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Veksler and Baldin laboratory of High Energy Physics

FINAL REPORT ON THE SUMMER STUDENT PROGRAM

*Modeling of the ion-ion cooling of highly charged ions in Electron
Beam Ion Sources using Ef software*

Supervisor:

Alexey Boytsov

Student:

Igor Getmanov, Russia
Saint-Petersburg State
University

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Abstract

Electron Beam Ion Sources (EBIS) are commonly used to produce beams of highly generated ions for application in particle physics. Their principle of operation is based on the ion retention in a potential well formed by dense electron flow while ions being ionized[1]. But such flow induces the acceleration of ions both in parallel or perpendicular direction of the electron flow which could make particles overcome the potential barrier and leave the ion bunch[2].

To research the behaviour of ions inside the dense electron beam the Ef software[3] based on particle-particle Coulomb interactions was created by the associates of Joint Institute for Nuclear Research. In this paper Ar¹⁶⁺ was used to obtain the heating rate of ions caused by Coulomb electron-ion encounters in EBIS being modeled with Ef software. Numerical results of the ion heating sufficiently approximate the theoretical dependencies. In order to decrease the mean perpendicular acceleration by ion-ion interaction, inducing of N⁶⁺ and O⁶⁺ separately was also simulated. The results regarding the cooling properties of the above mentioned coolant ions are represented.

1 Introduction

The development of the highly charged ion source is motivated by the JINR "Nuclotron-M" R&D program as a part of nuclotron-based ion collider facility (NICA) project. The primary purpose of NICA is to investigate the phase transitions in quark-gluon plasma formed under heavy ion collisions at the energies of 4,5 GeV/u. Thus, Electron String Ion Source has been developing and improving by the JINR ESIS group since 1994[4].

ESIS principle of operation is based on the potential well formation by the dense electron flow with injection energy $E_{inj} \approx 5$ keV. Then heavy ions become multiply charged by successive inelastic electron impacts while being injected to the electron string[1, 4]. But apart from inelastic interaction of electron beam with ion shell electrons, there is also ion-electron Coulomb interaction that causes ion acceleration in both parallel and perpendicular direction of the incident electrons. The phenomenon of electron-ion elastic Coulomb encounters increases the mean ion velocity[2], hence, making ion gas being heating and leaving the ion bunch. Therefore the percentage of ions yielding the source is very small because of the ion heating[5].

To prevent highly charged ion gas heating, the injection of lighter and less ionized ions as a coolant was proposed. This phenomenon was observed in the experiment with highly charged aurum ions, where the lighter ions of carbon and oxygen formed during evaporation of aurum from a tungsten surface were used as the coolants[4]. The purpose of this work, carried out during the summer student program at JINR, is to perform a simulation of the ion dynamics in an electron beam, depending in the characteristics of the injected coolant ions.

2 Background

The heating of highly charged heavy ions in the process of ionization by a dense electron beam leads to ion gas heating. A quantitative description of the ion gas heating due to its elastic collision with an electron flow was described by Becker[2] using the Rutherford scattering theory. Due to heating, some ions acquire a sufficiently high velocity to overcome the Coulomb barrier formed by the electron beam in the source. Potential energy in the cross section of the ion source, formed by an electron beam, is shown in Fig. 1. Assuming that the ions with a temperature T_{ion} are uniformly distributed in the electron beam, the loss rate R_{loss} for radial escape of an ion in charge state Z will be, according to Boltzmann's law[5]:

$$R_{loss,Z} = \nu_{loss} \exp\left(\frac{-ZeU_{res}}{kT_{ion}}\right), \quad (1)$$

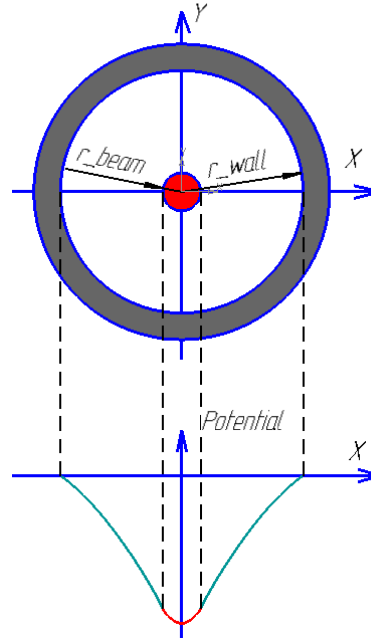


Figure 1: The profile of an Electron Beam Ion Source in a plane perpendicular to the direction of the electron beam[3].

where U_{res} is the residual potential depression in the compensated beam, ν_{loss} is the inverse of the compensation time. The reduction in the effectiveness of EBIS is the result of such losses, since lost ones can no longer be extracted from the source.

