CHAPTER III

Methodology [24, 25]

3.1. One Dimensional Simulation for Ions Motion in Plasma Field

This research create the model for describe phenomenal of one dimensional plasma system that has only Electric fielding in system and Magnetic induction or Magnetic flux density is neglected. The particle model system is used to calculate and forecasted plasma parameters. Poisson's equation is solved to find electrical field and electric potential by Fourier expansion and The Poisson's equation is

$$\nabla\vec{E} = \frac{q(n_i - n_e)}{\varepsilon_0} \tag{3.1}$$

For $\vec{E}$ = Electric field (V/m)

q = charge of particle (C)

n_i = Ion density (m^{-3})

n_e = Electron density (m^{-3})

ε_0 = Permittivity of free space or vacuum (F/m)

The result from Fourier expansion will be compared with the result from other method. After that, the electrical field from Poisson's equation solution is used to calculate in The Lorentz Force equation and Lorentz Force equation that zero Magnetic flux density is

$$\vec{F} = q\vec{E} \tag{3.2}$$

For $\vec{F}$ = Force (N)

$\vec{E}$ = Electric field (V/m)

q = charge of particle (C)

To solve Poisson's equation by Fourier series expansion method

Conceptual of Fourier series expansion is Periodic Function that is function has a period T and all of x in function $f(x)$ is equal $f(x+T)$. This method mention all function can be expanded in Fourier series form. That form is

$$f(x)=\frac{a_0}{2}+\sum_{n=1}^{\infty}\left[a_n\cos(\frac{i\pi x}{L})+b_n\sin(\frac{i\pi x}{L})\right] \tag{3.3}$$

$$a_n=\frac{1}{L}\int_0^{2L}f(x)\cos\frac{n\pi x}{L}dx \tag{3.4}$$

$$b_n=\frac{1}{L}\int_0^{2L}f(x)\sin\frac{n\pi x}{L}dx \tag{3.5}$$

The solution of Electrical potential and ion density is periodic function and the period of these function are $2L$ that L is system length in one dimension. So the Electrical potential ($\phi(x)$) can be expanded as

$$\phi(x)=\frac{a_0}{2}+\sum_{n=1}^{\infty}\left[a_n\cos(\frac{i\pi x}{L})+b_n\sin(\frac{i\pi x}{L})\right] \tag{3.6}$$

$$a_n=\frac{1}{L}\int_0^{2L}\phi(x)\cos\frac{n\pi x}{L}dx \tag{3.7}$$

Numerical form can be written as

$$a_n=\frac{1}{L}\sum_0^{2L}\Delta x\cdot\phi(x)\cos\frac{n\pi x}{L} \tag{3.8}$$

$$b_n=\frac{1}{L}\int_0^{2L}\phi(x)\sin\frac{n\pi x}{L}dx \tag{3.9}$$

Numerical form can be written as

$$b_n=\frac{1}{L}\sum_0^{2L}\Delta x\cdot\phi(x)\sin\frac{n\pi x}{L} \tag{3.10}$$

And ion density $(n_i(x))$ can be expanded as

$$n_i(x)=\frac{a'_0}{2}+\sum_{n=1}^{\infty}\left[a'_n\cos(\frac{i\pi x}{L})+b'_n\sin(\frac{i\pi x}{L})\right] \tag{3.11}$$

$$a'_n = \frac{1}{L}\int_0^{2L} n_i(x)\cos\frac{n\pi x}{L}dx \tag{3.12}$$

Numerical form can be written as

$$a'_n = \frac{1}{L}\sum_0^{2L} \Delta x \cdot n_i(x)\cos\frac{n\pi x}{L} \tag{3.13}$$

$$b'_n = \frac{1}{L}\int_0^{2L} n_i(x)\sin\frac{n\pi x}{L}dx \tag{3.14}$$

Numerical form can be written as

$$b'_n = \frac{1}{L}\sum_0^{2L} \Delta x \cdot n_i(x)\sin\frac{n\pi x}{L} \tag{3.15}$$

For One Dimensional Poisson's equation can be written as

$$\frac{dE}{dx} = \frac{q(n_i - n_e)}{\varepsilon_0} \tag{3.16}$$

And relation of Electrical field (E) and Electrical potential (ϕ) are

$$\vec{E} = -\nabla\phi \tag{3.17}$$

For One Dimensional can be written as

$$\frac{d\phi(x)^2}{dx^2} = -\frac{q(n_i(x) - n_e)}{\varepsilon_0} \tag{3.18}$$

From Fourier expansion of $\phi(x)$, $\frac{d\phi(x)^2}{dx^2}$ can be written in Fourier form as

$$\frac{d\phi(x)^2}{dx^2} = \sum_{n=1}^{\infty}\left[-\left(\frac{i\pi}{L}\right)^2 a_n\cos(\frac{i\pi x}{L}) - \left(\frac{i\pi}{L}\right)^2 b_n\sin(\frac{i\pi x}{L})\right] \tag{3.19}$$

From equation 3.18 can written as

$$\sum_{n=1}^{\infty}\left[-\left(\frac{i\pi}{L}\right)^2 a_n\cos(\frac{i\pi x}{L}) - \left(\frac{i\pi}{L}\right)^2 b_n\sin(\frac{i\pi x}{L})\right] = ...$$

$$...... = -\left(\frac{q}{\varepsilon_0}\right)\left[\frac{a'_0}{2} + \sum_{n=1}^{\infty}\left[a'_n\cos(\frac{i\pi x}{L}) + b'_n\sin(\frac{i\pi x}{L})\right] - n_e\right] \tag{3.20}$$

Comparing the coefficient between Fourier expansion of Electrical potential ($\phi(x)$) and ion density $(n_i(x))$

$$a_n = \left(\frac{L}{i\pi}\right)^2 \left(\frac{q}{\varepsilon_0}\right) a'_n \tag{3.21}$$

And

$$b_n = \left(\frac{L}{i\pi}\right)^2 \left(\frac{q}{\varepsilon_0}\right) b'_n \tag{3.22}$$

So, the Electrical potential can be solved by this method and this solution can be used to calculate the electrical field (E) by equation 3.23. From equation 3.23 that consider in One Dimensional can be written as

$$E(x) = -\frac{d\phi(x)}{dx} \tag{3.23}$$

The equation 3.23 is solved by finite different method. This method replaces differential equation by discrete difference approximation that is written in term of nodal evaluation of the unknown function. From equation 3.23 can be written in discrete difference approximation as

$$E_i = \frac{\phi_{i-1} - \phi_{i+1}}{2\Delta x} \tag{3.24}$$

For E_i = Electric field in position i

ϕ_{i+1} = Electric potential in Position i+1(forward position)

ϕ_{i-1} = Electric potential in Position i-1 (backward position)

Δx = Distance between Position i and Position i+1

To solve Lorentz Force equation by finite difference method

The solutions from Poisson's equation are used to calculate plasma particles displacement by Lorentz Force equation or equation 3.2. The first step to solve Lorentz Force equation is reform equation in t. The form of Lorentz Force equation in term of t can be written as

$$\frac{dx(t)^2}{dt^2} = \frac{q}{m}E(x,t) \tag{3.25}$$

That equation is second order differential equation. This equation is solved by Runge-Kutta Method that involves a weighted average of values of $f(x,t)$ taken at different point in the interval $t_n \le t \le t_{n+1}$.

