CHAPTER 3

SIMULATIONS OF DECELERATION LENS SYSTEM

This chapter shows simulations of the deceleration lens and the ion bending after passing through the parallel electric field plates using the SIMION program (version 8.0).

3.1 SIMION program version 8.0

The models in this thesis are simulated by the SIMION program version 8.0. The usefulness of the SIMION program is that the first, it reduces cost and time for construction a real model and the second, we can estimate the ion's trajectories. SIMION is an electrostatic and magnetic field modeling program. It is designed to study electrostatic and magnetic fields and forces created by a collection of shaped electrodes given certain symmetry assumptions (Manura and Dahl, 2008). Electrostatic and magnetic fields can be modeled as boundary value problem solutions of an elliptical partial differential equation called the Laplace equation. The specific method used within SIMION is a finite difference technique called over-relaxation which is applied to two or three dimensional potential arrays of points presenting electrode (pole) and non-electrode (non-pole) regions. The relaxation technique has

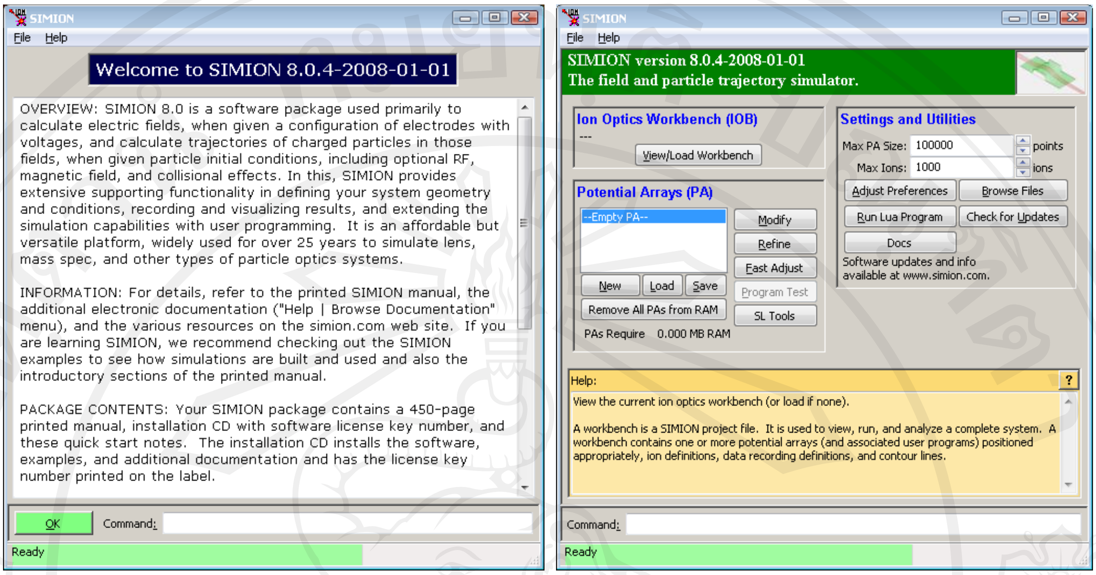

Figure 3.1. The features of SIMION program version 8.0 which is used for the simulations in this thesis.

the advantage that normal numerical computation errors are minimized, solutions are quite stable, and computer memory storage requirements are minimized. However, its disadvantage is that the exact number of iterations required for a given level of refining is quite variable and initially unknown for each specific solution. The feature of SIMION program version 8.0 is shown in Figure 3.1.

3.2 Deceleration lens simulation

The deceleration lens is designed by the SIMION program version 8.0 in order to use in the biophysics field for bombardment of biological materials at ultra low ion beam energy. The simulations used a retarding electrostatic field for decelerating ions to reduce their energies. The deceleration was aimed at: (1)

decreasing ion beam energies in orders of keV to 10 eV, (2) focusing the beam at the target, (3) maintaining high ion transmission, and (4) making mechanical simplicity for practical construction and alignment.

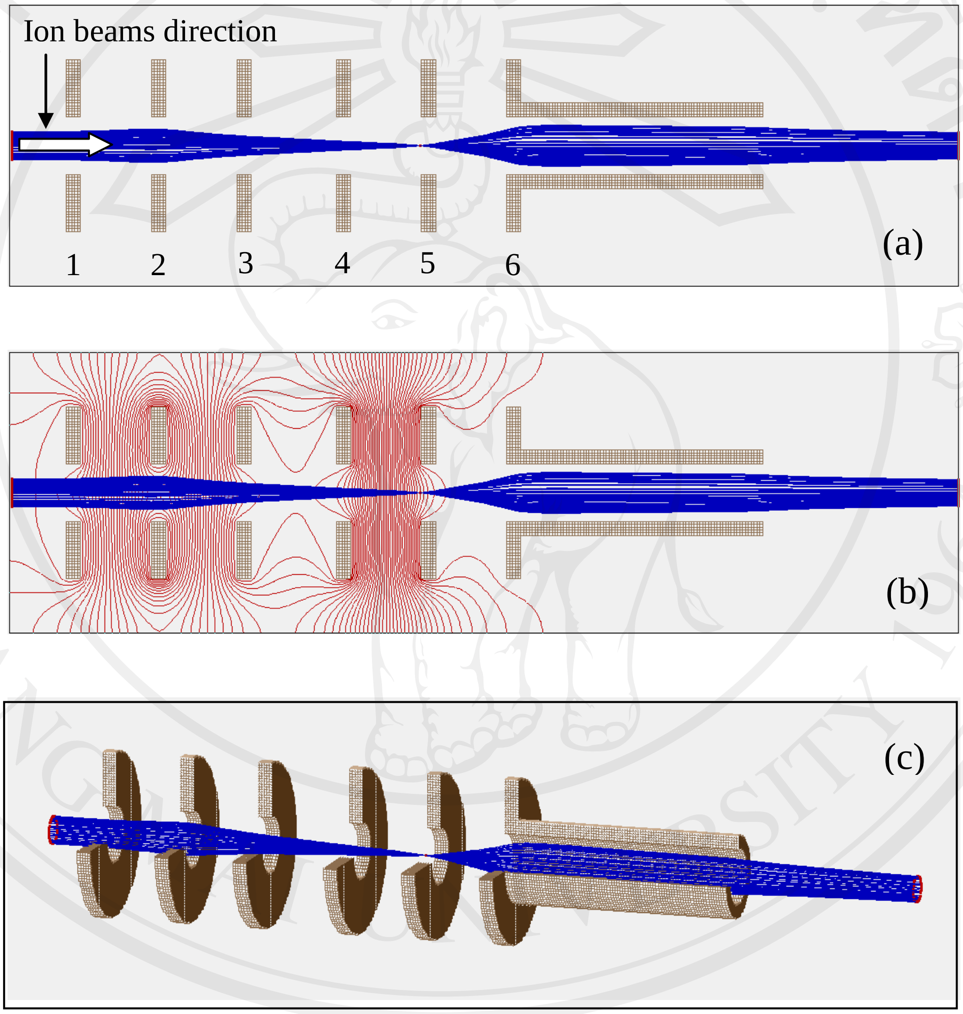

Figure 3.2. The SIMION simulated the deceleration lens which decreases the original energy of 20 keV to final energy 64 eV. (a) The electrodes and the beam optics. The electrodes are numbered with the numbers below them. (b) Equipotential surface. (c) The three-dimensional view. Blue color shows ion's trajectories and red color shows equipotential surface. The ions travel from the left to the right hand side.

