = F_0^\infty \frac{\sigma_{01}}{\sigma_{10}} \frac{\sigma_{12}}{\sigma_{21}}$$

$$F_3^\infty = F_2^\infty \frac{\sigma_{23}}{\sigma_{32}} = F_0^\infty \frac{\sigma_{01}}{\sigma_{10}} \frac{\sigma_{12}}{\sigma_{21}} \frac{\sigma_{23}}{\sigma_{32}}$$

$$F_0^\infty + F_1^\infty + F_2^\infty + F_3^\infty = 1$$

$$F_{q+1} = F_q \frac{\sigma_{EC}(q+1,q)}{\sigma_{EL}(q,q+1)}$$

$\sigma_{10}$ $\sigma_{21}$ $\sigma_{32}$ : EC cross sections
$\sigma_{01}$ $\sigma_{12}$ $\sigma_{23}$ : LOSS cross sections

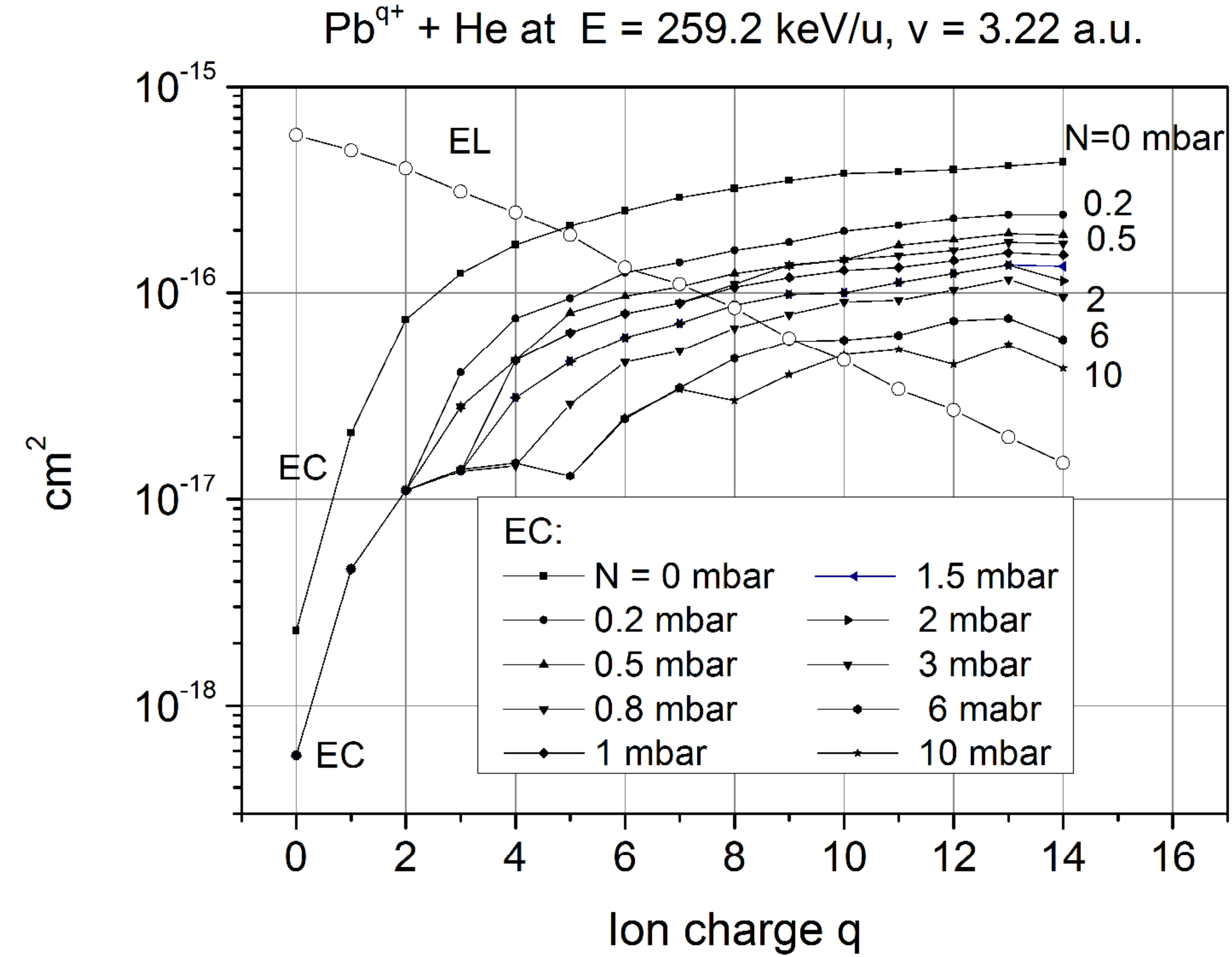
H.D.Betz. Rev. Mod. Phys. (1972)

# Charge-state eqilibration of heavy and superheavy ions

For the first time, atomic approach was applied in:

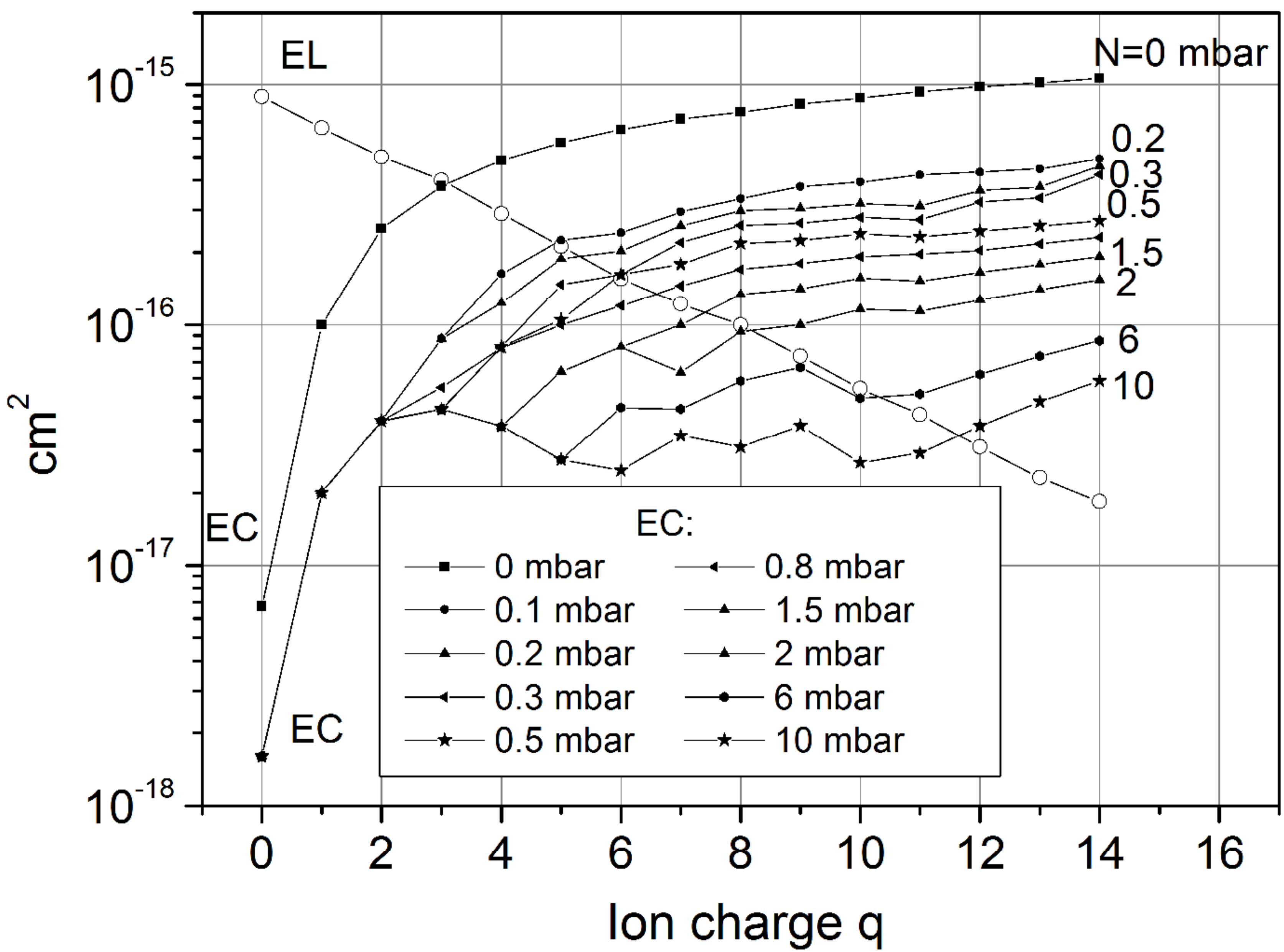
J. Khuyagbaatar, V.P.Shevelko et al., Phys. Rev. A 88, 042703 (2013)