Computing cycle

The calculations can be repeated to simulate the motion of plasma over time period. The position and velocity of particle is updated by calculating each round of time step. The position of particle change so, the ion density is changed. The update electrical potential is found by new ion density. The new electrical potential is solved by the new electric field, and the update position and velocity of particle are solved by new electric field. This process is repeated for many time steps.

The conditions of this plasma simulation are One Dimensional simulation, Ion particle is 10^{13} particles in 10 centimeters (0.1 meters) length system and 10^5 simulated particles were used to calculate and each simulated particles is 10^8 Ion particles. This system was divided in 100 parts and each part is 0.001 m. and time step is 10^{-7} sec. The boundary conditions correspond with Fourier series conditions.

3.2 Three Dimensional Simulations for Ions Motion in Plasma Field

This research creates the model to describe phenomenal of three dimensional plasma system that has only Electric fielding in system and Magnetic induction or Magnetic flux density is neglected. The particle model system is used to calculate and forecasted plasma parameters. Poisson's equation is solved to find electrical field and electric potential by Fourier expansion and The Poisson's equation is

$$\nabla\vec{E} = \frac{q(n_i - n_e)}{\varepsilon_0} \tag{3.26}$$

For $\quad \vec{E}$ = Electric field (V/m)

q = charge of particle (C)

n_i = Ion density (m^{-3})

n_e = Electron density (m^{-3})

ε_0 = Permittivity of free space or vacuum (F/m)

After that, the electrical field from Poisson Equation solution is used to calculate in The Lorentz Force equation. For zero Magnetic flux density, The Lorentz Force equation is

$$\vec{F} = q\vec{E} \tag{3.27}$$

For $\vec{F}$ = Force (N)

$\vec{E}$ = Electric field (V/m)

q = charge of particle (C)

To solve Poisson equation by finite different method

The relation of electrical field (E) and electrical potential (ϕ) are

$$\vec{E} = -\nabla\phi \tag{3.28}$$

So

$$\nabla^2\phi = -q\frac{(n_i - n_e)}{\varepsilon_0} \tag{3.29}$$

For Three Dimensional can write as

$$\frac{\partial^2\phi(x,y,z)}{\partial x^2}\hat{i} + \frac{\partial^2\phi(x,y,z)}{\partial y^2}\hat{j} + \frac{\partial^2\phi(x,y,z)}{\partial z^2}\hat{k} = -q\frac{(n_i - n_e)}{\varepsilon_0} \tag{3.30}$$

This equation is solved by finite different method that method, the differential equation is replaced by discrete difference approximate that is written in term of nodal evaluation of the unknown function. From equation 3.30 can be written in Finite different form that

$$\frac{\phi_{(i+1,j,k)} - 2\phi_{(i,j,k)} + \phi_{(i-1,j,k)}}{\Delta x^2} + \ldots$$
$$\ldots + \frac{\phi_{(i,j+1,k)} - 2\phi_{(i,j,k)} + \phi(_{i,j-1,k)}}{\Delta y^2} + \ldots$$
$$\ldots + \frac{\phi_{(i,j,k+1)} - 2\phi_{(i,j,k)} + \phi_{(i,j,k-1)}}{\Delta z^2} = \ldots \tag{3.31}$$
$$\ldots = -\frac{q}{\varepsilon_0}\left[n_{(i,j,k)ion} - n_{(i,j,k)electron}\right]$$

For $\phi_{(i,j,k)}$ = Electrical potential in position i, j and k

i equivalent with x

j equivalent with y

k equivalent with z

$\phi_{(i+1,j,k)}$ = Electrical potential in position i+1 (right position)

$\phi_{(i-1,j,k)}$ = Electrical potential in position i-1 (left Position)

$\phi_{(i,j+1,k)}$ = Electrical potential in position j+1 (forward position)

$\phi_{(i,j-1,k)}$ = Electrical potential in position j-1 (backward position)

$\phi_{(i,j,k+1)}$ = Electrical potential in position k+1 (up position)

$\phi_{(i,j,k-1)}$ = Electrical potential in position k-1 (down position)

Δx = Distance between Position i and i+1

Δy = Distance between Position j and j+1

Δz = Distance between Position k and k+1

From equation 3.31 If $\Delta x = \Delta y = \Delta z$, the relation of $\phi_{(i,j,k)}$ can be written as

$$\begin{aligned}6\phi_{(i,j,k)} &= \Delta x^2 \frac{q}{\varepsilon_0}\left[n_{(i,j,k)ion} - n_{(i,j,k)electron}\right] + \ldots \\ &\ldots + \phi_{(i+1,j,k)} + \phi_{(i-1,j,k)} + \ldots \\ &\ldots + \phi_{(i,j+1,k)} + \phi_{(i,j-1,k)} + \ldots \\ &\ldots + \phi_{(i,j,k+1)} + \phi_{(i,j,k-1)}\end{aligned} \tag{3.32}$$

This equation is solved by Jacobi iteration method. This solution is $\phi_{(i,j,k)}$ that is electrical potential.

$$\begin{aligned}\phi_{(i,j,k)} &= \frac{1}{6}\Delta x^2 \frac{q}{\varepsilon_0}\left[n_{(i,j,k)ion} - n_{(i,j,k)electron}\right] + \ldots \\ &\ldots + \phi_{(i+1,j,k)} + \phi_{(i-1,j,k)} + \ldots \\ &\ldots + \phi_{(i,j+1,k)} + \phi_{(i,j-1,k)} + \ldots \\ &\ldots + \phi_{(i,j,k+1)} + \phi_{(i,j,k-1)}\end{aligned} \tag{3.33}$$

This solution can be used to calculate the electrical field $(\vec{E})$ by equation 3.28. From equation 3.28 that consider in Three Dimensional can be written as

$$\vec{E}_x(x,y,z) = -\frac{\partial \phi(x,y,z)}{\partial x} \tag{3.34}$$

$$\vec{E}_y(x,y,z) = -\frac{\partial \phi(x,y,z)}{\partial y} \tag{3.35}$$

$$\vec{E}_z(x,y,z) = -\frac{\partial \phi(x,y,z)}{\partial z} \tag{3.36}$$

The equations 3.34 to 3.36 are solved by finite different method. This method replaces differential equation by discrete difference approximations that are written in term of nodal evaluation of the unknown function. From equation 3.34 to 3.36 can be written in discrete difference approximation as

$$E_{x[i][j][k]} = \frac{\phi_{(i-1,j,k)} - \phi_{(i+1,j,k)}}{2\Delta x} \tag{3.37}$$

$$E_{y[i][j][k]} = \frac{\phi_{(i,j-1,k)} - \phi_{(i,j+1,k)}}{2\Delta y} \tag{3.38}$$

$$E_{y[i][j][k]} = \frac{\phi_{(i,j,k-1)} - \phi_{(i,j,k+1)}}{2\Delta z} \tag{3.39}$$

For $E_{x[i][j][k]}$ = Electrical field in position i equivalent with $E_{x(x,y,z)}$

$E_{y[i][j][k]}$ = Electrical field in position j equivalent with $E_{y(x,y,z)}$

$E_{z[i][j][k]}$ = Electric field in position k equivalent with $E_{z(x,y,z)}$

$\phi_{(i+1,j,k)}$ = Electrical potential in position i+1 (right position)