After many times of simulations using varied parameters, deceleration lens was designed in Figure 3.2. The deceleration lens was designed as of six electrodes. The electrodes had 2 sets.

The first set consists of 3 cylindrical plates playing a role of an Einzel lens for focusing beam while the ion beam energy is not changed but the beam diameter is decreased before entering the deceleration part. The second set consists of 3 cylindrical plates with the last one in a tube shape, in which the first 2 cylindrical plates for decelerating ions beam and the last electrode (cylindrical connected with tube) for focusing beam and making the exiting beam more parallel.

The configuration of deceleration lens consists of 6 electrodes, as shown in Figure 3.2. The electrodes are in cylindrical shape with an outer diameter of 60 mm, an inner diameter of 20 mm and a thickness of 5 mm. The last electrode is a cylindrical plate connected with a tube in a length of 85 mm. The spaces between electrodes are 25 mm, except between the third- and the fourth-electrodes which is 30 mm.

The role of electrostatic field depends on the shape of ion beam, as shown in Figure 3.3. In this case, the simulation has included the deceleration lens with cover in order to show the equipotential surfaces (the SIMION program version 8.0 can't show electric field's directions, but can show equipotential surfaces) of each area. From the equipotential surface (an electric's direction perpendicular with an equipotential surface away), the ion beam is diverged by an electric field at before entrance the 2nd electrode and after pass the 5th electrode. The ion beam is converged

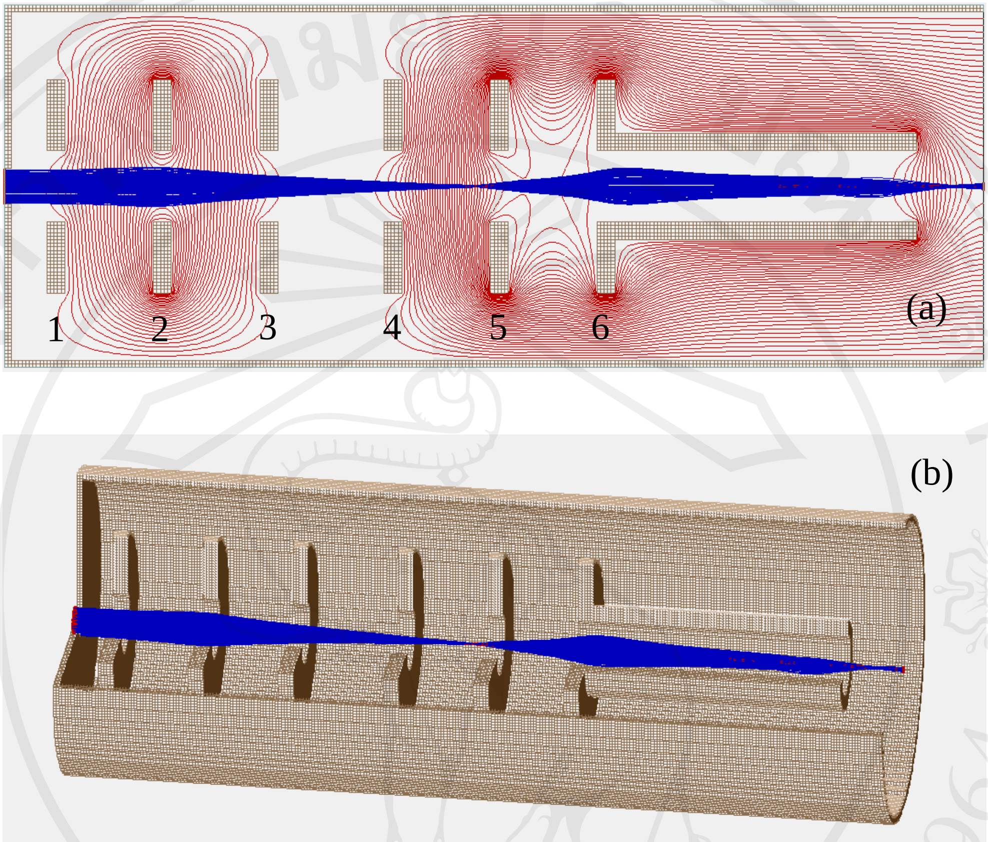

Figure 3.3. The SIMION simulated the deceleration lens with the cover. (a) Equipotential surface. (b) The three-dimensional view.

at after pass the 2nd electrode, before entrance and after pass the 6th electrode. The 6th electrode is the conductor therefore the electric field inside the tube is zero. This simulation, I would like to show the equipotential surfaces of each area of the deceleration lens only.

The simulations in this research for bombardment of DNA have 5 models in which each model has the same electrode configurations but different parameters as described in the following.

In the first model, the simulation needs to reduce energy from 20 keV to 64 eV, as seen in Figure 3.4. The procedure of creating model is described by David J Manura and David A. Dahl in "SIMION® Version 8.0 User Manual" on pages 2-16 to 2-30. The potentials of electrodes are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 14.00 kV, and the fifth- and sixth-electrodes are 20.56 kV, respectively.

After the deceleration lens was simulated, we must determine the parameters of an ion beam in the Particle Define mode, as shown in Figure 3.5 (a). We can adjust the parameters in the green area only. This simulation defines the parameters for ion beam as follows: (1) selected particle group is photon, (2) number of particles are 100, (3) mass is 28 (molecule of nitrogen), (4) charge is 1, showing that positive ion

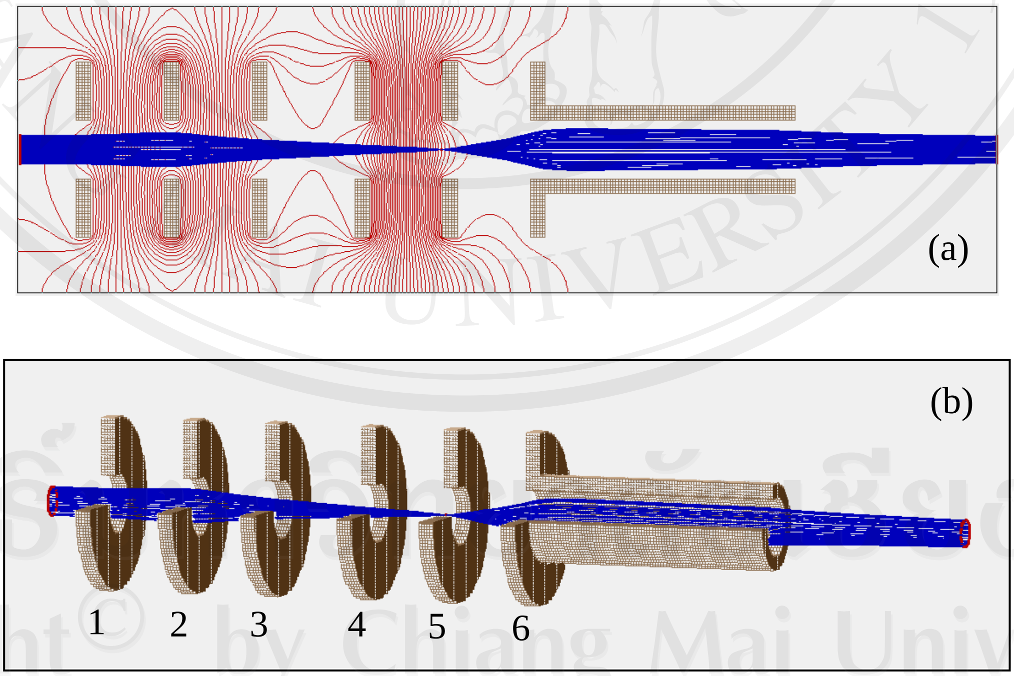

Figure 3.4. The first simulation reduces ion beam energy from 20 keV to 64 eV. (a) A two-dimensional view with equipotential surfaces, and (b) a three-dimensional view.