for determination of the equilibrium charges <q> for heavy and superheavy elements with Z = 80 – 120, measured at TASCA/GSI, where 20 % agreement between theory and experiment was achieved.



Pb$^{q+}$ + He at E = 259.2 keV/u, v = 3.22 a.u.
EL
N=0 mbar
0.2
0.5
2
6
10
EC
EC
EC:
N = 0 mbar
0.2 mbar
0.5 mbar
0.8 mbar
1 mbar
1.5 mbar
2 mbar
3 mbar
6 mabr
10 mbar
cm$^2$
Ion charge q

# $No^{q+}$ + He at E = 144 keV/u, v = 2.4 a.u.

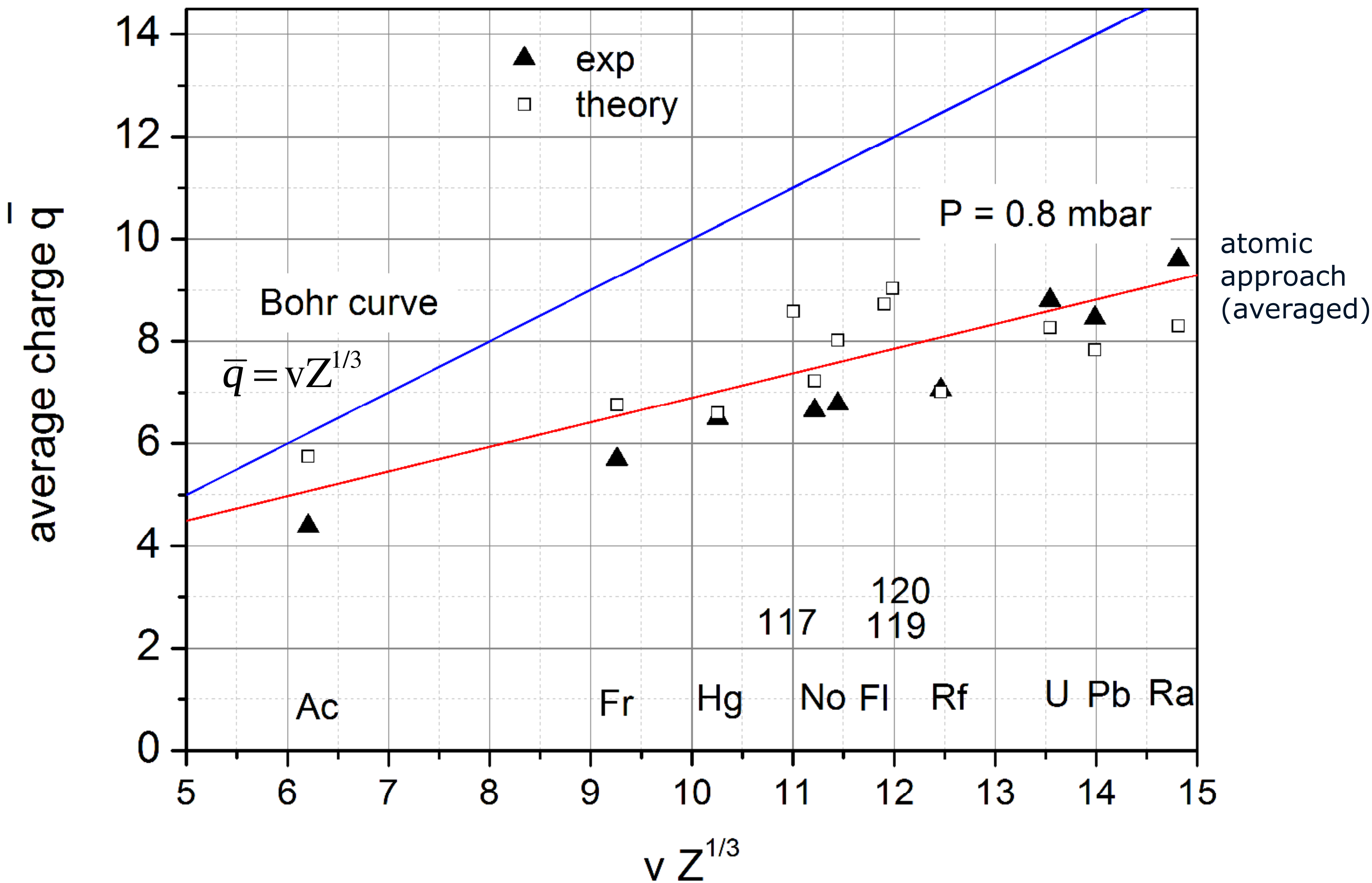


# Equilibrium mean charges <q> of heavy and super heavy elements

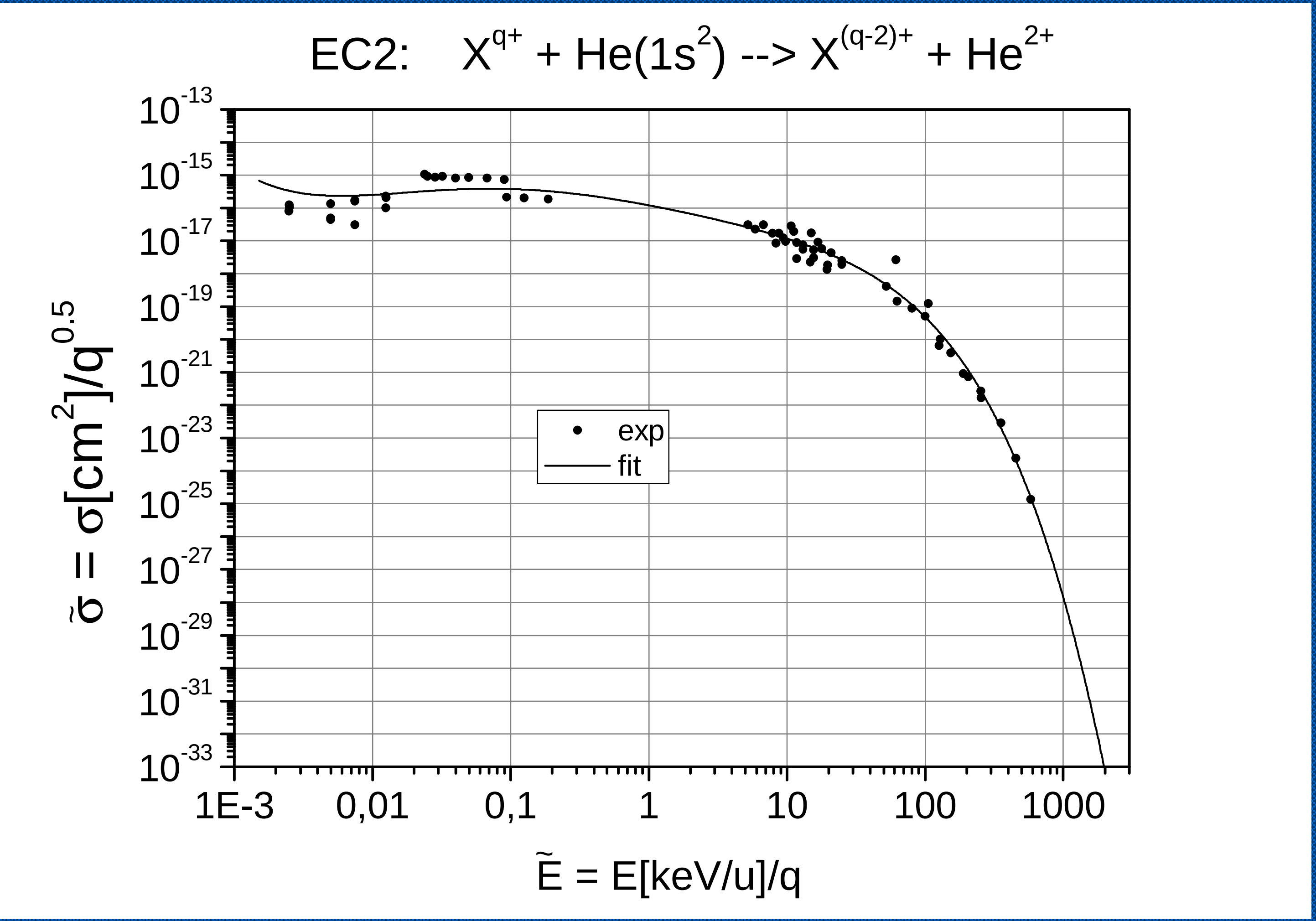
J. Khuyagbaatar et al., Phys. Rev. A 88, 042703 (2013)

| Element | Z | v a.u. | <q>exp | <q>th | $\|\Delta q\|$ | Bohr | Schiwietz |
|---|---|---|---|---|---|---|---|
| Hg | 80 | 2.38 | 6.50 | 6.60 | 0.10 | 12.2 | 9.07 |
| Pb | 82 | 3.22 | 8.45 | 7.83 | 0.62 | 14.0 | 10.6 |
| Fr | 87 | 2.09 | 5.70 | 6.76 | 1.06 | 9.26 | 6.46 |
| Ra | 88 | 3.33 | 9.60 | 8.30 | 1.30 | 14.8 | 10.5 |
| Ac | 89 | 1.39 | 4.40 | 5.75 | 1.35 | 6.21 | 4.22 |
| U | 92 | 3.00 | 8.80 | 8.27 | 0.50 | 13.5 | 9.80 |
| No | 102 | 2.40 | 6.65 | 7.23 | 0.58 | 11.2 | 8.30 |
| Rf | 104 | 2.65 | 7.06 | 7.02 | 0.04 | 12.5 | 9.37 |