$\phi_{(i-1,j,k)}$ = Electrical potential in position i-1 (left Position)

$\phi_{(i,j+1,k)}$ = Electrical potential in position j+1 (forward position)

$\phi_{(i,j-1,k)}$ = Electrical potential in position j-1 (backward position)

$\phi_{(i,j,k+1)}$ = Electrical potential in position k+1 (up position)

$\phi_{(i,j,k-1)}$ = Electrical potential in position k-1 (down position)

Δx = Distance between Position i and i+1

Δy = Distance between Position j and j+1

Δz = Distance between Position k and k+1

Magnetic field concerned is regarded as the relationship with electrical field. That relation ship is

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{3.40}$$

It can be written in discrete difference approximation as

$$-\frac{\partial \vec{B}}{\partial t} = -\frac{\left[\vec{B}_{new} - \vec{B}_{old}\right]}{\Delta t} \tag{3.41}$$

$$-\frac{\partial \vec{B}}{\partial t} = \frac{\left[\vec{B}_{old} - \vec{B}_{new}\right]}{\Delta t} \tag{3.42}$$

$$-\frac{\partial \vec{B}}{\partial t} = \frac{\left[B_{x_{old}} - B_{x_{new}}\right]}{\Delta t}\hat{i} + \frac{\left[B_{y_{old}} - B_{y_{new}}\right]}{\Delta t}\hat{j} + \frac{\left[B_{z_{old}} - B_{z_{new}}\right]}{\Delta t}\hat{k} \tag{3.43}$$

$$-\frac{\partial B}{\partial t}=\frac{\left[B_{x[i][j][k]_{old}}-B_{x[i][j][k]_{new}}\right]}{\Delta t}\hat{i}+\ldots$$
$$\ldots+\frac{\left[B_{y[i][j][k]_{old}}-B_{y[i][j][k]_{new}}\right]}{\Delta t}\hat{j}+\frac{\left[B_{z[i][j][k]_{old}}-B_{z[i][j][k]_{new}}\right]}{\Delta t}\hat{k} \tag{3.44}$$

$$\nabla\times E=\left(\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}\right)\hat{i}+\left(\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}\right)\hat{j}+\left(\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}\right)\hat{k} \tag{3.45}$$

$$\left(\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}\right)\hat{i}+\left(\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}\right)\hat{j}+\left(\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}\right)\hat{k}=-\frac{\partial B}{\partial t} \tag{3.46}$$

$$\left[\left(\frac{E_{z[i][j][k]}-E_{z[i][j-1][k]}}{\Delta y}\right)-\left(\frac{E_{y[i][j][k]}-E_{y[i][j][k-1]}}{\Delta z}\right)\right]=\frac{B_{x[i][j][k][t_0]}-B_{x[i][j][k][t_1]}}{\Delta t} \tag{3.47}$$

$$\left[\left(\frac{E_{x[i][j][k]}-E_{x[i][j][k-1]}}{\Delta z}\right)-\left(\frac{E_{z[i][j][k]}-E_{z[i-1][j][k]}}{\Delta x}\right)\right]=\frac{B_{y[i][j][k][t_0]}-B_{y[i][j][k][t_1]}}{\Delta t} \tag{3.48}$$

$$\left[\left(\frac{E_{y[i][j][k]}-E_{y[i-1][j][k]}}{\Delta x}\right)-\left(\frac{E_{x[i][j][k]}-E_{x[i][j-1][k]}}{\Delta y}\right)\right]=\frac{B_{z[i][j][k][t_0]}-B_{z[i][j][k][t_1]}}{\Delta t} \tag{3.49}$$

Therefore, the electrical potential, electrical field and magnetic field parameters are determined by the method mention above.

To solve Lorentz Force equation by finite difference method

The Electrical fields from these solutions are used to calculate plasma particles displacement by Lorentz Force equation or equation 3.2. This equation will be reformed in term of t .The form of Lorentz Force equation in t relation can be written as

$$\ddot{x}=\frac{q}{m}E_x(x,y,z,t) \tag{3.50}$$

$$\frac{\partial^2 x}{\partial t^2}=\frac{q}{m}E_x(x,y,z,t) \tag{3.51}$$

$$\ddot{y}=\frac{q}{m}E_y(x,y,z,t) \tag{3.52}$$

$$\frac{\partial^2 y}{\partial t^2}=\frac{q}{m}E_y(x,y,z,t) \tag{3.53}$$

$$\ddot{z}=\frac{q}{m}E_z(x,y,z,t) \tag{3.54}$$

$$\frac{\partial^2 z}{\partial t^2}=\frac{q}{m}E_z(x,y,z,t) \tag{3.55}$$

The Electrical fields and Magnetic field from these solutions are concern and they are used to calculate plasma particles displacement by Lorentz Force equation

$$\vec{F}=q(\vec{E}+\vec{v}\times\vec{B}) \tag{3.56}$$

$$\vec{v}=v_x\hat{i}+v_y\hat{j}+v_z\hat{k} \tag{3.57}$$

$$\vec{B}=B_x\hat{i}+B_y\hat{j}+B_z\hat{k} \tag{3.58}$$

$$\vec{E}=E_x\hat{i}+E_y\hat{j}+E_z\hat{k} \tag{3.59}$$

In x component

$$\vec{F}_x=q\left[E_x+\left(v_yB_z-v_zB_y\right)\right]\hat{i} \tag{3.60}$$

$$\vec{F}_x=m\frac{\partial^2 x}{\partial t^2}\hat{i} \tag{3.61}$$

$$\frac{\partial^2 x}{\partial t^2}\hat{i}=\frac{q}{m}\left[E_x(x,y,z,t)+\left(v_y(x,y,z,t)B_z(x,y,z,t)-v_z(x,y,z,t)B_y(x,y,z,t)\right)\right]\hat{i} \tag{3.62}$$

$$\ddot{x} = \frac{q}{m}\left[E_{x[i][j][k]} + \left(\dot{y}B_{z[i][j][k]} - \dot{z}B_{y[i][j][k]}\right)\right] \tag{3.63}$$

In *y* component

$$\vec{F}_y = q\left[E_y + \left(v_z B_x - v_x B_z\right)\right]\hat{j} \tag{3.64}$$

$$\vec{F}_y = m\frac{\partial^2 y}{\partial t^2}\hat{j} \tag{3.65}$$

$$\frac{\partial^2 y}{\partial t^2}\hat{j} = \frac{q}{m}\left[E_y(x,y,z,t) + \left(v_z(x,y,z,t)B_x(x,y,z,t) - v_x(x,y,z,t)B_z(x,y,z,t)\right)\right]\hat{j} \tag{3.66}$$

$$\ddot{y} = \frac{q}{m}\left[E_{y[i][j][k]} + \left(\dot{z}B_{x[i][j][k]} - \dot{x}(x,y,z,t)B_{z[i][j][k]}\right)\right] \tag{3.67}$$

In *z* component

$$\vec{F}_z = q\left[E_z + \left(v_x B_y - v_y B_x\right)\right]\hat{k} \tag{3.68}$$

$$\vec{F}_z = m\frac{\partial^2 z}{\partial t^2}\hat{k} \tag{3.69}$$

$$\frac{\partial^2 z}{\partial t^2}\hat{k} = q\left[E_z(x,y,z,t) + \left(v_x(x,y,z,t)B_y(x,y,z,t) - v_y(x,y,z,t)B_x(x,y,z,t)\right)\right]\hat{k} \tag{3.70}$$

$$\ddot{z} = q\left[E_{z[i][j][k]} + \left(\dot{x}B_{y[i][j][k]} - \dot{y}B_{x[i][j][k]})\right)\right] \tag{3.71}$$

These equations are second order differential equation. These equations are solved by Runge-Kutta Method that involves a weighted average of values of $f(x,y,z,t)$ taken at different point in the interval $t_n \le t \le t_{n+1}$.

