Abstract. Together with space-charge neutralization, ionization and charge exchange in the heavy ion beam fusion (HIBF) chamber can change beam quality and final focusing. Our research here supports simulation of these interactions through exploring theoretical approaches and developing improved models. This study is focused on the multi-electron processes which play an important role for these low-charged high-energy heavy ions. An improved classic trajectory Monte Carlo model and corresponding codes have been developed to simulate the heavy ion-atom collisions, which require intensive computations to solve many-body Hamiltonian Equations. Currently the results from the ion $Xe^q+$ ($q=1$-$18$) colliding with $Xe$ gas show that multi-electron effects are significant, and this cross section can reach about 40% of the total. The improved code is expected to be an integral part of a plasma simulation package designed to study the atomic effects in beam transport and focusing in HIBF using plasma neutralization techniques. This should help provide improved physical insight into current HIBF experiments and future studies.

1. Introduction

In heavy ion beam fusion (HIBF), the ion beams with energies 10-40 MeV/amu are dominated by a strong space charge [1]. This causes a major limitation on the ability to focus all of the beams onto the target. To minimize space charge forces in the accelerator and the reactor chamber, the ion beams should have a low charge state. However, the interaction of fast heavy ions with background gases or plasma used for neutralization involves a combination of electron loss and capture, increasing or decreasing charge states. Thus it neutralization of the high-energy heavy ion beam is very challenging because the electron loss cross-sections largely dominate the electron capture.

Thus, to model beam transport, including space-charge neutralization in the chamber, it is essential to have an accurate knowledge of the beam charge state evolution, which requires cross sections for electron loss and capture. However, to date no accurate experimental or sufficient theoretical data exists for high-energy, low-charge-state, heavy ion cross-sections [2-4]. More measurements and theoretical work are required to provide the data needed for HIBF studies.

2. Theoretical Description

Collisions between the ions such as $Cs^+$, $Xe^+$, $Bi^+$, $U^+$, and $Rb^+$, and the noble gas or Flibe vapor, which is mainly contains $BeF_2$ in a power reactor chamber are the typical scenario in heavy ion fusion. The present study is focused on the interactions between $Xe^q+$ and gases $Xe$ or $N_2$.

The Hamiltonian for these heavy ion-atom systems is given by

\[ H = H_0 + V_{NP-NP} + V_{NP-e} + V_{NT-e} + V_{e-e} \]  

where

\[ H_0 \]  

is the initial Hamiltonian of the ions in the absence of collisions.

\[ V_{NP-NP} \]  

is the potential energy due to the non-parallel interaction between the ions.

\[ V_{NP-e} \]  

is the potential energy due to the non-parallel interaction between the ions and the electrons.

\[ V_{NT-e} \]  

is the potential energy due to the non-parallel interaction between the ions and the neutral atoms.

\[ V_{e-e} \]  

is the potential energy due to the parallel interaction between the electrons.
Here, $p$ is the particle momentum, and $n$ is the number of active electrons in the target $n_T$ or projectile $n_P$. The subscripts $N$ and $e$ indicate nucleus and electron, $P$ and $T$ denote projectile and target respectively.

Among various theoretical approaches for ion-atom collisions, such as the Continuum- Distorted-Wave (CDW) model, semi-classical ones, and classical models such as the classical trajectory Monte Carlo (CTMC) method [2-5], the CTMC is simpler for modelling where couplings are strong. Also it allows all types of collision events. This method has been shown capable of producing satisfactory results for total cross sections. Our calculations are based on an improvement of this approach. In our approach, the cross sections for different events can be expressed through the following sampling equation,

$$
\sigma_{Eve} = \frac{N_{Eve}}{N_{Tot}} \pi b_{\text{max}}^2 \left[ 1 \pm \left( \frac{N_{Tot} - N_{Eve}}{N_{Tot} N_{Eve}} \right)^{0.5} \right]
$$

Here subscript $Eve$ represents specific reactions, such as ionization, excitation and charge exchange, and $b_{\text{max}}$ is the assumed maximum impact parameter.