| Fl | 114 | 2.36 | 6.78 | 8.02 | 1.24 | 11.4 | 8.28 |
| Uus | 117 (Ts) | 2.25 | - | 8.58 | - | 11.0 | 8.19 |
| Uue | 119 | 2.42 | - | 8.73 | - | 11.9 | 8.92 |
| Ubn | 120 | 2.43 | - | 9.03 | - | 12.0 | 9.02 |

TASCA Z = 117: J.Khuyagbaatar et al., Phys. Rev. Lett. 112, 172501 (2014)


exp
theory
P = 0.8 mbar
atomic
approach
(averaged)
Bohr curve
$\bar{q} = vZ^{1/3}$
average charge $\bar{q}$
$v Z^{1/3}$
120
117
119
Ac
Fr
Hg
No
Fl
Rf
U
Pb
Ra
0
2
4
6
8
10
12
14
5
6
7
8
9
10
11
12
13
14
15

# Scaled double-electron capture cross sections of heavy ions in He




V.P. Shevelko et al. NIMB 330, 82 (2014)

# 4. Dynamics of charge-state fractions of heavy and superheavy ions. The BREIT code.

**BREIT** code:

Balance Rate Equations of Ion Transportation –

to solve numerically the balance equations as a function of the target thickness in the **analytical** form using the matrix-diagonalization method:

$$\frac{dF_q}{dx} = \sum_{q' \neq q} F_{q'}(x)\,\sigma_{q'q} - F_q(x) \sum_{q' \neq q} \sigma_{qq'}$$

$$\sum_q F_q(x) = 1$$

Description of the **BREIT** code:
N.Winckler, V.Shevelko et al NIMB 392, 67 (2017)
BREIT is available on-line: http://breit.gsi.de