To prevent such losses more lighter and less charged ions are used as in Electron Beam Ion sources as coolants. The light ions are favorable as coolants because of the fact that their maximum charge state is limited and they completely ionize much faster than heavy ions, while still remaining cold[5]. The experimental research of ion beam cooling in EBIS using CO gas as a coolant was carried out by Donets[4]. The Fig. 2 illustrates the benefit of the ion-ion cooling in terms of ions yield under various time of coolant gas injection. According to the TOF spectra, the number of ions

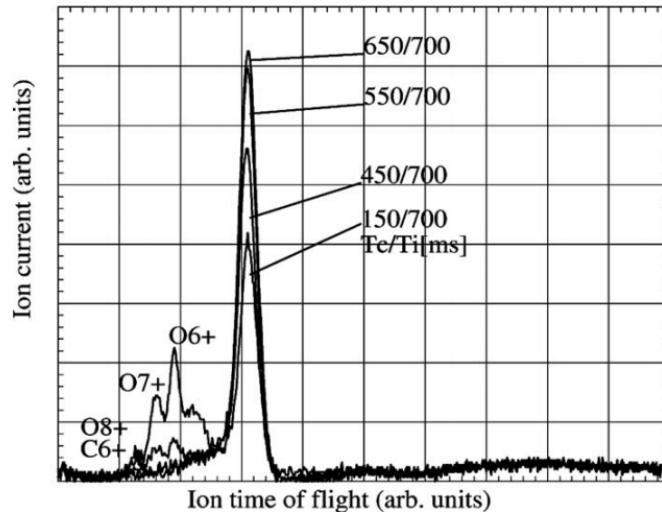


Figure 2: Au ion yield and TOF spectra (mean $q_{Au} = 50.2$) for various injection time of the cooling (CO) gas. $E_{inj} = 4.4$ keV. Total ionization time is $T_i = 700$ ms. The injection time for cooling gas, as shown on corresponding curves, $T_c = 150$ ms, $T_c = 450$ ms, $T_c = 550$ ms, and $T_c = 650$ ms[4].

in the beam increases, with the cooling time of highly charged heavy ions. This fact indicates that, while cooling, a smaller number of ions leaves a potential trap formed by electrons, which leads to an increase in the efficiency of the source.

3 Methods & Techniques

The numerical analysis of the ion dynamics was carried out using Ef software[3], which was created by JINR ESIS group. Ef is a software that is open and available for downloading and modification. It is designed to simulate the dynamics of particles with non-relativistic energies in external electromagnetic fields that is relevant for accelerator and particle physics. Particle self-consistent problem is numerically solved with particle-in-cell method[3].

To model an ion-ion cooling of heavily charged ions, the binary Coulomb interaction model had been implemented as a modification of Ef software during the summer program time. Its principle of operation is based on taking into account all Coulomb forces applied to each simulated particle. It can be easily explained with the equation of motion for i -th particle:

$$m_i \frac{d\vec{v}_i}{dt} = q_i \left(\vec{E}_{ext} + \frac{1}{c} [\vec{v}_i \times \vec{B}_{ext}] \right) + \sum_{j \neq i}^N q_i \vec{E}_j, \quad i = 1, 2, \dots, N \quad (2)$$

where m_i , \vec{v}_i , q_i are the i -th particle mass, velocity, and charge respectively; \vec{E}_{ext} , \vec{B}_{ext} are the electric and magnetic vectors of an external electromagnetic field, \vec{E}_j is the electric field if the point charge of the j -th particle in the point of i -th particle. During the simulation, Ef solves the equation of motion for all N particles each dt time step. This algorithm was successfully tested using the example of the Maxwell-Boltzmann distribution with the variation of the initial conditions, such as: number of initial particles, their momenta and the isolated system scale size.

