Simulation of charge breeding for trapped ions

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Abstract. The well established program SUK (Sukze ssive Ionisierung) for the evaluation and graphical presentation of charge state evolution has been improved by including RR (radiative recombination) and CX (charge exchange). It has options for continuous or pulsed feed of single charged ions, ion heating by Coulomb collisions of electrons limited by loss, residual gas pressure and plotting controls. SUK recently has been renamed to CBSIM (charge breeding simulation) and is run from a GUI (graphical user interface). Future developments are intended to make the program universal for any charge breeding simulation, including ECRs.

1. Introduction
For the simulation of the time dependent evolution of charge states in an EBIS (electron beam ion source) [1,2] the program SUK (sukzessive Ionisierung) has been developed many years ago and distributed to interested people around the world. Some feedback [3] has been received, like the extension to 21 different atomic species. In contrast to similar programs, which are around in the EBIS and EBIT community SUK integrates the balance equations for each charge state after transforming time to a logarithmic scale [4]. This is appropriate for the large span of the time evolution, which typically runs from $10^{-6}$ to $10^{4}$ s for singly charged ions to fully stripped heavy ones at a normalized electron current density of 1 A/cm². Besides providing high accuracy this method also reduces the computation time considerably. For sake of simplicity those collision processes have been directly taken into account, which lead to a change of the charge state by more than one. The cross sections used therefore should be considered as effective ones. This approach is also reasonable, when comparing them with measured values [5].

2. Simulation physics
A complete set of differential equations for successive charge states $n_{i-1}$, $n_i$, and $n_{i+1}$, describing the balance of any ion charge state $i$ takes into account ionisation, radiative recombination (RR), charge exchange, and the loss of heated ions by Coulomb collisions from an ion trap (eq. 1): This set of coupled differential equations produces the well known time dependent solutions of stepwise ionization, familiar to EBIS/T and ECRs, which describe the charge state abundances, observed in charge spectra after a given time of confinement. Besides the change of charge state, losses of ions from the trap can also be treated with the term in the second line of eq. 1. The ions are heated by either
\[
\frac{dn}{dt} = n_e \nu_e \left[ \sigma_{i-1 \rightarrow i}^{\text{ion}} n_{i-1} - \left( \sigma_{i-1 \rightarrow i}^{\text{ion}} + \sigma_{i-1 \rightarrow i}^{\text{RR}} \right) n_i + \sigma_{i-1 \rightarrow i}^{\text{RR}} n_{i+1} \right] - n_o \nu_{\text{ion}} \left[ \sigma_{i-1 \rightarrow i}^{\text{chech}} n_i - \sigma_{i-1 \rightarrow i}^{\text{chech}} n_{i+1} \right] - \nu_{\text{coll}} \frac{eU_w}{kT_{\text{ion}}} n_i 
\]

where \( n_e \nu_e \) are density and velocity of the electrons, 
\( n_o \) is the neutral density, 
\( \nu_{\text{ion}} \) is the average thermal ion velocity, \( \nu_{\text{ion}} = \frac{\sqrt{2kT_{\text{ion}}/M_{\text{ion}}}}{kT_{\text{ion}}} \)
\( \sigma \) are the cross sections for ionization, RR, and charge exchange
\( \nu_{\text{coll}} \) is the collision rate for all Coulomb collisions of ions with charge \( i \)
\( U_w \) is the depth of the electrostatic potential well
\( kT_{\text{ion}} \) is the thermal energy of Coulomb heated ions

falling through the radial potential well or by Coulomb collisions with the ionising electrons. The comparison of the well depth \( U_w \) with their thermal energy defines the loss rate according to Boltzmann’s law. The ionisation cross sections used are those from Lotz [6] as described in [7], where also the cross sections for RR are given. The charge exchange cross sections are calculated with the formula of Mueller and Salzborn [8] and the ion heating with a formula derived from Spitzer [2].

3. Simulation results

3.1. EBIS and EBIT mode of stepwise ionisation

Typical charge state evolutions are shown in figures 1 and 2. In EBIS mode all ions are trapped from the beginning of successive ionisation, while for EBIT mode of operation trapping is continuous.

**Figure 1.** Ionisation of an injected amount of argon atoms at an energy of 3.9 keV, which excludes ionisation to \( \text{Ar}^{17+} \) (EBIS mode with shell effect)

**Figure 2.** Trapping and ionisation from a continuous influx of argon atoms at an energy of 6 keV (EBIT mode without radiative recombination and charge exchange)
3.2 Neutralisation and charge exchange in EBIT mode
The effect of space charge neutralisation, which limits the accumulation of more positive charges is shown in figure 3. After reaching the maximum of accumulated charge at $J \times \text{TAU} = 10$ the ionisation balance is determined by self-cooling: $\text{Ar}^{17+}$ and $\text{Ar}^{18+}$ suffer from more electron heating than lower charge states, hence are lost preferentially. Without any losses from the trap, but with charge exchange ionisation will continue, but with much longer ionisation time, as seen in figure 4.

Figure 3. Ionisation and trapping of argon atoms at an electron energy of 6 keV from background gas; neutralisation at $J \times \text{Tau}=10$

Figure 4. Ionisation and trapping of argon atoms at an energy of 6 keV from background gas; charge exchange by a pressure of $10^{-10}$ mbar.

3.3 Limitation of charge evolution by radiative recombination and charge exchange in EBIS mode

Figure 5. Ionisation of lead at an energy of 5.025 keV, which excludes ionisation to Pb$^{55+}$ (EBIS mode with shell effect), but reduced by radiative recombination.

Figure 6. Ionisation of lead at an energy of 5.025 keV but additional charge exchange by a background pressure of $10^{-11}$ mbar.
Charge breeding with an EBIS seems to be most attractive by selecting a charge state, where a closed shell is reached. For lead the electron beam energy then may be selected to 5.025 keV just below the ionisation energy to Pb\(^{55+}\), resulting in highest abundance for Pb\(^{54+}\). This ideal goal is missed due to RR and charge exchange. In figure 5 the reduction of the abundance by RR from 100\% to about 62\% can be seen and in figure 6 the additional reduction by charge exchange at a very low pressure of 10\(^{-11}\) mbar to 45\%. At 10\(^{-9}\) mbar the most abundant charge state would become limited to Pb\(^{51+}\).

4. Future developments

4.1. Different atomic species
While the extension to all atoms of the periodic table has been done recently, the simultaneous charge breeding simulation of different ion species needs to be done. The idea will be that by the strong coupling of Coulomb collisions all ions will have the same temperature, but according to their charge state will differ in their loss rate. This will allow simulation of evaporative cooling.

4.2. Self consistent Poisson solutions
In order to calculate the loss rates unambiguously it will be necessary to compare the kinetic energy of trapped ions with the radial potential well of the partially neutralised electron beam. This will also allow to take into account a radial distribution of the electron beam and its influence on the time dependent overlap of electrons and charge bred ions.

4.3. Incorporation of measured cross sections
A special feature, which has been already tested for carbon, will be the use of measured cross sections. This will result in more accurate simulations and also provide the means to deduce cross sections from time-dependent measurements of charge breeding measurements.

5. Conclusions
The simulation of charge breeding with the program CBSIM exhibits many different results by the choice of parameters. The future development will make the program very general for all charge breeders, including ECR sources. The program is in the public domain and the authors will be happy for any response from users, inviting them to join for the further development.

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