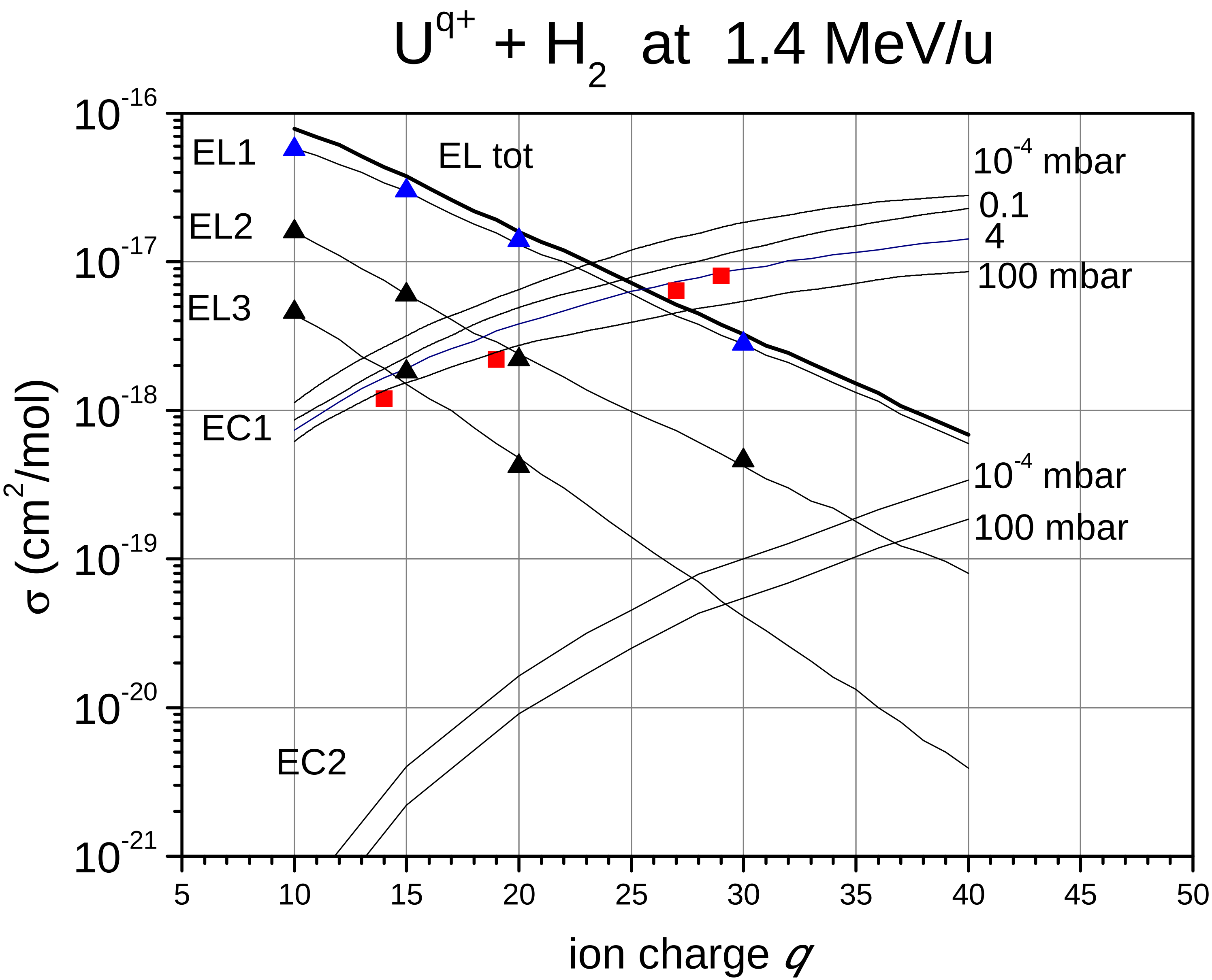
The code can make calculations of up to 200 charge-state fractions at energies 50 keV/u –50 GeV/u. The cross-section values are given in the BREIT input file as theoretical or/and experimental data.

Other codes:

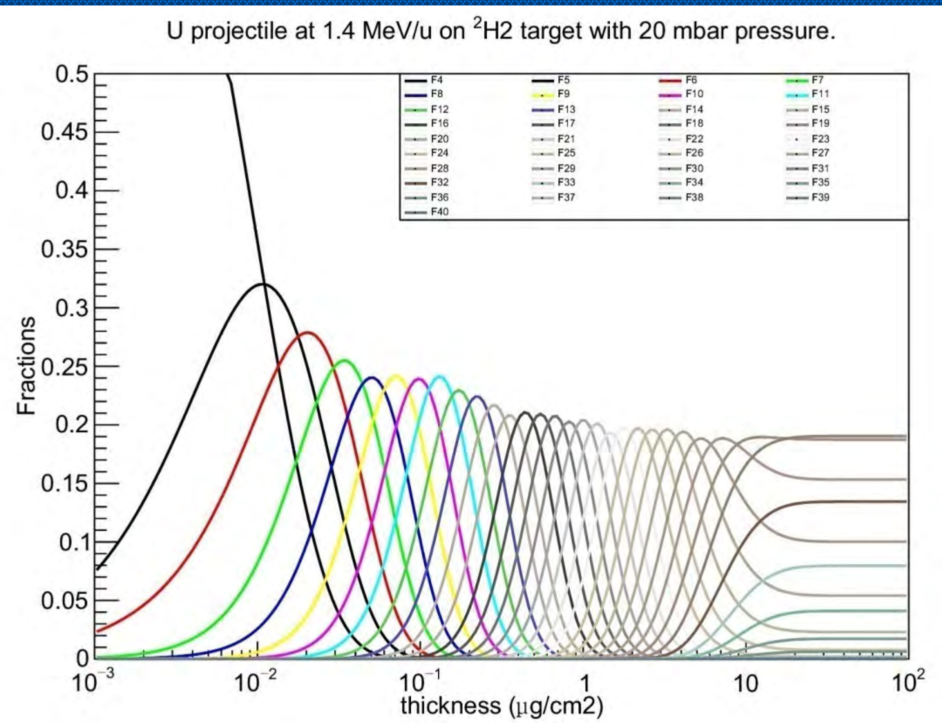
**CLOBAL and CHARGE -** Scheidenberger, C., Stöhlker, et al. NIMB 142, 441 (1998)

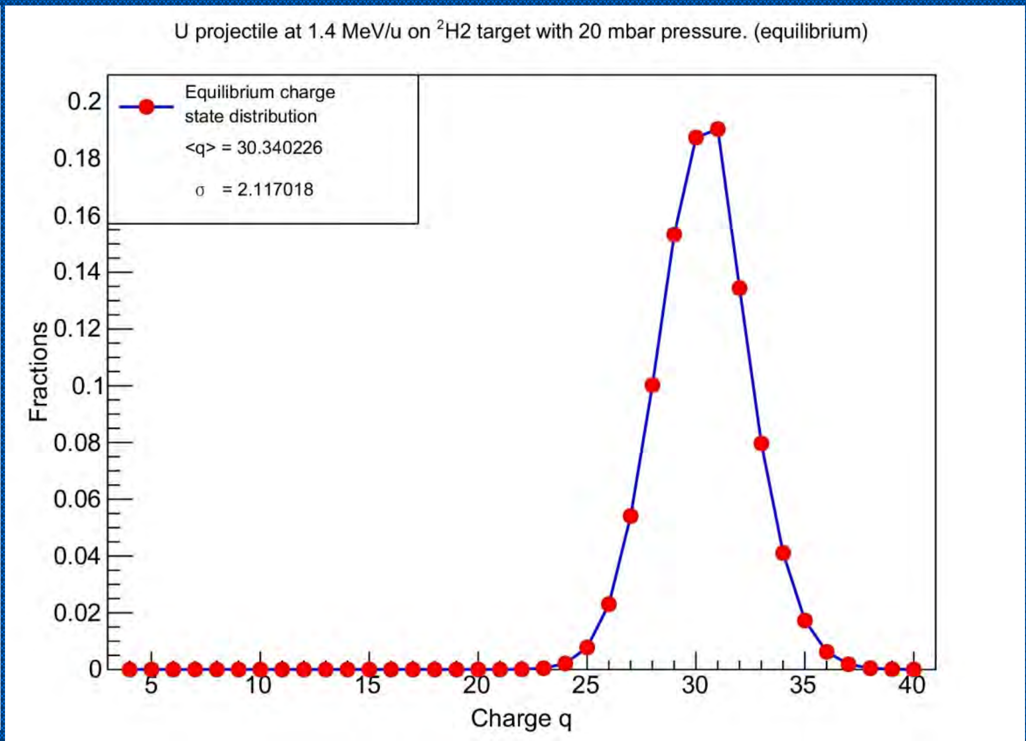
**ETACHA –** Lamour, E., Fainstein, et al. Phys. Rev. A92, 042703 (2015)