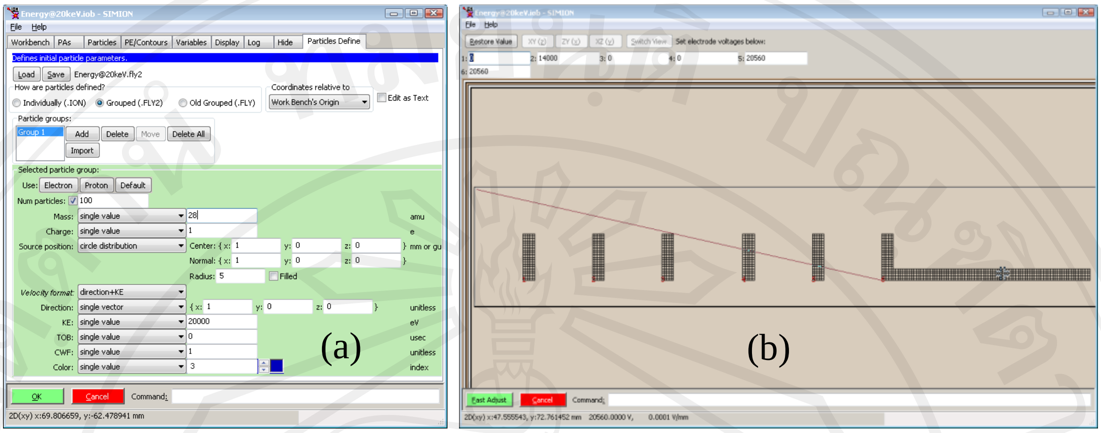

Figure 3.5. The features of (a) the Particles Define mode which defines the properties of ion beams and (b) Adjustment Voltages mode.

beam which link with selected particle group, (5) source position is Gaussian 3d distribution, determining the radius of source or ion beams as 5 mm, (6) kinetic energy is 20 keV, and (7) color of ion's trajectories is blue. The ion beam was first defined. We can adjust the voltages of electrodes in order to correspond with the objectives mentioned above. This simulation is used for bombardment of DNA as the ion species is nitrogen. From simulation, we can verify the diameters of ion beams, as shown in Figure 3.6. The diameters of ion beam before entrance and pass through the target are the same as 10 mm.

The second to the fifth models have the same configurations and some parameters except the potentials of electrodes. The data of potentials of each model are shown in Table 3.1. The original ion's kinetic energies of the second to the fifth models are 15 keV. Argon (mass number is 40 amu) was used for simulations and

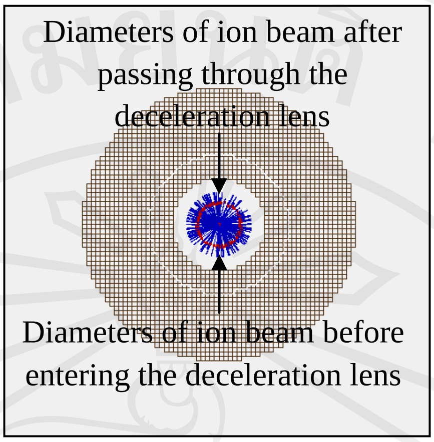

Figure 3.6. The diameters of the first model before ion beam enters and after it passes through the deceleration lens. The red circles are diameters of ion beam (this case diameters of ion beam before entering and after passing through the deceleration lens same).

experiments in these models. The ion's trajectories and deceleration lens models simulated by the SIMION program are shown in Figure 3.7 to Figure 3.10.

As seen in Figure 3.7, the second model reduces energy from 15 keV to 230 eV. The potentials of electrodes are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 11.20 kV, and the fifth- and sixth-electrodes are 15.27 kV, respectively. The ion beam diameters are 10 mm and 6 mm at the entrance and after passing though the deceleration lens, respectively.

The third model reduces energy from 15 keV to 304 eV, as shown in Figure 3.8. The potentials of electrodes are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 11.30 kV, and the fifth- and sixth-electrodes are 15.20 kV,

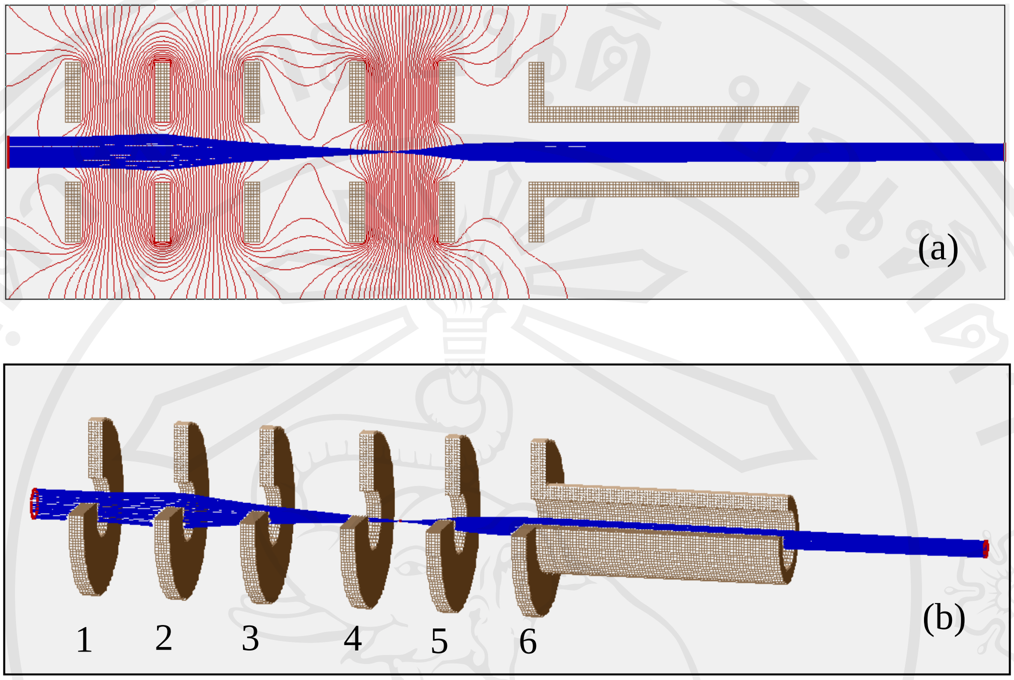

Figure 3.7. The second simulation reduces ion beam energy from 15 keV to 230 eV. (a) A two-dimensional view with equipotential surfaces and (b) a three-dimensional view.

respectively. The ion beam diameters are 10 mm and 6.1 mm at the entrance and after passing though the deceleration lens, respectively.

The fourth model reduces energy from 15 keV to 408 eV, as shown in Figure 3.9. The potentials of electrodes are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 11.40 kV, and the fifth- and sixth-electrodes are 15.10 kV, respectively. The ion beam diameters are 10 mm and 7.8 mm at the entrance and after passing though the deceleration lens, respectively.