In this paper, we used parameters corresponding to the real characteristics of EBIS, reduced in scale, in order to increase the counting rate of Ef software. The example of Electron Beam simulation that was used in this work is illustrated in Fig. 3. In a simulation with such geometry,

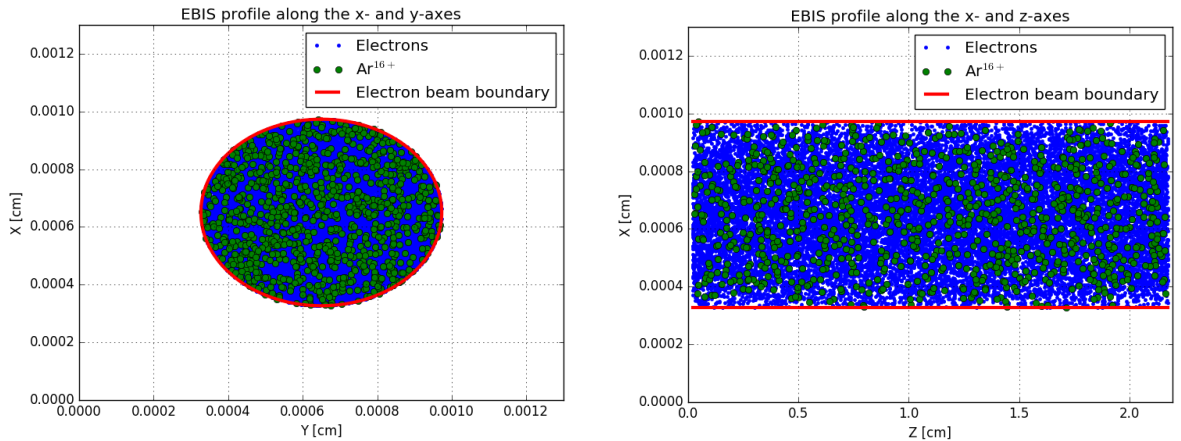


Figure 3: The profiles of the electron beam and injected ions modeled with Ef software, in the XY and XZ planes respectively.

$N_i = 1000$ Ar^{16+} ions are uniformly distributed in a beam of $N_e = 20000$ electrons moving with energies $E_{inj} = 5$ keV. In order to take into account the changes of ion momentum caused by the Coulomb interactions of the particles, with sufficient accuracy, the time step dt was chosen equal to $2 \cdot 10^{-18}$ s.

The next step in this simulation is the injection of the lighter O and N ions as coolers into the beam to estimate the reduction in the increase of the mean highly charged heavy ions over time.

In the course of research the heating and cooling of argon by different ions, the simulation of each case with the same characteristics of problems will perform several times to collect statistics and to approach the actual heating and cooling law. Assuming this, the average velocity value as a function of time will be estimated as the average value of the mean velocities of all M experiments at each time point:

$$\langle v_{\perp\parallel} \rangle = \frac{1}{M} \sum_{k=1}^M (\bar{v}_{\perp\parallel})_k, \quad \delta \bar{v}_{\perp\parallel} = \sqrt{\frac{1}{M-1} \sum_{k=1}^M (\langle v_{\perp\parallel} \rangle - (\bar{v}_{\perp\parallel})_k)^2}, \quad (3)$$

where $(\bar{v}_{\perp\parallel})_k$ is the mean value of either parallel or perpendicular component of ion velocity obtained in k-th experiment, $\langle v_{\perp\parallel} \rangle$ is the average value of all the mean velocities obtained in M experiments, $\delta \bar{v}_{\perp\parallel}$ is the unbiased sample standard deviation of $\langle v_{\perp\parallel} \rangle$.

4 Results

4.1 Ion heating

According to Becker's theoretical studies[2], based on the fact that the increase in the ion velocity in EBIS is due to an electron-ion elastic collision, the variation of the perpendicular and parallel component of the ion velocities can be represented in the following form:

$$\Delta v_{i\parallel} = \frac{2 \frac{m_e}{M_i} v_e}{1 + \left(\frac{\rho}{\rho_0}\right)^2} \quad (4)$$

$$\Delta v_{i\perp} = \frac{2 \frac{m_e}{M_i} v_e \frac{\rho}{\rho_0}}{1 + \left(\frac{\rho}{\rho_0}\right)^2} \quad (5)$$