# Example of MEL and MEC data for the BREIT.



# Output of the BREIT code for U4+ + H2 collisions at 1.4 MeV/u and 20 mbar pressure of H2.



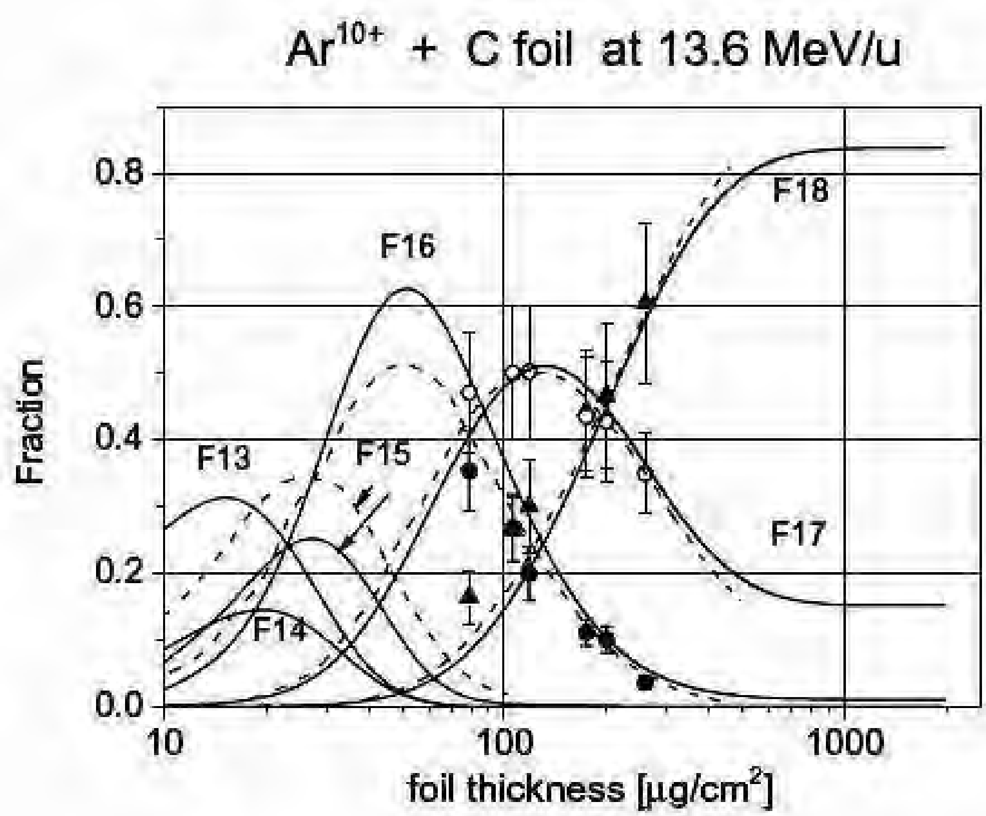



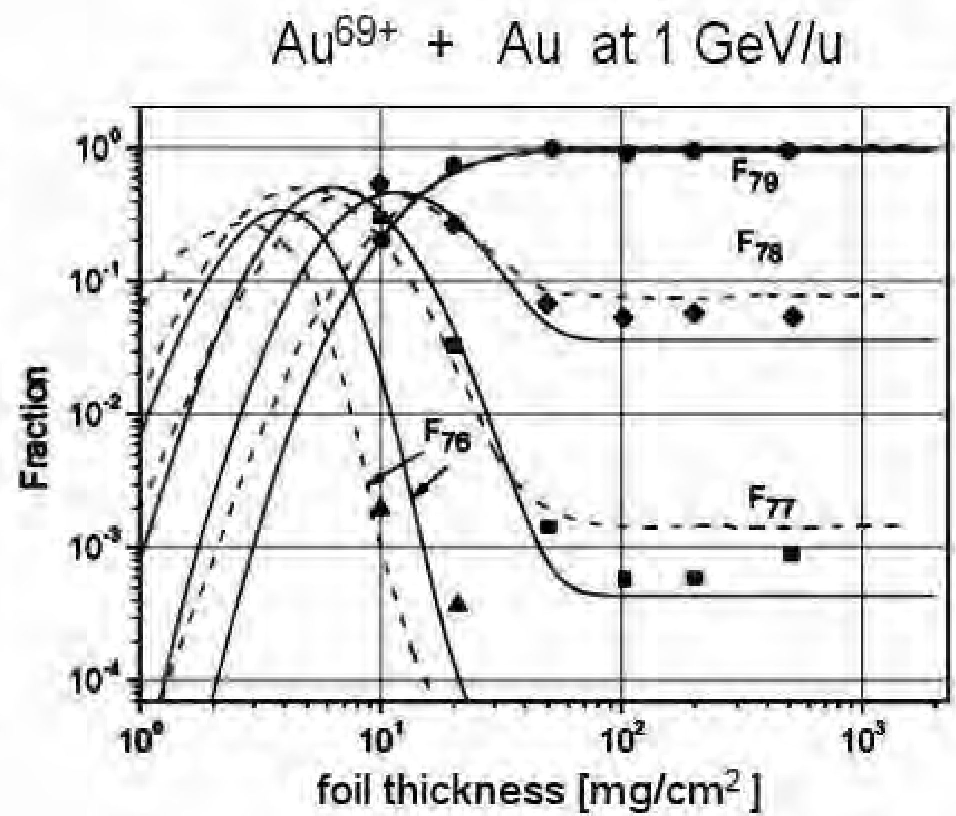

Measuremenst of **non-equilibrium** charge-state fractions in stripping of heavy ions (U, Bi, Ti and Ar) in H2 and He have been recently performed at GSI (**P. Scharrer, Ch. Düllmann et al., Phys. Rev. Acc, and Beams 20, 043503 (2017)**). Preliminary calculations by the BREIT show quite good agreement with experimental data.