As shown in Figure 3.10, the fifth model reduces energy from 15 keV to 511

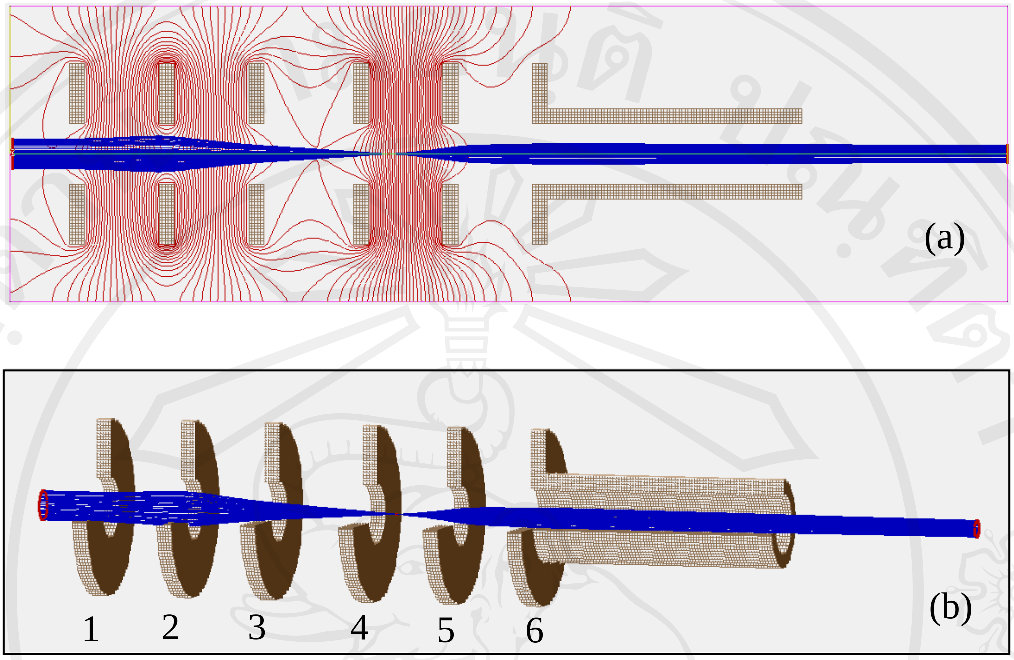

Figure 3.8. The third simulation reduces ion beam energy from 15 keV to 304 eV. (a) A two-dimensional view with equipotential surfaces and (b) a three-dimensional view.

eV. The potentials of electrodes are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 11.50 kV, and the fifth- and sixth-electrodes are 15.00 kV, respectively. The ion beam diameters are 10 mm and 7.4 mm at the entrance and after passing though the deceleration lens, respectively.

Conclusions, the parameters were defined for ion beam in the deceleration lens models:

(1) particle group is photon,

(2) particles' number are 100,

(3) ion masses are 28 (nitrogen's molecule) for the first simulation and 40 (ion of argon) for the other simulations,

(4) charge is 1,

(5) source is Gaussian 3d distribution,

The potentials of each electrode, original and final kinetic energies of each model, and diameters of ion beam are shown in Table 3.1.

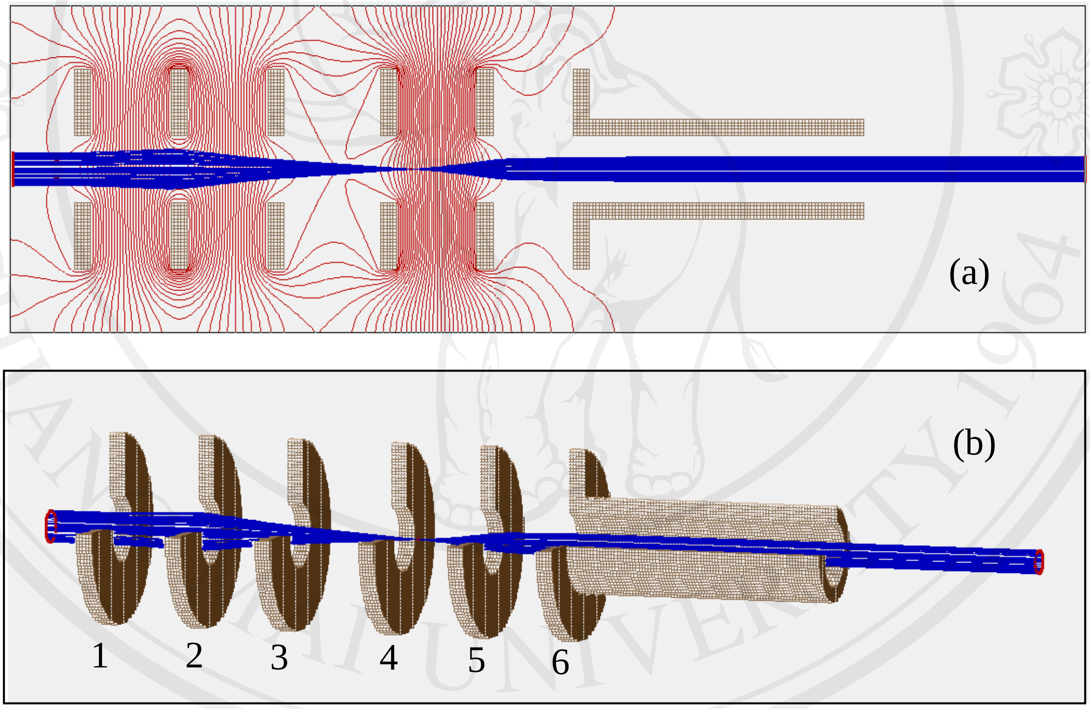

Figure 3.9. The fourth simulation reduces ion beam energy from 15 keV to 408 eV. (a) A two-dimensional view with equipotential surfaces and (b) a three-dimensional view.

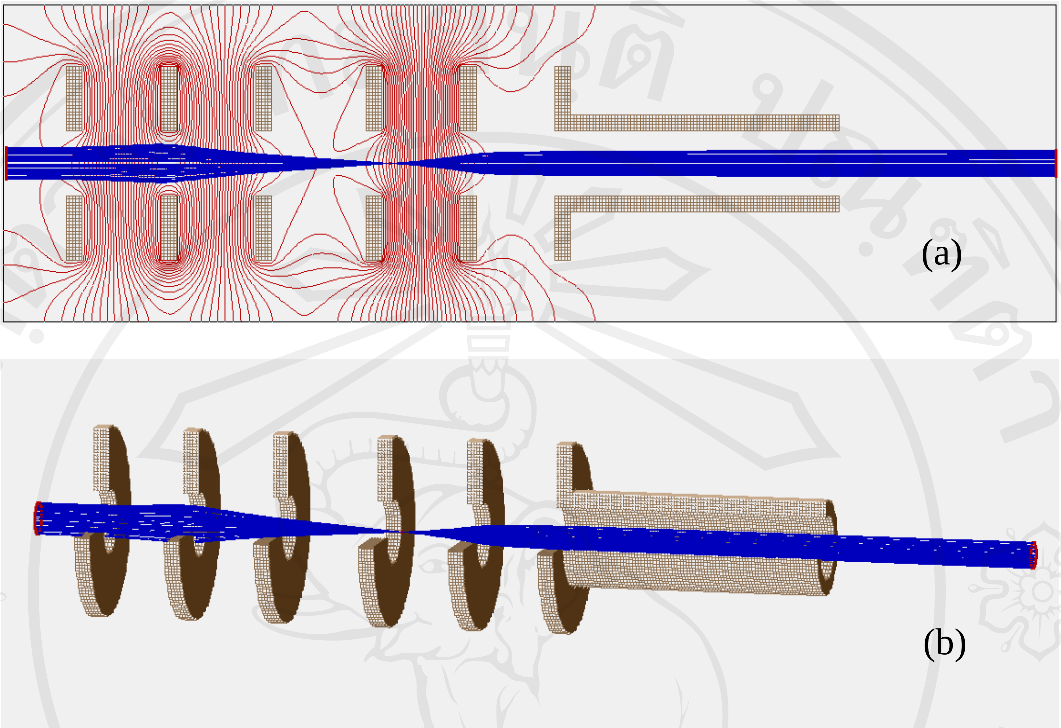

Figure 3.10. The fifth simulation reduces ion beam energy from 15 keV to 511 eV. (a) A two-dimensional view with equipotential surfaces and (b) a three-dimensional view.