$$\rho_0 = \frac{Z e^2}{m_e v_e^2}$$

where m_e and M_e are the electron and ion masses respectively, v_e is the electron speed, ρ is an impact parameter. Since the temperature is proportional to the square of the mean velocity of all particles in the ensemble, in this work the measure of particle heating will be characterized as an increase in their average velocity. The averaging of both velocity components will be performed over all impact parameters in the circular cross section of a cylindrical electron beam[2]:

$$\langle v_{\perp\parallel} \rangle_{\rho} = \frac{\int_0^R v_{\perp\parallel} 2\pi\rho d\rho}{\int_0^R 2\pi\rho d\rho}, \quad (6)$$

where R is the beam radius. To obtain the average acceleration acquired by ions at each moment of time, we multiply the components of average velocities by the electron-ion collision frequency:

$$\nu = n_e v_e \pi R^2 \quad (7)$$

Calculating the integrals (6) for both components of the velocities, multiplying by the frequency, we obtain:

$$\langle a_{\parallel} \rangle_{\rho} = 2\pi \frac{m_e}{M_i} n_e v_e \rho_0^2 \ln \left(1 + \frac{R^2}{\rho^2} \right) \quad (8)$$

$$\langle a_{\perp} \rangle_{\rho} = 4\pi \frac{m_e n_e \rho_0^2 v_e^2}{M R^2 \left(\frac{M}{\rho_0} \right)^{3/2}} \left(R \rho_0 \left(\frac{M}{\rho_0} \right)^{3/2} - M \sqrt{M \rho_0} \arctan \left(\frac{R}{\rho_0} \right) \right) \quad (9)$$

Before proceeding to the simulation of the ion-ion cooling, it is necessary to check the correctness of the performance of the created algorithm based on Coulomb interactions. To do this, we simulate the situation of heating an highly charged ion gas with an electron beam.

The Fig. 4 illustrates the results of calculations of the average ion velocities in both perpendicular and parallel directions of the electron flow during the process of electron beam heating in seven identical simulations. The averaged values, according to the formula, over all experiments at each moment of time give a result corresponding to the theoretical function.

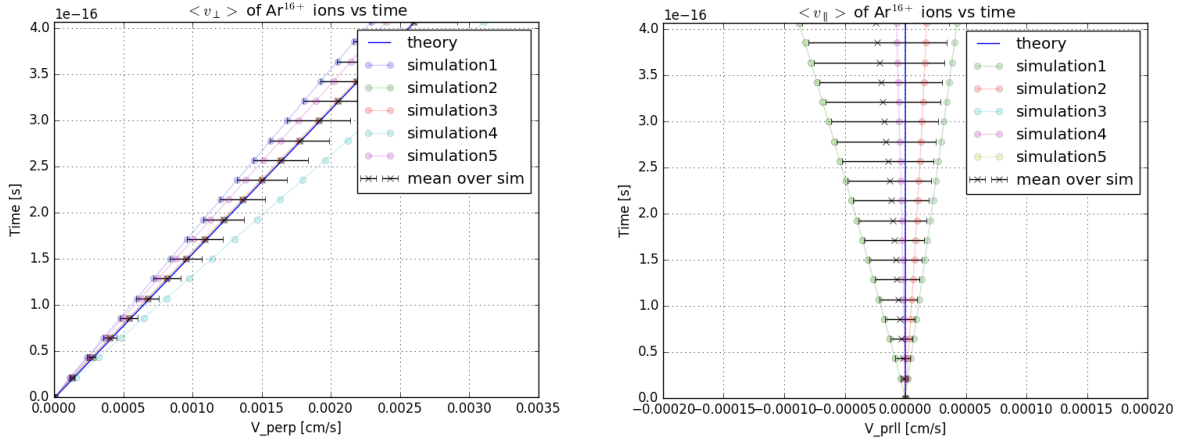


Figure 4: On the left, the average value of the perpendicular velocity component of Au¹⁶⁺ ions to the electron beam direction as a function of time. On the right, the average value of the ion velocity components along the direction of the electron beam in the source.