# 5. Numerical calculations and prediction of the optimal conditions for charge equilibration of heavy ions

NEW ETACHA - BREIT

GLOBAL - BREIT

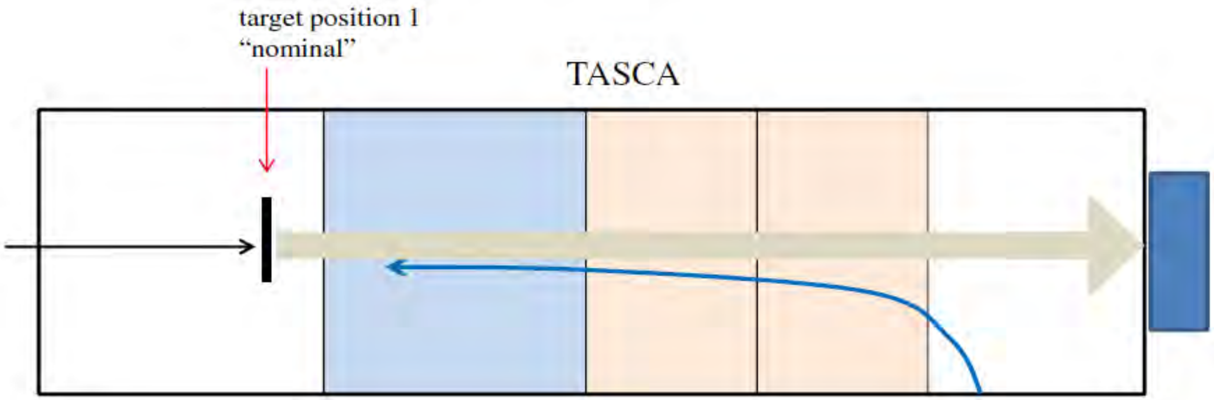



(from N.Winckler, V.Shevelko et al NIMB 392, 67 (2017))

# Heavy ion deflection at gas-filled separators

Observed single Gaussian type of distributions at the focal plane indicates that an average charge state have been established.



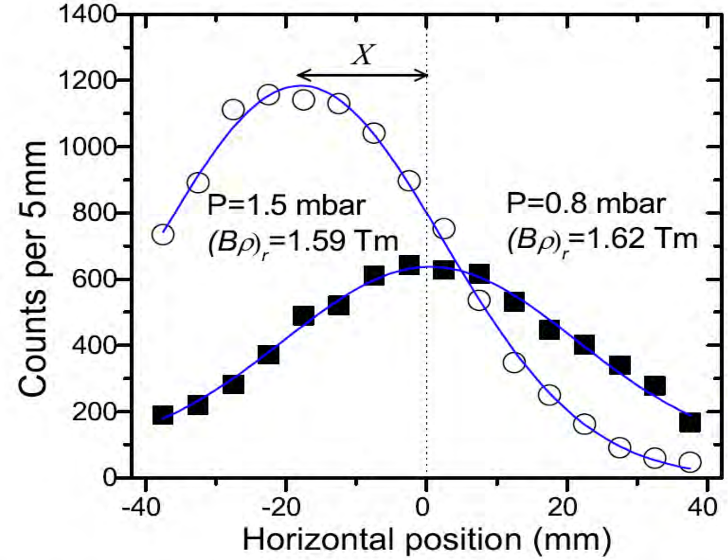
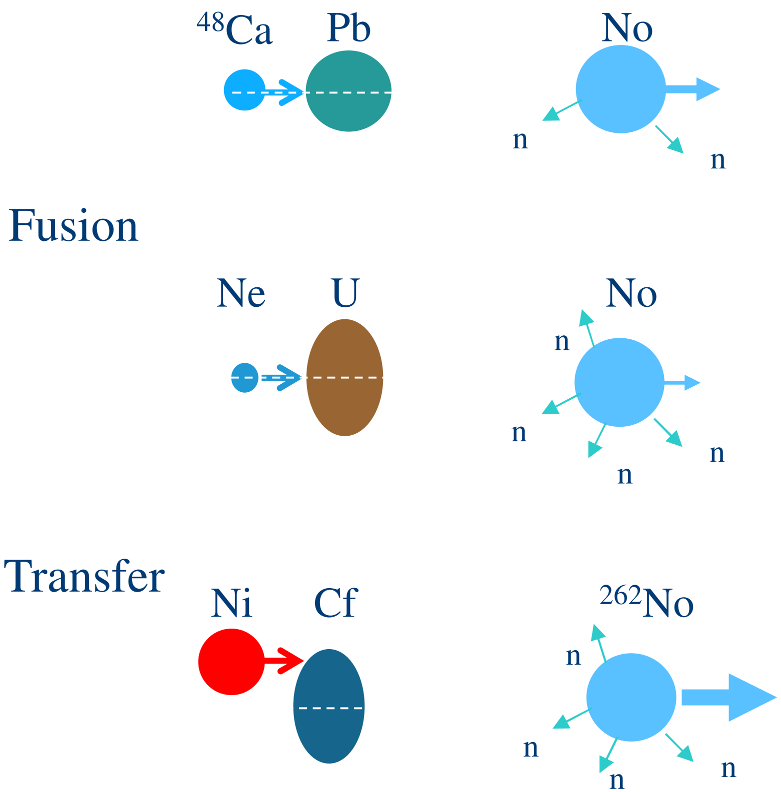




FIG. 1. Experimental distributions of $^{188}Pb$ in the focal plane detector at 0.8 (solid symbols) and 1.5 mbar (open symbols) He pressure. In both cases TASCA was set to the same magnetic rigidity of $(B\rho)_0$=1.62 Tm. Lines show the fitted Gaussians. See text for details.

Total length of TASCA is 350 cm.
An average flight path of ions before entering dipole is about **30 cm**.

**What is the dynamics of charge-state fractions of heavy ions in TASCA ?**

# Which highly charged ions can be produced in gas-filled separators? Nobelium as an example (Z = 102).




$V \approx 177$ keV/u
$\bar{q}_{in} = 20$

$V \approx 39$ keV/u
$\bar{q}_{in} = 10$

$V \approx 500$ keV/u (130MeV)
$\bar{q}_{in} = 31$

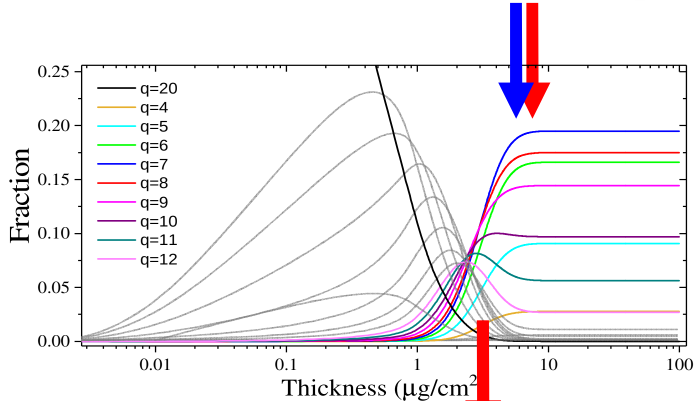
How these No (SHE) ions will behave
in the dilute He gas ?