3.3 Simulation the deceleration lens with space charge

This topic, I would like to show that the shape of ion beam pass through the deceleration lens depend on space charge effect. When ion beam is low energy and high ion beam current the space charge effect will dominate.

The SIMION program version 8.0 supports three estimates of charge repulsion: Beam, columbic and factor repulsion (Abdelrahman, 2012). In general charge repulsion estimations involve determining the forces between the current ion in question and all other currently flying ions (Manura and Dahl, 2008). The SIMION

Table 3.1. Simulation data. (a) The potentials of each electrode of each model. (b) The original, final kinetic energies and diameters of each model.

Models	Electrode 1 (kV)	Electrode 2 (kV)	Electrode 3 (kV)	Electrode 4 (kV)	Electrode 5 (kV)	Electrode 6 (kV)
1	0.00	14.00	0.00	0.00	20.56	20.56
2	0.00	11.20	0.00	0.00	15.27	15.27
3	0.00	11.30	0.00	0.00	15.20	15.20
4	0.00	11.40	0.00	0.00	15.10	15.10
5	0.00	11.50	0.00	0.00	15.00	15.00

(a)

Models	Original energies (keV)	Final energies (eV)	Original diameters of ion beam (mm)	Final diameters of ion beam (mm)
1	20	64	10	10
2	15	230	10	6
3	15	304	10	6.1
4	15	408	10	7.8
5	15	511	10	7.4

(b)

program version 8.0 uses the sum of the accelerations to represent the estimate of charge repulsion effects on the current ion.

This work, the charge repulsion of simulations had used the mode of Beam. The beam repulsion for each ion is assumed to represent a line charge. The line charge density (coulombs/mm) is determined by apportioning the beam current between the ion trajectories according to their charge adjusted by their charge weighting factor and dividing it by the ion's velocity [coulombs/mm=(coulombs/µ sec)/(mm/µ sec)]. The numerical beam repulsion acceleration is given by:

$$A_{accelbeam} = \frac{Scale \times T_g \times T_f \times r_{fac}}{v} \tag{3.1}$$

$$Scale = \frac{-1.734 \times 10^9 \times I(Amp) \times q}{(m \times T_{total})} \tag{3.2}$$

$$r_{fac}beam = \frac{r_e^2}{(0.341 + r_e^3) r_{avg}} \tag{3.3}$$

$$r_e = \frac{r}{r_{avg}}. \tag{3.4}$$

Where $A_{accelbeam}$ is the acceleration components computed using unit vector for distance r between the two ions where:

$I(Amp)$ = total beam (amps)

q = charge on current ion (real charge)

m = rest mass of current ion (amu)

T_{total} = sum of all ion's cwf x their absolute charge

T_g = test ion's charge (real charge)

T_f = test ion's charge weighting factor

r = distance between the two ions

r_{avg} = average min distance between ions

v = speed of the test ion.

However, we can give an ion beam current for estimation the shape of ion beam, as shown in Figure 3.11. The ion beam repulsion is included in the simulation of beam's shape by the first step selects Particles tab, the second check the Grouped button, the third select the types of repulsion (None, Beam, Colu, and Fact) which this work select the Beam repulsion, and the last step gives beam current in the box unit of A.

The simulations of the deceleration lens depends on the ion beam current, as shown in Figure 3.12, when an original energy is 15 keV and final energy after pass through the deceleration lens is 230 eV. The simulations vary beam currents: 1 A, 0.1 A, 0.01 A, 1 mA, 0.1 mA, 10 μA, 1 μA, 100 nA, and 10 nA, respectively.

The potentials of each electrode: the 1st-, 3rd-, and 4th-electrode is 0 V, the 2nd-electrode is 11.2 kV, and the 5th- and 6th-electrode is 15.27 kV, respectively.

From the simulations are shown in Figure 3.12, ion beam trajectories are disturbed by the beam repulsion when the beam current more than 1 μA at the energy 230 eV. In the experiment, we had measured the beam current about 10-100 nA therefore the beam repulsion has influence to the shape of beam very little.

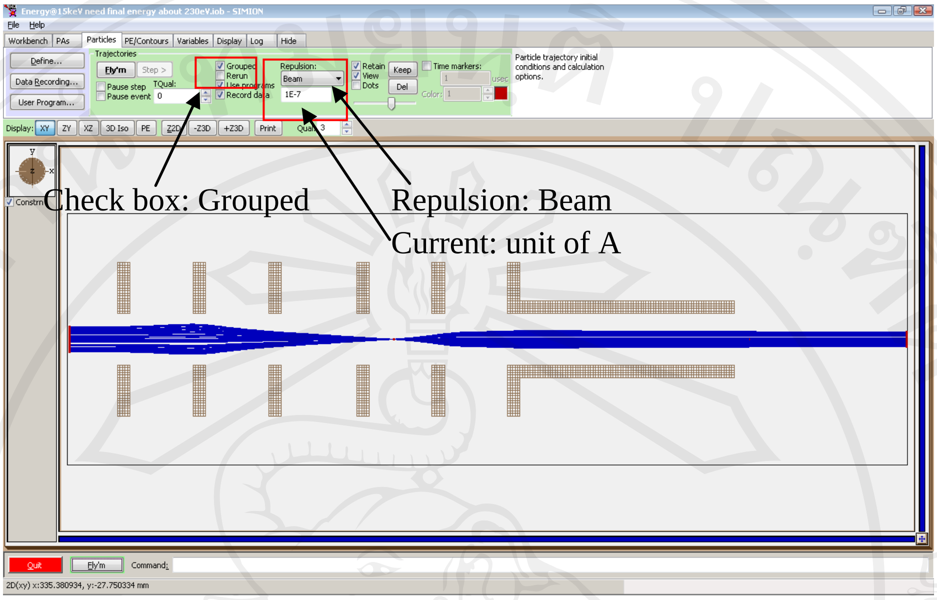

Figure 3.11. Mode of ion beam repulsion of the SIMION program version 8.0.