In heavy ion-atom collisions, the multi-electron processes play a very important role, but are very complex. For example, each ionization or transfer event is actually a combination of many different reaction channels. Also, inner shell electrons must be considered as well as outer-shell ones [6]. These complexities present a major complexity in the study of heavy ion collisions. Different approaches are examined to describe the potentials $V$ between particles, including electron-electron effects in several sub-shells. This is done to obtain accurate results while reducing the number of interactions.

### 3. Results

Based on the above assumptions, the cross sections for Xe$^{q+}$ + Xe collisions are calculated and given below in the energy range of 1-40 MeV/amu. Figure 1 illustrates the target ionization cross-section in the order of $10^{-16}$ ~ $10^{-15}$ cm$^2$ as a function of ion energy, and electron-loss numbers ranging from 1-8. It can be seen that ionization cross section decreases as the charge states increase, mainly due to the increase of ionization energy. The cross sections also drop with increasing energy faster for higher order ionizations. For example, for single ionization, it decreases as $\sigma \sim 1/E^{1.5}$ or $1/v$, and for double ionization, $\sigma$ is $\sim 1/E$.

![Figure 1. Target ionization for Xe$^{q+}$ + Xe](image-url)
Projectile stripping is similar to target ionization, which is shown in Figure 2. At high energies, the projectile ion easily loses an electron instead of undergoing electron capture, especially with a loosely bound outer-shell electron. Together with the target ionization shown above, more electrons are produced. The loss of low-charged heavy ions and electron production compete with each other, changing the net space-charge in the HIBF chamber.

![Figure 2. Ion stripping for Xe\(^{+}\) + Xe](image)

From the above figures, it is seen from the total electron production cross section that the collisions are dominated by the loss of one to three electrons, either from the target or the projectile, especially at higher energies. However, multi-electron loss can account to around 40% of the total loss at lower energies. In addition, both ionization and stripping demonstrate very similar behaviour, except the difference of the cross section amplitude. This is mainly because both centres are very similar in the atomic structure. Some abnormal data that is seen in high-order ionizations may be explained by the more complex multi-electron effects that violate some of the approximations employed.

The calculated cross sections for charge exchange (electron capture) are very small (mostly below \(10^{-18}\) cm\(^2\)), especially at high energies. Thus these are not shown here.

![Figure 3. Projectile Stripping for Xe\(^{18+}\) + N\(_2\) at 2MeV/amu](image)
However, experimental data for Xe$^+ +$ Xe is currently not available. Thus a scaling law derived from other available data (such as Xe$^{18+}$ + N$_2$) is used to test the accuracy and the validity of the CTMC method. This study will be provided in the near future. Here, we calculated the cross sections for as Xe$^{18+}$ + N$_2$ collisions, where the corresponding experimental data are available at 2 MeV/amu [3]. The projectile ions are in the range of 1– 40 MeV/amu. Different approaches for potential calculations are also provided and compared, including Thomas-Fermi, Hartree-Fock, and modified Columbic models. These results are shown in Figures 3 and benchmarked with experimental data. Due to the large statistic errors for higher order ionizations (such as those above 4), those data are not shown in Figure 3. From the results it is obvious that the calculated cross sections are over-estimated, in some cases up to 5 times the experimental data. The Hartree-Fock model gives better performance among these three approaches, mainly due to the improved description of the potential distribution in heavy ions provided by this approach.

4. Conclusions
Using of an improved CTMC method, we calculated the cross sections Xe$^q+$ + Xe (q = 1, 8, 18), and Xe$^{18+}$ + N$_2$ at energies 1 – 40 MeV/amu. Some of these results are shown in Figures 1-3. The figures clearly show that multi-electron effects are significant. The comparison of calculated data with experimental data demonstrates that the Hartree-Fock approach represents the potentials for the multi-electron system better. These results demonstrate the utility of the extended CTMC method developed here. Thus this provides an attractive approach for further study of these important reactions and their effect on beam transport in HIBF chambers.

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