## $^{48}Ca+^{208}Pb$, $^{254}No$, 177 keV/u, $\bar{q}_{in}$=20(2)

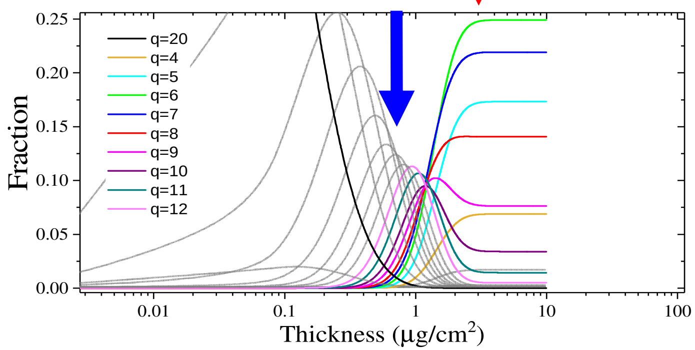
equilibration

30 cm distance to enter TASCA dipole

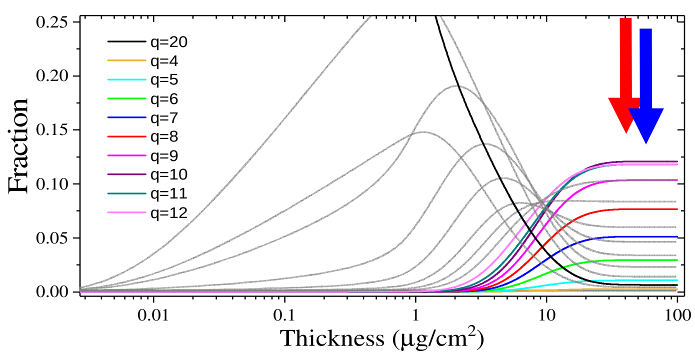
$P_{He}$=0.8 mbar,
d=4.6 μg/cm²

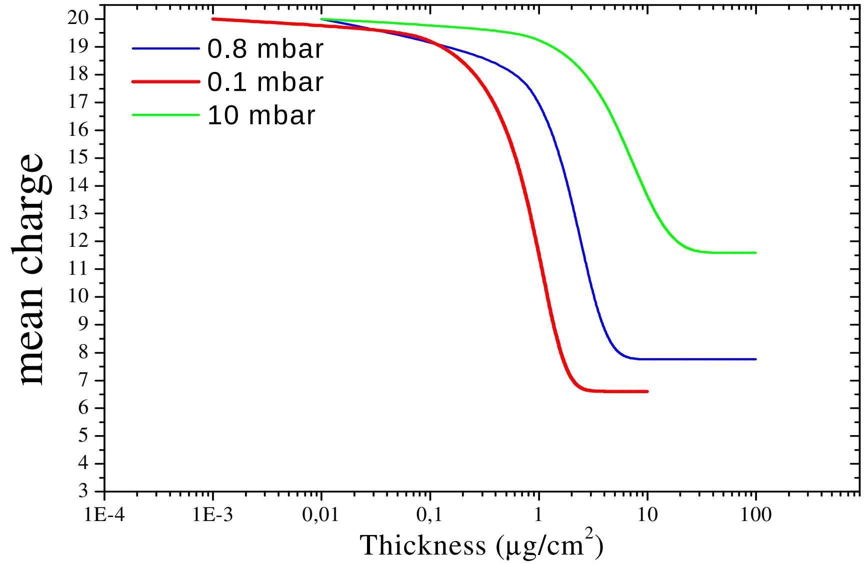



$P_{He}$=0.1 mbar,
d=0.55 μg/cm²




$P_{He}$=10 mbar,
d=54 μg/cm²




equilibration occurs at different thickness and $\bar{q}$ are different due to the density effect which was experimentally observed at **TASCA**

During the deflection in the dipole
**0.8 mbar: Well equilibrated and seems to be optimal**
0.1 mbar: Not yet fully equilibrated and might still have a dynamical effects
10 mbar: Well equilibrated but with wider distribution

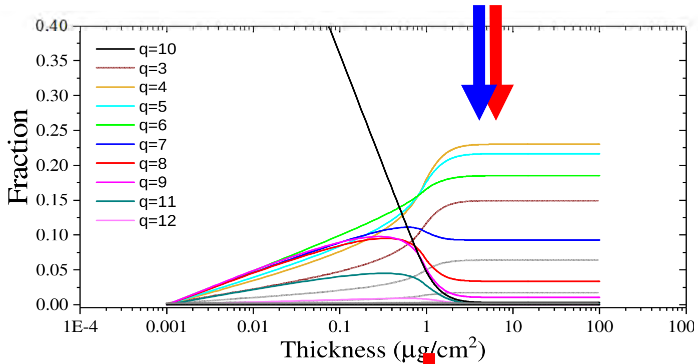
# $^{22}$Ne+$^{238}$U, $^{256}$No, 39 keV/u, $\bar{q}_{in}$=10(2)