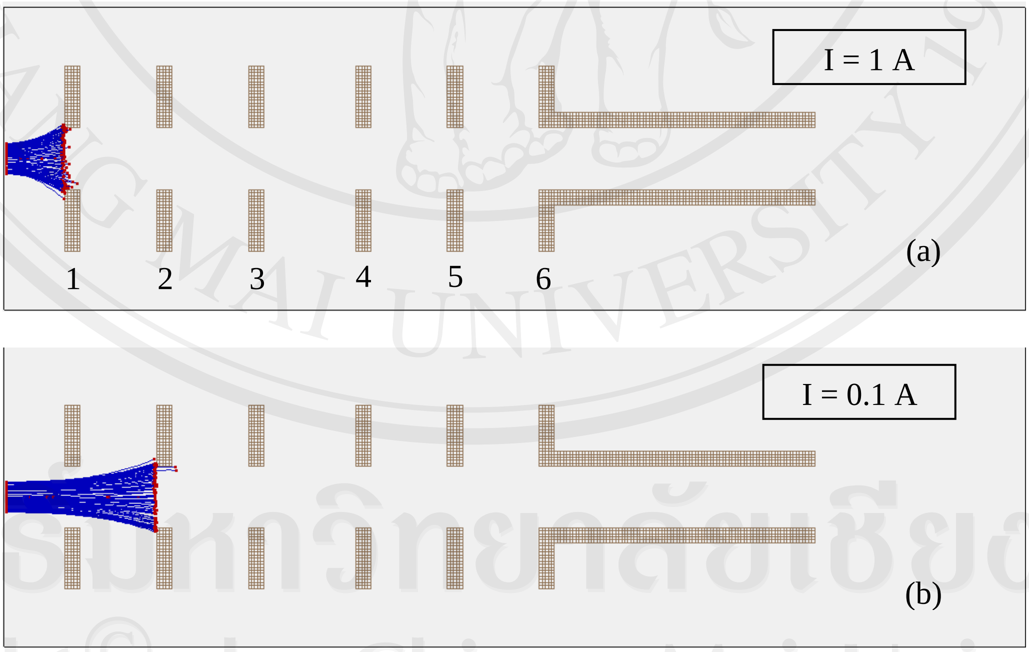

Figure 3.12. The deceleration lens simulations vary the beam current: (a) 1 A, (b) 0.1 A, (c) 0.01 A, (d) 1 mA, (e) 0.1 mA, (f) 10 μA, (g) 1 μA, (h) 100 nA, and (i) 10 nA, respectively.

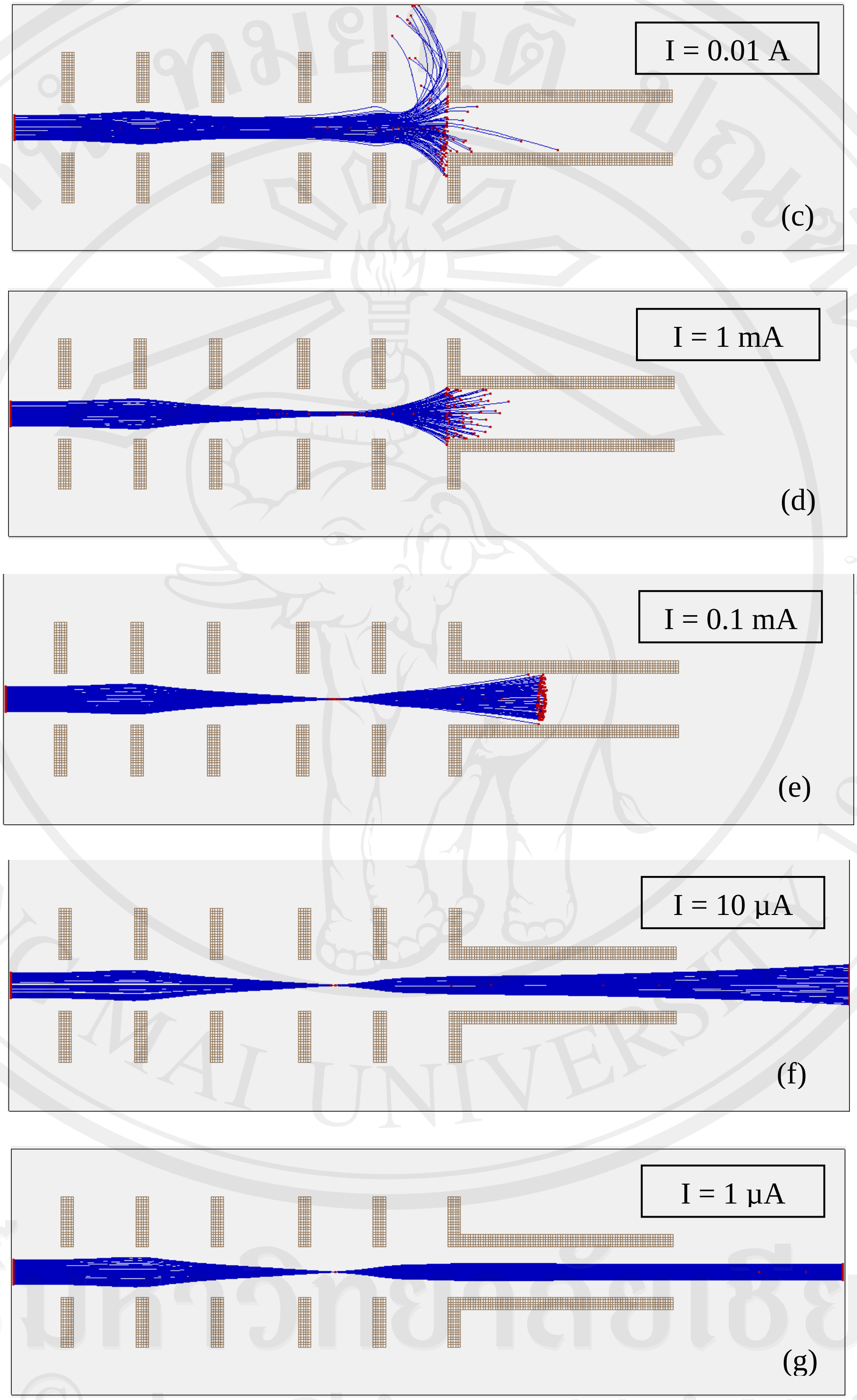

Figure 3.12. The deceleration lens simulations vary the beam current: (a) 1 A, (b) 0.1 A, (c) 0.01 A, (d) 1 mA, (e) 0.1 mA, (f) 10 µA, (g) 1 µA, (h) 100 nA, and (i) 10 nA, respectively (Continued).

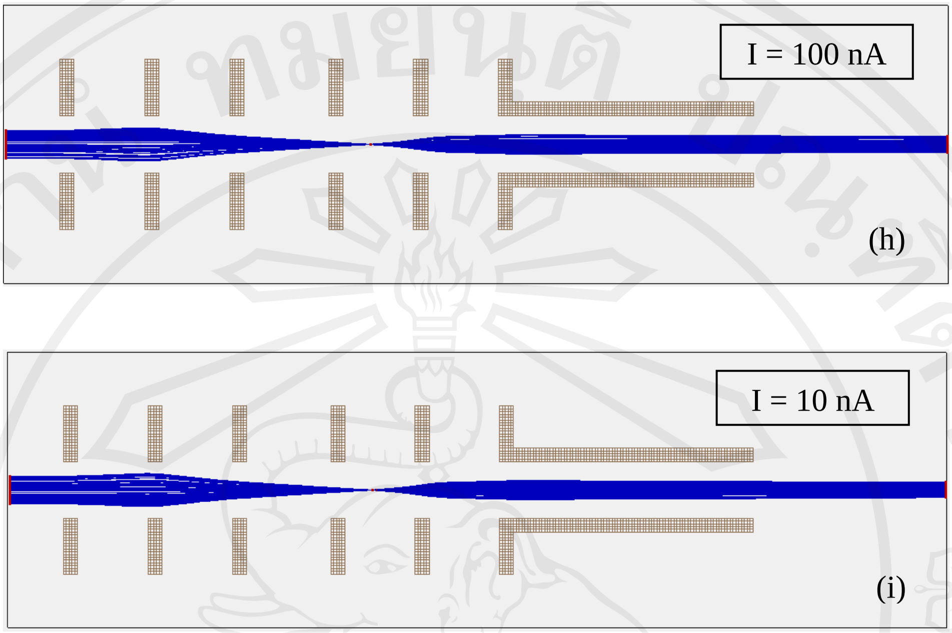

Figure 3.12. The deceleration lens simulations vary the beam current: (a) 1 A, (b) 0.1 A, (c) 0.01 A, (d) 1 mA, (e) 0.1 mA, (f) 10 µA, (g) 1 µA, (h) 100 nA, and (i) 10 nA, respectively (Continued).