Computing cycle

The calculation can be repeated to simulate the motion of plasma over time period. The position and velocity of ion particle in plasma field is updated by calculating each round of time step. The position of particle is changed by electrical influences of potential and electrical field. As a result, the ion density in plasma field is changed. The update electrical potential is calculated by new ion density. The new electrical field is solved by electrical potential, and the ion position and velocity of particles are updated by electrical field variables that are used to solve in Lorentz force equation. All processes are repeated for many time steps.

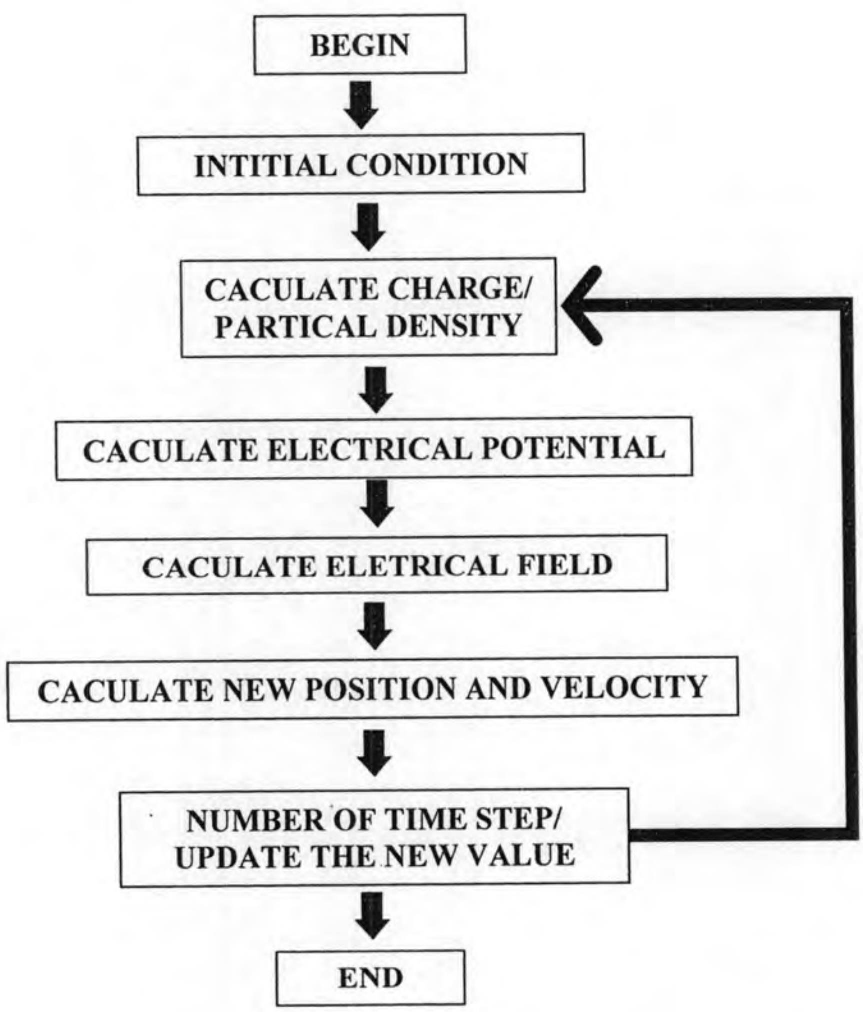

Fig. 3.1 Flow chart of Plasma source ion implant calculation

3.3 Plasma Source Ion Implantation

The numerical plasma particle model is used for determining the frequency of the electrical pulse. It can describe the ion movements in the plasma system. At first, the electrical potential is determined from Poisson's equation, which is the relationship between the Laplacian of electrical potential and ions electrons density. The equation is shown in equation 3.72, where ϕ is the electrical potential; q is the elementary charge, n_i is ion plasma density, n_e is electron plasma density and ε_0 is vacuum permittivity.

$$\nabla^2\phi = -q\frac{(n_i - n_e)}{\varepsilon_0} \tag{3.72}$$

This equation is solved by the method of finite difference to identify the electrical potential. Furthermore, the initial condition for the simulation is the assumption that the system is in thermal equilibrium for electron distribution. In such case, electron density can be described by Boltzmann equation, equation 3.73.

$$n_e = n_0 \exp(q\phi / KT_e) \tag{3.73}$$

Where n_0 is the uniform initial density of the plasma, K is the Boltzmann constant, and T_e is the electron temperature at thermal equilibrium.

Subsequently, the electrical potential is employed to determine the electrical field according to equation 3.74.

$$\vec{E} = -\nabla\phi \tag{3.74}$$

Afterward, the electrical field is employed to determine the ion movement in the plasma system as described by Lorentz force equation 3.75, where F is the force that reacts with ion in plasma field. The solution of this equation is then solved with the Runge-Kutta method.

$$\vec{F} = q\vec{E} \tag{3.75}$$

Under the periodic boundary condition, it is assumed that as the ions move out of the boundary on end side, they move into the system again from the other side of the system. For example, when some ions move out from the left side of system, it then moves in to right the system from the right handed side. The collision between ions in the system is neglected. The electrical pulse is stipulated by the internal boundary condition, where the frequency and the magnitude of the pulse can be manipulated. The plasma chamber is depicted as a cube with the size of 10 cm. The cube contains the hydrogen plasma (density = 10^{10} m^{-3}) as shown in figure 3.2. Moreover, a cubic sample (5 cm) is placed inside the plasma chamber at its center and the pulse is set at -2000 volt. Figure 3.3 shows the characteristic of the electrical pulse. .