equilibration

30 cm distance to enter TASCA dipole

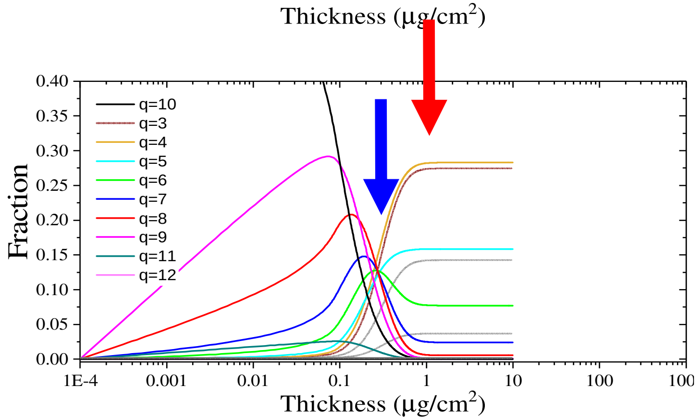
$P_{He}$=0.8 mbar,

d=4.6 μg/cm$^2$



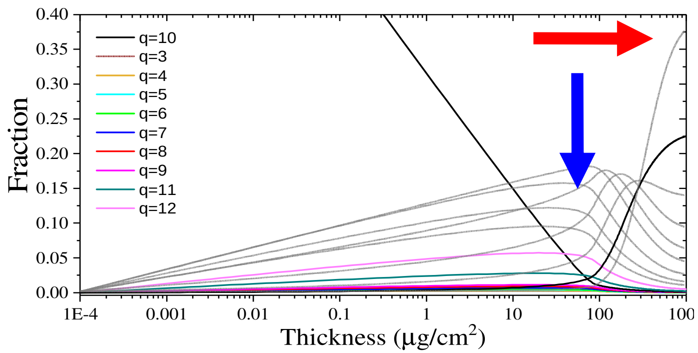

$P_{He}$=0.1 mbar,

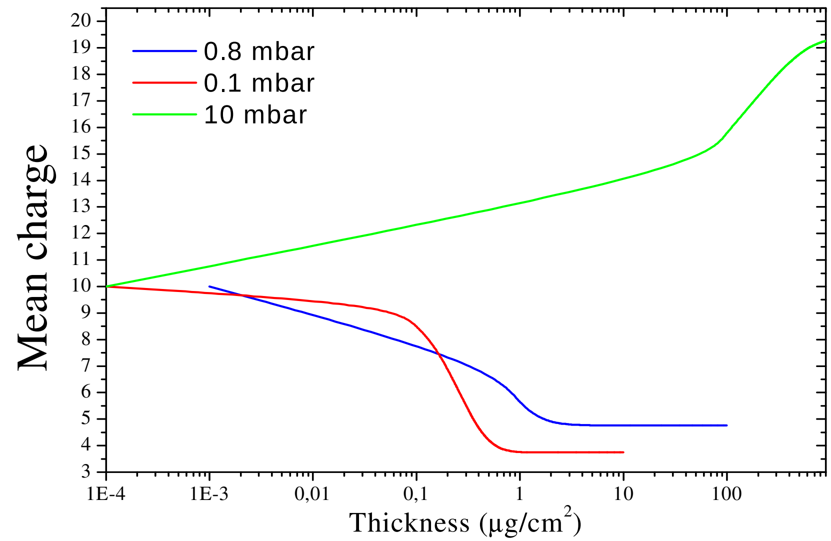
d=0.55 μg/cm$^2$




$P_{He}$=10 mbar,

d=54 μg/cm$^2$




During the deflection in the dipole
0.8 mbar: Well equilibrated
**0.1 mbar: Well equilibrated and narrower distribution. Seems to be optimal**
10 mbar: No equilibration but now the gas is as stripper

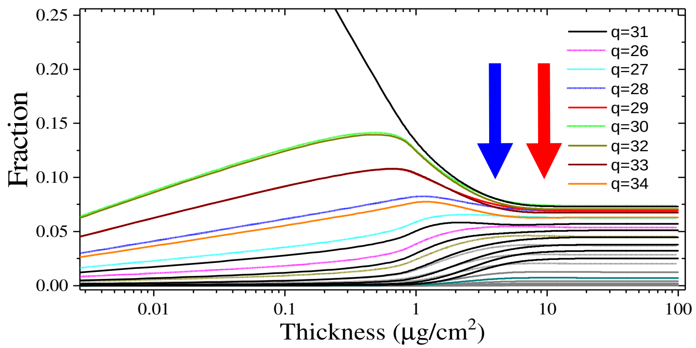
# Ni+Cf, No, 500 keV/u, $\bar{q}_{in}$=31(4)

equilibration

30 cm distance to enter TASCA dipole

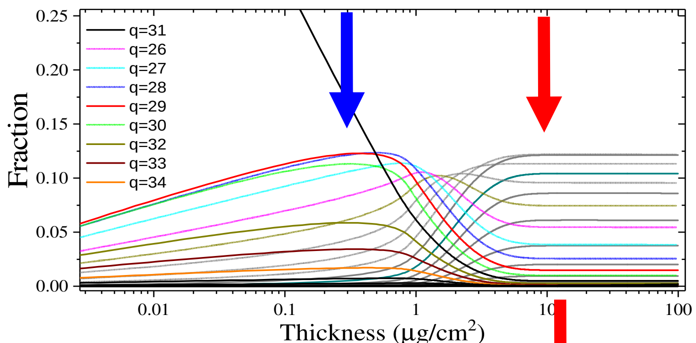
$P_{He}$=0.8 mbar,

d=4.6 µg/cm²



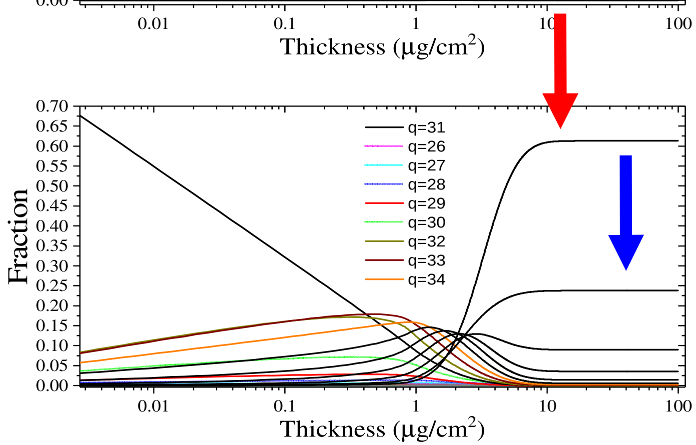

$P_{He}$=0.1 mbar,

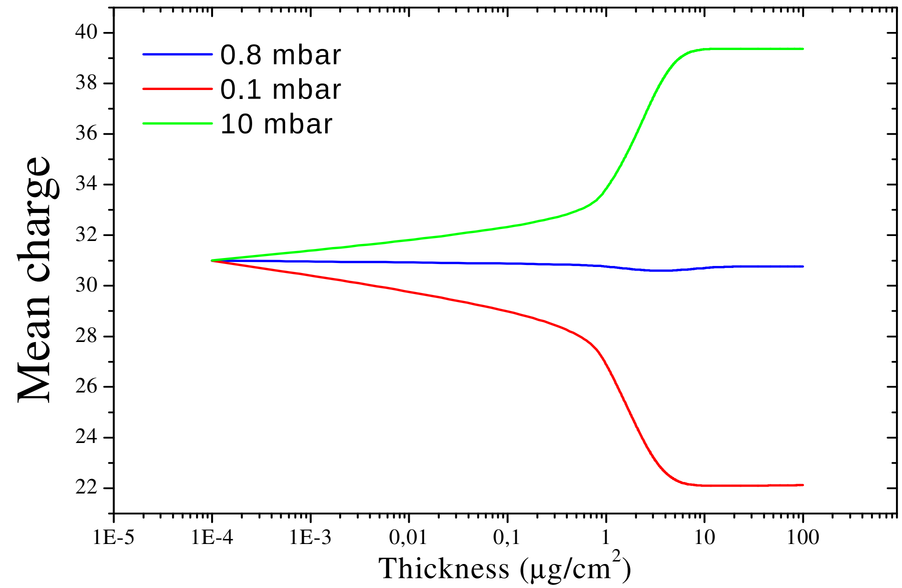
d=0.55 µg/cm²




$P_{He}$=10 mbar,

d=54 µg/cm²




equilibration occurs but still very high $\bar{q}$ (> 11)
and density effect

During the deflection in the dipole
**He pressure can not give a typical charge state for the separation. They will strongly be deflected at TASCA**

# Conclusion

- **Atomic approach**, first applied for description of the equilibrium charge state of heavy and superheavy ions showed a good agreement with experimental data obtained at TASCA/GSI. These results show that the imput cross sections should take into account the target density effect and multiple-electron cross sections.

- Further steps were made to create a new (BREIT) code to investigate **dynamics** of the charge-state fractions
- in collisions of heavy and superheavy ions with matter. The use of the BREIT code provides quite accurate results for description for dynamics of the charge-state fractions and mean charge as a function of the target thickness.

- These results help to understand the observed mean charges of heavy and superheavy ions measured at TASCA separator on the atomic (microscopic) level.

# In collaboration with:

- Ch. Düllmann (HIM and GSI)
- W. Barth (HIM and GSI)
- A. Yakushev (GSI)
- P. Scharrer (GSI)
- N. Winckler (QuanoX, Luxemburg)
- A. Borschevsky (Univ. Groningen, NL)
- I. Tolstikhina (LPI, Russia)
- I. Tupitsyn (St-PSU, Russia)

**Spasibo !**