Approximation of the data obtained from all five simulations by linear regression gives us the value of average ion acceleration:

$$\langle a_{\perp} \rangle_{num} = (6.390 \pm 0.008) \cdot 10^{12} [cm/s^2] \quad (10)$$

Comparing this value with the theoretical:

$$\langle a_{\perp} \rangle_{theor} = 6.384 \cdot 10^{12} [cm/s^2] \quad (11)$$

it can be verified that the experimental data within the error limits correspond to the theoretical values of radial ion acceleration.

4.2 Ion-ion colling

After verifying the correctness of the algorithm operation for heating the ions in EBIS, we proceed to the simulation of ion-ion heating. In this paper, the cooling ions are distributed uniformly over the entire volume of the electron beam at the initial instant of time. The number of cooling

ions is equal to the number of heavy ions ($N_c = 1000$). At the initial time, the ion-coolants are stationary.

Let us consider the effect of cooling ions of two species with the same charge state number Z and different masses M_i on the velocity of heavy highly charged ions in the source. Since the loss of ions in the source occurs predominantly in its radial direction of the velocity, in this paper we will consider the dependence of the perpendicular component of the ion velocity in the direction of motion of the electron beam. The Fig. 5 illustrates the dependence of the O^{6+} ion-velocity component perpendicular to the motion of the electron beam on time, formed by initializing seven simulations with identical initial conditions.

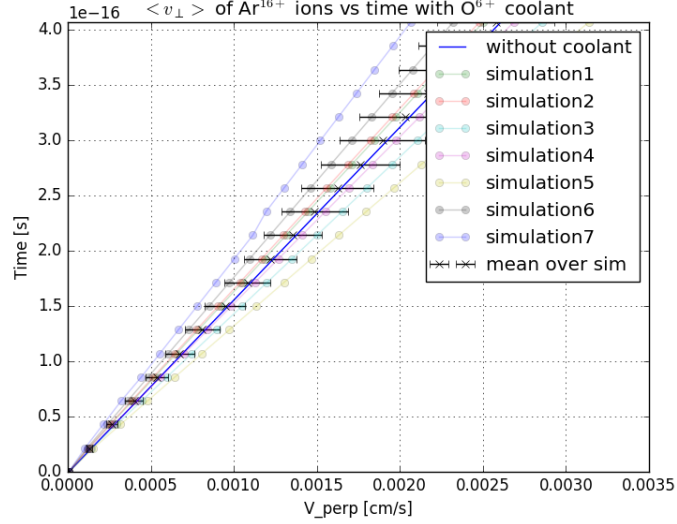


Figure 5: The average value of the Ar^{16+} velocity components perpendicular to the direction of electron beam motion in the source with O^{6+} coolant as a function of time

The linear regression, based on data averaged over all seven experiments, according to (3) formulas has the form:

$$\begin{aligned} \langle v_{\perp} \rangle (O^{6+}) &= 6.337 \cdot 10^{12} \cdot t + 6.387 \cdot 10^{-6} \\ \langle a_{\perp} \rangle_{num} (O^{6+}) &= (6.337 \pm 0.011) \cdot 10^{12} [cm/s^2] \end{aligned} \quad (12)$$

The parallel component of the ion velocity, according to a sample of seven identical simulations, illustrated in Fig. 6 has a greater scatter, but the average value is slightly different from zero.

In the following example, five simulations of electron-ion heating of Ar^{16+} were initialized with the same conditions as in the previous examples, but now, N^{6+} was taken as a coolant. The results of the average values of perpendicular component of highly charged argon ion velocities are represented in Fig. 7.

The linear regression approximating the averaged data of the average perpendicular velocity components of Ar^{16+} for all five simulations has the following form:

$$\begin{aligned} \langle v_{\perp} \rangle (O^{6+}) &= 6.173 \cdot 10^{12} \cdot t + 4.184 \cdot 10^{-6} \\ \langle a_{\perp} \rangle_{num} (O^{6+}) &= (6.173 \pm 0.009) \cdot 10^{12} [cm/s^2] \end{aligned} \quad (13)$$

According to the data obtained during the simulation, the slope of the direct regression of the mean value of the perpendicular velocity component of high-charge heavy ions when heated by an electron beam is smaller in the presence of coolants. Since the gas temperature is a measure of the