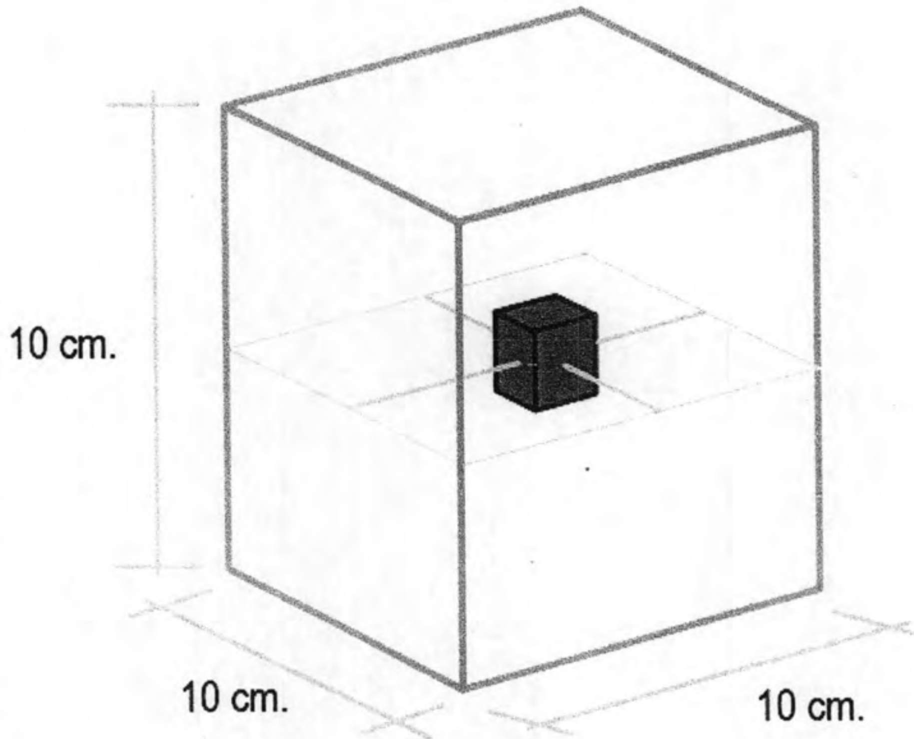

Fig. 3.2 Schematic of simulation plasma container

The electron temperature at its thermal equilibrium is 4 eV. Only the hydrogen is simulated in the system. The 10^7 hydrogen ion particles are assumed in this system. The simulated particles are used to calculate in this model and each simulated particles is equivalent to 10^2 hydrogen ion particles. Therefore this model uses 10^5 simulated particles in simulating ion motion in the plasma field. The position and velocity of an ion particle are updated by in each time step. It is found that when the positions of the particles changed, the ion density is also changed. The updated electrical potential is then found from the new ion density. The new electrical potential is solved for the new electric field, and the updated positions and velocities of particles are solved by the new electric field. The simulation process is repeated for many time steps. For this simulation, 3000 steps which each step is 10^{-8} second are employed.

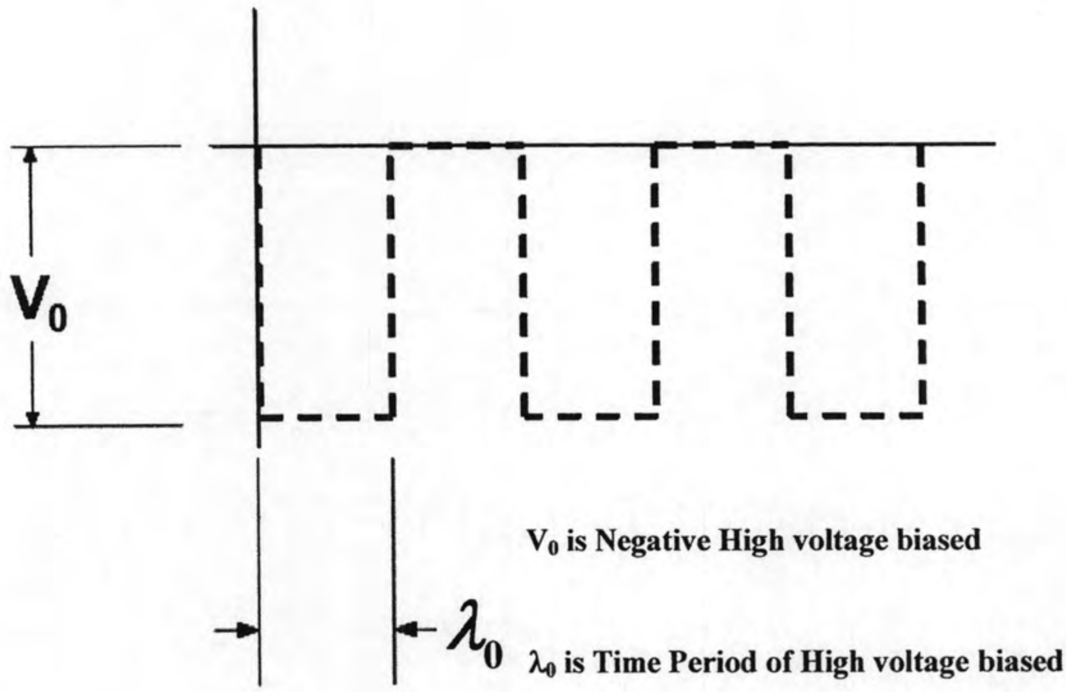

Fig. 3.3 Configuration of negative high voltage pulse biased

3.4 Ion Implantation

For this study, the molecular dynamic model was numerically used to determine the ion range in the lattice medium and to describe the motion of an ion in the medium. It was assumed that all ions and lattice particles involved in the calculation were pointed like. Two types of atomic interaction potentials between the ion and the lattice particles were implemented. One was the ZBL potential for the long range interaction. The other one was LJ potential for the short range one. Subsequentially, the net atomic force was computed from all of the interacting forces between each atomic pairs in the system. The interacting force between the ion and lattice particles was determined by Hamiltonian function (H) where

$$H = \frac{1}{2m} p^2 + f_{IPE}(x,y,z) \tag{3.76}$$

$$\vec{F} = -\nabla H \tag{3.77}$$

$$\vec{F} = -(\frac{\partial f_{IPE}(x,y,z)}{\partial x}\hat{i} + \frac{\partial f_{IPE}(x,y,z)}{\partial y}\hat{j} + \frac{\partial f_{IPE}(x,y,z)}{\partial z}\hat{k}) \tag{3.78}$$

F was the interatomic force. For the above relation, the parameter x, y, and z indicated the position in Cartesian coordinate and $f_{IPE}(x,y,z)$ was the interatomic potential the ion and the lattices. There are two types of potential energy in interatomic potential. One is long range ZBL potential ($V_{ZBL}(x,y,z)$). Another one is short range Landard Jone potential ($V_{LJ}(x,y,z)$) .Both of them is shown below. ZBL potential ($V_{ZBL}(x,y,z)$) is showed.

$$V_{ZBL}(r) = \frac{1}{4\pi\varepsilon_0}\left(\frac{q_1 q_2}{r}\right)\phi(r) \tag{3.79}$$

$$V_{ZBL}(x,y,z) = \frac{1}{4\pi\varepsilon_0}\left(\frac{q_1 q_2}{(x^2+y^2+z^2)^{1/2}}\right)\phi(x,y,z) \tag{3.80}$$

$$V_{ZBL}(x,y,z) = \delta(x,y,z)\phi(x,y,z) \tag{3.81}$$

$$\frac{\partial \delta(x,y,z)}{\partial x} = \frac{q_1 q_2}{4\pi\varepsilon_0}\left(-\frac{1}{2}\right)\left(x^2+y^2+z^2\right)^{-\frac{3}{2}}(2x) \tag{3.82}$$

$$\frac{\partial\delta(x,y,z)}{\partial x}=-\frac{q_1q_2}{4\pi\varepsilon_0}x\left(x^2+y^2+z^2\right)^{-\frac{3}{2}} \tag{3.83}$$

$$\frac{\partial\delta(x,y,z)}{\partial y}=\frac{q_1q_2}{4\pi\varepsilon_0}\left(-\frac{1}{2}\right)\left(x^2+y^2+z^2\right)^{-\frac{3}{2}}(2y) \tag{3.84}$$