3.4 Simulation of measurement of low ion-beam energy

The deceleration lens was designed for reducing ion beam energy to keV to around 10 eV. The principle of measuring deceleration-lens-reduced ion beam energy is using an electrostatic field in order to deflecting ions. From Section 2.6, the basic idea is to use an electrostatic field to bend the beam with the beam bending depending on the ion beam energy, as shown in Figure 2.8. The parameters in Figure 2.8 are: E_0 is the original ion energy (after the ion passes the deceleration lens), d is the distance between two electrode plates of the electrostatic field, b is the plate length, y_1 is the

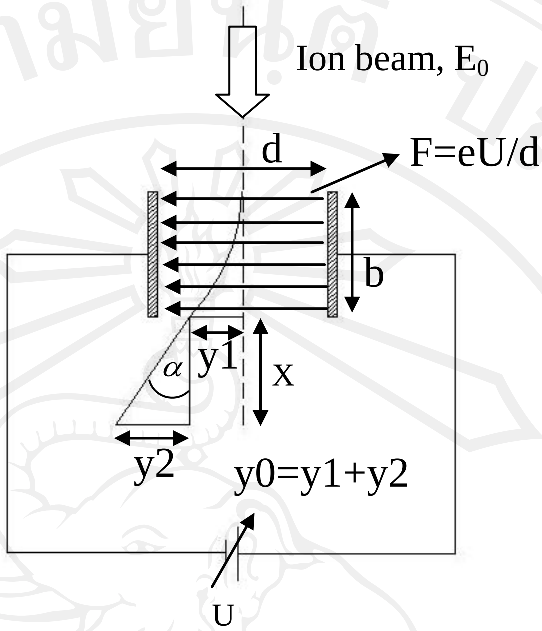

Figure 2.8. Schematic diagram of the method used to measure the ion beam energy.

bending distance by the electric field, y_2 is the distance between the end exit of the bent beam from the field and the measurement point, y_0 is the total bending distance, x is the distance between the end of electric plate to the point (perpendicular) of measurement, and U is the potential of the electric field.

From Section 2.6 and Figure 2.8, an ion has a quadratic trajectory inside the electric field resulting in the bending distance depending on time square during the ion travels in the field. After the ion exits from the field, if the edge effect of the electrode plates is ignored, the ion has a straight trajectory. The distance of an ion bending is

$$y_0 = \frac{1}{2}\frac{eUb}{E_0 d}\left(\frac{b}{2}+x\right). \tag{2.80}$$

In the experiment, we can measure the distance of ion beam bending. From relation of equation (2.80), the ion beam energy can be calculated by

$$E_0 = \frac{1}{2}\frac{eUb}{y_0 d}\left(\frac{b}{2}+x\right). \tag{2.81}$$

There are 4 simulations applied in experiment for verifying that the deceleration lens reduces ion beam energy.

The configuration of plates and parameters for measurement of ion beam energy are defined as following: b = 30 mm, d = 20 mm, and x = 40 mm. The ion species are argon for the first and the second simulations, while nitrogen for the third and the fourth simulations.

In the first simulation, the original ion beam energy before entering the deceleration lens is 15 keV, and after the ions are decelerated, the ion beam energy is 230 eV (E_0). Ions with the ion beam energy of 230 eV will be bent by the electrostatic field. The first simulation is shown in Figure 3.13.

The electrodes' potentials of the deceleration lens are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 11.20 kV, and the fifth- and sixth-electrodes are 15.27 kV. The potentials of the electric plates are 50 V and 0 V, (U = 50 V) respectively. The distance of ion bending by the electrostatic field in theory is 8.9 mm (equation 2.80) and in simulation is 9 mm. In experiment, we can measure the distance of ion beam bending using equation 2.81, the relation between the distance and the ion energy, and finally we can know ion beam energy.

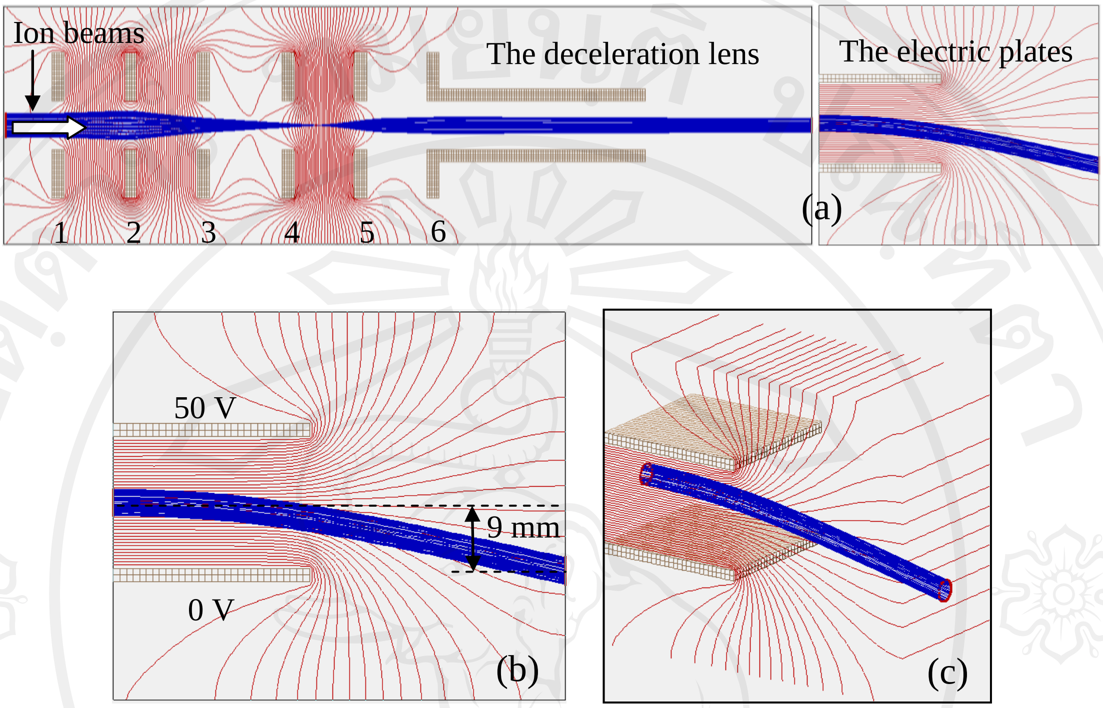

Figure 3.13. The first simulation of measurement of ion beam energy. (a) Configuration of the deceleration lens with the electric plates. (b) The ion beam bending by an electrostatic field in two-dimension view, and (c) Three-dimension view. Ions travel from the left to the right hand side. The red lines are the equipotential surfaces and the blue color is the ion's trajectories.