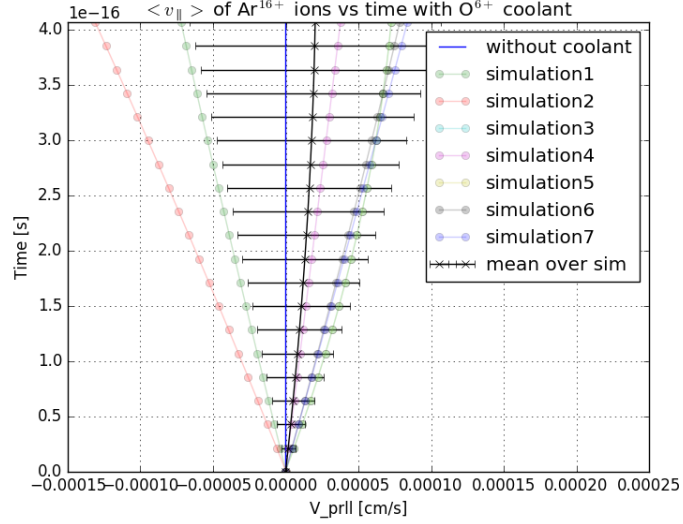


Figure 6: The average value of the Ar^{16+} velocity components parallel to the direction of electron beam motion in the source with O^{6+} coolant as a function of time

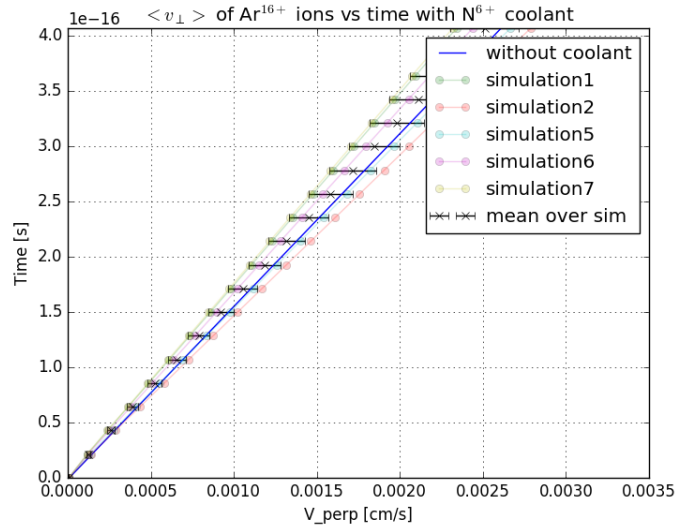


Figure 7: The average value of the Ar^{16+} velocity components perpendicular to the direction of electron beam motion in the source with N^{6+} coolant as a function of time

average motion of its particles, then, referring to the simulation results, light ions show themselves as good coolers of gas consisting of heavier ions. Comparing the coefficients of the slope of the velocity perpendicular component average value of argon ions, being cooled by O^{6+} and N^{6+} ions, it can be said that ions with a lower mass are better coolants. This can be demonstrated from the relations of the average acceleration of particles (10, 13,) in the perpendicular direction to the electron beam:

$$\langle a_{\perp} \rangle_{num} > \langle a_{\perp} \rangle_{num} (\text{O}^{6+}) > \langle a_{\perp} \rangle_{num} (\text{N}^{6+})$$

$$M_{\text{O}^{6+}} > M_{\text{N}^{6+}}$$

This result can be physically interpreted by the fact that the lighter ions are less inert, and take the greater part of the kinetic energy transferred during the ion-ion interaction with the heated heavy ion. Thus, as a result of this interaction, the heavier ion gas heats up more slowly.

5 Conclusions

To sum up, during the summer program at JINR, the following results regarding the modeling of the dynamics of charged particles have been obtained:

1. The Ef software was mastered and modified taking into account the particle-particle Coulomb interaction. The modification was successfully tested for determining of the Maxwell-Boltzmann distribution.
2. The heating of highly charged heavy ions in EBIS by the electron-ion interaction was simulated in accordance with the real parameters of the problem. The results show sufficient correlations with theoretical predictions.
3. Through the simulation, the effect of gases consisting of ions of different masses on cooling of the investigated highly charged heavy ions was observed. According to the results, the better coolants are likely to be lighter ions, rather than heavy ones.

During the summer program in JINR, the abstracts of the report were submitted at an open physical forum at PNPI in Gatchina that will be held on November, 21-23, where the results of this paper are planning to be presented.

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