$$\frac{\partial\delta(x,y,z)}{\partial y}=-\frac{q_1q_2}{4\pi\varepsilon_0}y\left(x^2+y^2+z^2\right)^{-\frac{3}{2}} \tag{3.85}$$

$$\frac{\partial\delta(x,y,z)}{\partial z}=\frac{q_1q_2}{4\pi\varepsilon_0}\left(-\frac{1}{2}\right)\left(x^2+y^2+z^2\right)^{-\frac{3}{2}}(2z) \tag{3.86}$$

$$\frac{\partial\delta(x,y,z)}{\partial z}=-\frac{q_1q_2}{4\pi\varepsilon_0}z\left(x^2+y^2+z^2\right)^{-\frac{3}{2}} \tag{3.87}$$

$$\phi(r)=0.1818e^{-3.2\frac{r}{a}}+0.5099e^{-0.9423\frac{r}{a}}+0.2802e^{-0.4029\frac{r}{a}}+0.02817e^{-0.2016\frac{r}{a}} \tag{3.88}$$

$$\begin{aligned}\phi(x,y,z)&=0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots\\ &\ldots+0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\end{aligned} \tag{3.89}$$

For X component, those are shown below.

$$\frac{\partial\phi(x,y,z)}{\partial x}=\frac{\partial\left(0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial x}+\frac{\partial\left(0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial x}+\ldots$$
$$\ldots+\frac{\partial\left(0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial x}+\frac{\partial\left(0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial x} \tag{3.90}$$

$$\frac{\partial\phi(x,y,z)}{\partial x}=\left(\frac{\partial\left[\frac{-3.2}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial x}\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{\partial\left[\frac{-0.9423}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial x}\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{\partial\left[\frac{-0.4029}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial x}\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{\partial\left[\frac{-0.2016}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial x}\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} \tag{3.91}$$

$$\frac{\partial\phi(x,y,z)}{\partial x}=\left(\frac{-3.2}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2x)\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.9423}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2x)\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.4029}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2x)\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots \tag{3.92}$$
$$\ldots+\left(\frac{-0.2016}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2x)\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}$$

$$\frac{\partial\phi(x,y,z)}{\partial x}=\left(\frac{-3.2x}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.9423x}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.4029x}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots \tag{3.93}$$
$$\ldots+\left(\frac{-0.2016x}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}$$

$$\frac{\partial V_{ZBL}(x,y,z)}{\partial x}=\phi(x,yz)\frac{\partial\left(\delta(x,y,z)\right)}{\partial x}+\delta(x,y,z)\frac{\partial\left(\phi(x,y,z)\right)}{\partial x} \tag{3.94}$$

For $\boldsymbol{Y}$ component, those are shown below.

$$\frac{\partial\phi(x,y,z)}{\partial y}=\frac{\partial\left(0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial y}+\frac{\partial\left(0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial y}+\ldots$$
$$\ldots+\frac{\partial\left(0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial y}+\frac{\partial\left(0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial y} \tag{3.95}$$

$$\frac{\partial\phi(x,y,z)}{\partial y}=\left(\frac{\partial\left[\frac{-3.2}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial y}\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{\partial\left[\frac{-0.9423}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial y}\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{\partial\left[\frac{-0.4029}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial y}\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots \tag{3.96}$$
$$\ldots+\left(\frac{\partial\left[\frac{-0.2016}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial y}\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}$$

$$\frac{\partial\phi(x,y,z)}{\partial y}=\left(\frac{-3.2}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2y)\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.9423}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2y)\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.4029}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2y)\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.2016}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2y)\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} \tag{3.97}$$

$$\frac{\partial\phi(x,y,z)}{\partial y}=\left(\frac{-3.2y}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.9423y}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.4029y}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$
$$\ldots+\left(\frac{-0.2016y}{a}(x^2+y^2+z^2)^{-\frac{3}{2}}\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} \tag{3.98}$$

$$\frac{\partial V_{ZBL}(x,y,z)}{\partial y}=\phi(x,yz)\frac{\partial\left(\delta(x,y,z)\right)}{\partial y}+\delta(x,y,z)\frac{\partial\left(\phi(x,y,z)\right)}{\partial y} \tag{3.99}$$

For X component, those are shown below.

$$\frac{\partial\phi(x,y,z)}{\partial z}=\frac{\partial\left(0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial z}+\frac{\partial\left(0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial z}+\ldots$$

$$\ldots+\frac{\partial\left(0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial z}+\frac{\partial\left(0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}\right)}{\partial z} \quad (3.100)$$

$$\frac{\partial\phi(x,y,z)}{\partial z}=\left(\frac{\partial\left[\frac{-3.2}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial z}\right)0.1818e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$

$$\ldots+\left(\frac{\partial\left[\frac{-0.9423}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial z}\right)0.5099e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots$$

$$\ldots+\left(\frac{\partial\left[\frac{-0.4029}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial z}\right)0.2802e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}+\ldots \quad (3.101)$$

$$\ldots+\left(\frac{\partial\left[\frac{-0.2016}{a}(x^2+y^2+z^2)^{\frac{1}{2}}\right]}{\partial z}\right)0.02817e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}$$

$$\frac{\partial \phi(x,y,z)}{\partial z} = \left(\frac{-3.2}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2z) \right) 0.1818 e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} + \dots$$
$$\dots + \left(\frac{-0.9423}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2z) \right) 0.5099 e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} + \dots$$
$$\dots + \left(\frac{-0.4029}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2z) \right) 0.2802 e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} + \dots \quad (3.102)$$
$$\dots + \left(\frac{-0.2016}{a}\frac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}(2z) \right) 0.02817 e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}$$

$$\frac{\partial \phi(x,y,z)}{\partial z} = \left(\frac{-3.2z}{a}(x^2+y^2+z^2)^{-\frac{3}{2}} \right) 0.1818 e^{-3.2\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} + \dots$$
$$\dots + \left(\frac{-0.9423z}{a}(x^2+y^2+z^2)^{-\frac{3}{2}} \right) 0.5099 e^{-0.9423\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} + \dots$$
$$\dots + \left(\frac{-0.4029z}{a}(x^2+y^2+z^2)^{-\frac{3}{2}} \right) 0.2802 e^{-0.4029\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}} + \dots \quad (3.103)$$
$$\dots + \left(\frac{-0.2016z}{a}(x^2+y^2+z^2)^{-\frac{3}{2}} \right) 0.02817 e^{-0.2016\frac{(x^2+y^2+z^2)^{\frac{1}{2}}}{a}}$$

$$\frac{\partial V_{ZBL}(x,y,z)}{\partial z} = \phi(x,yz)\frac{\partial\left(\delta(x,y,z)\right)}{\partial z} + \delta(x,y,z)\frac{\partial\left(\phi(x,y,z)\right)}{\partial z} \quad (3.104)$$

Landard Jone potential ($V_{LJ}(x,y,z)$) is showed.