In the second simulation, the original ion beam energy is 15 keV and is reduced after passing through the deceleration lens to 56.5 eV. The electrodes' potentials of the deceleration lens are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 10.65 kV, and the fifth- and sixth-electrodes are 15.417 kV. The potentials of the electric plates are 12 V and 0 V (U = 12 V), respectively. The distance bent by the electrostatic field in theory is 8.8 mm and in simulation is 9.1 mm. The second simulation is shown in Figure 3.14.

In the third simulation, the original ion beam energy is 13 keV and is reduced after passing through the deceleration lens to 39 eV. The electrodes' potentials of the deceleration lens are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 9.10 kV, and the fifth- and sixth-electrodes are 13.365 kV. The potentials of the electric plates are 10 V and 0 V (U = 10 V), respectively. The distance bent by the electrostatic field in theory is 10.6 mm and in simulation is 10.4 mm. The third simulation is shown in Figure 3.15.

The Figure 3.16, in the fourth simulation the original ion beam energy is 10 keV and is reduced after passing through the deceleration lens to 32 eV. The electrodes' potentials of the deceleration lens are: the first-, third-, and fourth-electrodes are 0 V, the second-electrode is 7.0 kV, and the fifth- and sixth-electrodes are 10.257 kV. The potentials of the electric plates are 9 V and 0 V $(U = 9V)$, respectively. The distance bent by the electrostatic field in theory is 11.6 mm and in simulation is 11.5 mm.

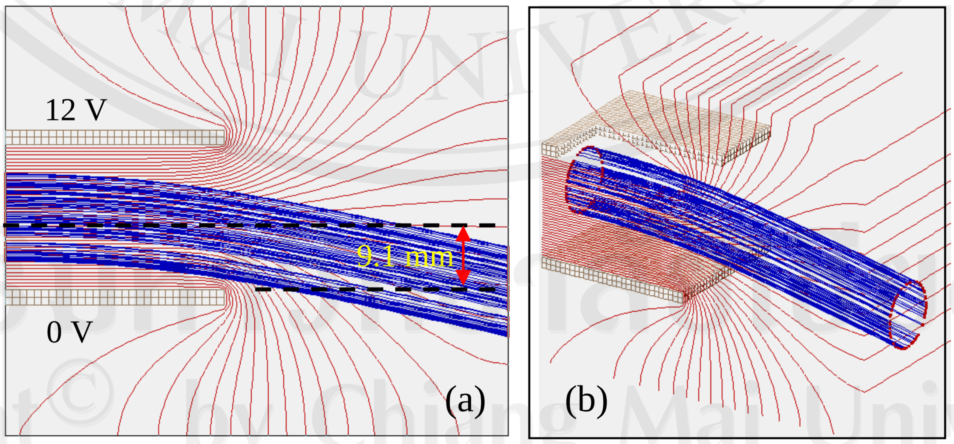

Figure 3.14. The second simulation of measurement of ion beam energy. (a) The ion beam bending by the electrostatic field in 2-D view, and (b) 3-D view.

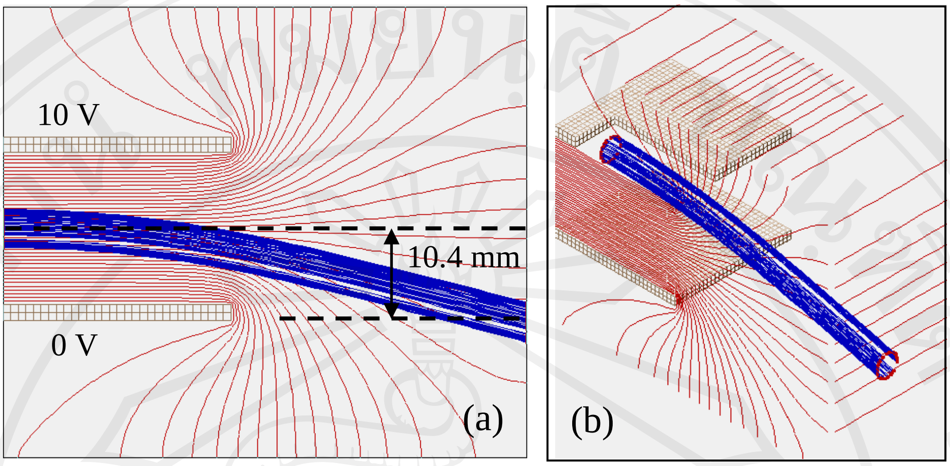

Figure 3.15. The third simulation of measurement of ion beam energy. (a) The ion beam bending by an electrostatic field in 2-D view, and (b) 3-D view.

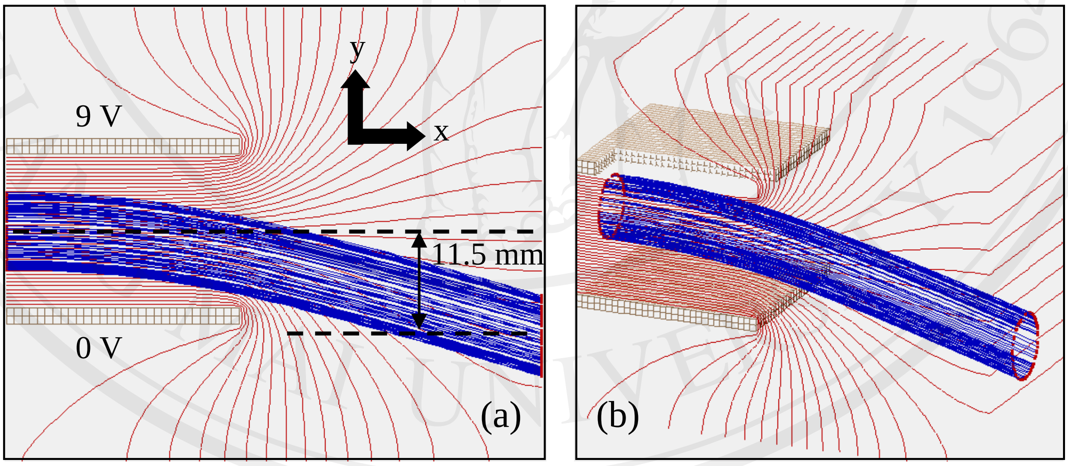

Figure 3.16. The fourth simulation of measurement of ion beam energy. (a) The ion beam bending by an electrostatic field in 2-D view, and (b) 3-D view.

The equipotential surfaces in the case symmetry of planar can't show since the SIMION program must define an area for simulation (the ions travelling are positive x-direction, as shown in Figure 3.16 (a)) which the electrode is drawn in x-and y-direction only and a dimension in z-direction same with define from the area, then the equipotential can't show in the z-direction.

Conclusions on the simulations of measurement of low ion beam energy are shown in Table 3.2.

Table 3.2. Summary. (a) The potentials of each electrode in each model. (b) The original, final ion energies and the distance bending by theory and simulations.

Models	Electrode 1 (kV)	Electrode 2 (kV)	Electrode 3 (kV)	Electrode 4 (kV)	Electrode 5 (kV)	Electrode 6 (kV)
1	0.00	11.20	0.00	0.00	15.27	15.27
2	0.00	10.65	0.00	0.00	15.42	15.42
3	0.00	9.10	0.00	0.00	13.365	13.365
4	0.00	7.00	0.00	0.00	10.275	10.275

(a)

Models	Original energies (keV)	Final energies, E_0 (eV)	Distance bending by theory (equation 2.80) (mm)	Distance bending by simulations (mm)
1	15.0	230.0	8.9	9.0
2	15.0	56.5	8.8	9.1
3	13.0	39.0	10.6	10.4
4	10.0	32.0	11.6	11.5

(b)