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad (3.105)$$

$$V_{LJ}(x,y,z) = 4\varepsilon\left[\left(\frac{\sigma}{(x^2+y^2+z^2)^{1/2}}\right)^{12} - \left(\frac{\sigma}{(x^2+y^2+z^2)^{1/2}}\right)^{6}\right] \tag{3.106}$$

$$V_{LJ}(x,y,z) = 4\varepsilon\left[\frac{\sigma^{12}}{\left(x^2+y^2+z^2\right)^6} - \frac{\sigma^6}{\left(x^2+y^2+z^2\right)^3}\right] \tag{3.107}$$

X axis.

$$\frac{\partial V_{LJ}(x,y,z)}{\partial x} = 4\varepsilon\left[\sigma^{12}\frac{\partial\left(x^2+y^2+z^2\right)^{-6}}{\partial x} - \sigma^6\frac{\partial\left(x^2+y^2+z^2\right)^{-3}}{\partial x}\right] \tag{3.108}$$

$$\frac{\partial V_{LJ}(x,y,z)}{\partial x} = \left(\left(24\varepsilon\sigma^6 x\right)\left(x^2+y^2+z^2\right)^{-4}\right) - \left(\left(48\varepsilon\sigma^{12} x\right)\left(x^2+y^2+z^2\right)^{-7}\right) \tag{3.109}$$

Y axis.

$$\frac{\partial V_{LJ}(x,y,z)}{\partial y} = 4\varepsilon\left[\sigma^{12}\frac{\partial\left(x^2+y^2+z^2\right)^{-6}}{\partial y} - \sigma^6\frac{\partial\left(x^2+y^2+z^2\right)^{-3}}{\partial y}\right] \tag{3.110}$$

$$\frac{\partial V_{LJ}(x,y,z)}{\partial y} = \left(\left(24\varepsilon\sigma^6 y\right)\left(x^2+y^2+z^2\right)^{-4}\right) - \left(\left(48\varepsilon\sigma^{12} y\right)\left(x^2+y^2+z^2\right)^{-7}\right) \tag{3.111}$$

Z axis.

$$\frac{\partial V_{LJ}(x,y,z)}{\partial z} = 4\varepsilon\left[\sigma^{12}\frac{\partial\left(x^2+y^2+z^2\right)^{-6}}{\partial z} - \sigma^6\frac{\partial\left(x^2+y^2+z^2\right)^{-3}}{\partial z}\right] \tag{3.112}$$

$$\frac{\partial V_{LJ}(x,y,z)}{\partial z}=\left(\left(24\varepsilon\sigma^{6}z\right)\left(x^{2}+y^{2}+z^{2}\right)^{-4}\right)-\left(\left(48\varepsilon\sigma^{12}z\right)\left(x^{2}+y^{2}+z^{2}\right)^{-7}\right) \quad (3.113)$$

Inter atomic force is shown belown.

$$f_{IPE}(x,y,z)=V_{ZBL}+V_{LJ} \quad (3.114)$$

X axis

$$\frac{d^{2}x}{dt^{2}}\hat{i}=-\frac{1}{m}\frac{\partial f_{IPE}(x,y,z)}{\partial x}\hat{i} \quad (3.115)$$

$$\frac{d^{2}x}{dt^{2}}\hat{i}=-\frac{1}{m}\left[\frac{\partial V_{ZBL}(x,y,z)}{\partial x}+\frac{\partial V_{LJ}(x,y,z)}{\partial x}\right]\hat{i} \quad (3.116)$$

Y axis

$$\frac{d^{2}y}{dt^{2}}\hat{j}=-\frac{1}{m}\frac{\partial f_{IPE}(x,y,z)}{\partial y}\hat{j} \quad (3.117)$$

$$\frac{d^{2}y}{dt^{2}}\hat{j}=-\frac{1}{m}\left[\frac{\partial V_{ZBL}(x,y,z)}{\partial y}+\frac{\partial V_{LJ}(x,y,z)}{\partial y}\right]\hat{j} \quad (3.118)$$

Z axis

$$\frac{d^{2}z}{dt^{2}}\hat{k}=-\frac{1}{m}\frac{\partial f_{IPE}(x,y,z)}{\partial z}\hat{k} \quad (3.119)$$

$$\frac{d^{2}z}{dt^{2}}\hat{k}=-\frac{1}{m}\left[\frac{\partial V_{ZBL}(x,y,z)}{\partial z}+\frac{\partial V_{LJ}(x,y,z)}{\partial z}\right]\hat{k} \quad (3.120)$$

For the simulation, the calculation with the Runge-Kutta technique was attempted. For the boundary condition, was assumed to an ion that moved out of one boundary immediately entered the system again from the opposite boundary. This was called the periodic boundary condition.

As it was not possible to model the full size medium, even with the periodic boundary condition, it was then necessary to simplify the lattice system to that of the cubic type with only 1000 lattices. The size of the system was not defined by the physical length but by the number of the lattice and the distance between two adjacent lattices.

The collisions between the ions and the medium lattices were neglected. No lattice defects and all other irregular formation were considered. For this study, the lattices types of simple cubic (SC), body center cubic (BCC) and face center cubic (FCC) were considered for the calculation of the ion motion.

The position and the velocity of an ion particle were updated in each time step under the influence of the lattice interaction potential. It was found that when the ion changed the position, the lattice interaction potential was also changed. The updated interatomic force was then recalculated for the new ion position. Then the updated position and the velocity of the ion were solved for the new interatomic force. The simulation process was repeated for many time steps. For this simulation, amount 3000 time steps, each step was 10^{-17}- 10^{-15} second, were used.

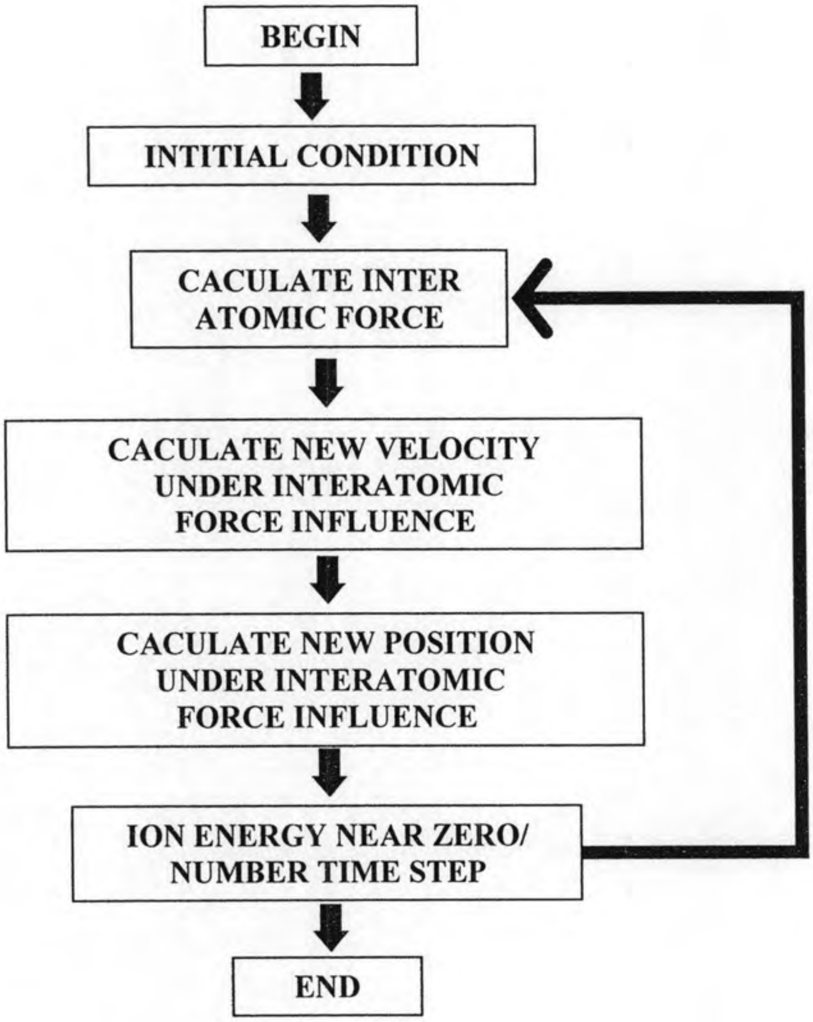

Fig. 3.4 Flow chart of ion implantation calculation

3.5 Ion Coating Model

For this study, the molecular dynamic model was used to describe the mechanism of the coating of the ion on the basement material and the implantation of that ion in the basement. The energy of the coating ion was accelerated by the plasma source ion implantation process. From the result, the predicted mechanism described the motion of the ion. The behavior of the ion coating in the first period, ions will embed in the substance atom. Then when all of the substance space were filled with the coating atom, the next ion embedded overlie on previous embedded ion. For the embedded process continuously happen for the long period of time, the process caused the ion coating cover the entire substance surface. It was assumed that all ions and lattice particles involved in the calculation were pointed like. Two types of atomic interactions potential between the ion and the lattice particles were implemented. One was the ZBL potential for long range interaction. The other one was LJ potential for short range. Subsequentially, the total atomic force was computed from all of the interacting forces between atomic pairs in the system. The interacting force between the ion and lattice particles was determined by Hamiltonian function (H) where

$$H = \frac{1}{2m} p^2 + f_{IPE}(x,y,z) \tag{3.121}$$

Moreover, the study had modified the interatomic force calculation by addition the embedded ion force (F_D).Based on the concept of Hamiltonian system and the artificial damping, the force acting on the coating ion was described as

$$\vec{F} = -\nabla H + \vec{F}_D \tag{3.122}$$

With the microconvergence model, the above equation was written as

$$\vec{F} = -\nabla H + K\vec{v}(x,y,z) \tag{3.123}$$

In the Cartesian coordinate, the equation became

$$\vec{F} = -(\frac{\partial f_{IPE}(x,y,z)}{\partial x}\hat{i} + \frac{\partial f_{IPE}(x,y,z)}{\partial y}\hat{j} + \frac{\partial f_{IPE}(x,y,z)}{\partial z}\hat{k}) + K(v_x\hat{i} + v_y\hat{j} + v_z\hat{k}) \tag{3.124}$$

F was the interatomic force. For the above relation, the parameter X , Y , and Z indicated the position in Cartesian coordinate and $f_{IPE}(x,y,z)$ was the interatomic forced the ion and the lattices. $v(x,y,z)$ indicated the function of the coating ion velocity in Cartesian coordinate. K was the negative value depended on the type of the medium, the type of the ion and the ion energy. For this study, K was determined by trialed K value in the simulation until got through the ion range from the standard TRIM/SRIM model.

The relationship between the basement atom and the coating ion can be described by the schematic in figure 3.5.

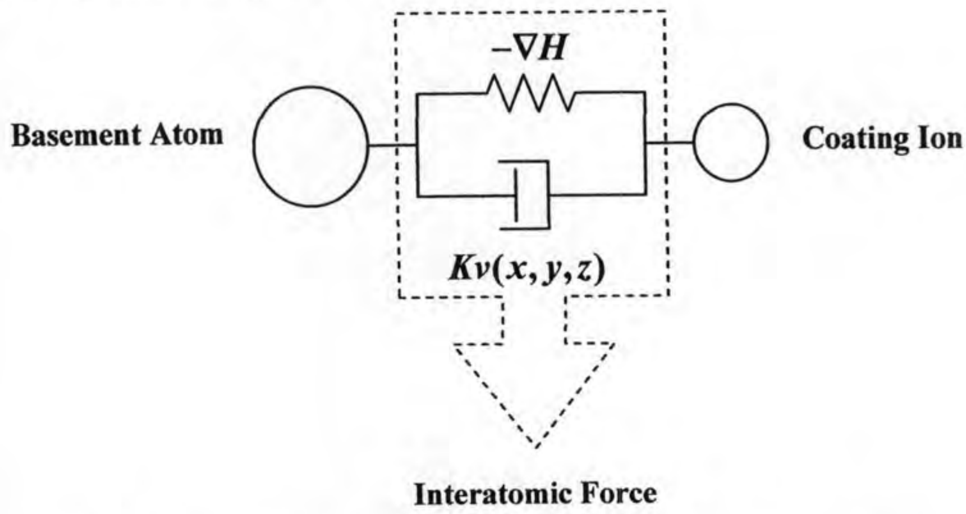

Fig. 3.5 Schematic of two body interatomic force equivalent between implanted ion and atom basement

For the simulation, the integration at each time steps was done with Runge-Kutta technique and the periodic boundary condition was assumed for the system.
In the term of the boundary condition, it was assumed to an ion that moved out of one boundary immediately entered the system again from the opposite boundary.

As it was not possible to model the full size medium, even with the periodic boundary condition, it was then necessary to simplify the lattice system to that of the cubic type with only 1000 lattices. The size of the system was not defined by the physical length but by the number of the lattice and the distance between two adjacent lattices.
The collisions between the ions and the medium lattices were neglected. No lattice defects and all other irregular formation were considered. For this study, the lattices types of simple cubic (SC), body center cubic (BCC) and face center cubic (FCC) were considered for the calculation of the ion motion.

The position and the velocity of an ion particle were updated in each time step under the influence of the lattice interaction potential. It was found that when the ion changed the position, the lattice interaction potential was also changed. The updated interatomic force was then recalculated for the new ion position. Then the updated position and the velocity of the ion were solved for the new interatomic force. The simulation process was repeated for many time steps. For this simulation, amount 3000 time steps, each step was 10^{-17}- 10^{-15} second, were used.

To test the concept, the system of interest had the coating of the target whose the mass number was 56 and the atomic number was 26 by the ions whose the mass and the atomic number were 195 and 78. The crystalline structures of target were figured to either SC, BCC or FCC. Such configurations were chosen because of the large values of the mass and the atomic numbers. This allowed their effects on the potential field, which governed the interaction forces, to be clearly demonstrated. At the same time, such configurations were common enough that they could be examined and compared by TRIM/SRIM code. In addition, the heavy ion had high energy lost ratio due to the interaction with the matter but with the small angle of scattering. Such condition allowed the comparison between the obtained results from the simulation with that for TRIM/SRIM to be more possible.

In the coating material, there were consist of 3 layers. The study divided those layers by the concept of the ion range. The mixed layer started from the upper surface of the target material to the ion range within the material. Above that layer was the coating layer started from the upper surface outside of the target material in the opposite direction with the ion range. For the sustaining or the basement layer, the layer was inside the target material defined from the ion range to the lower surface of the material.

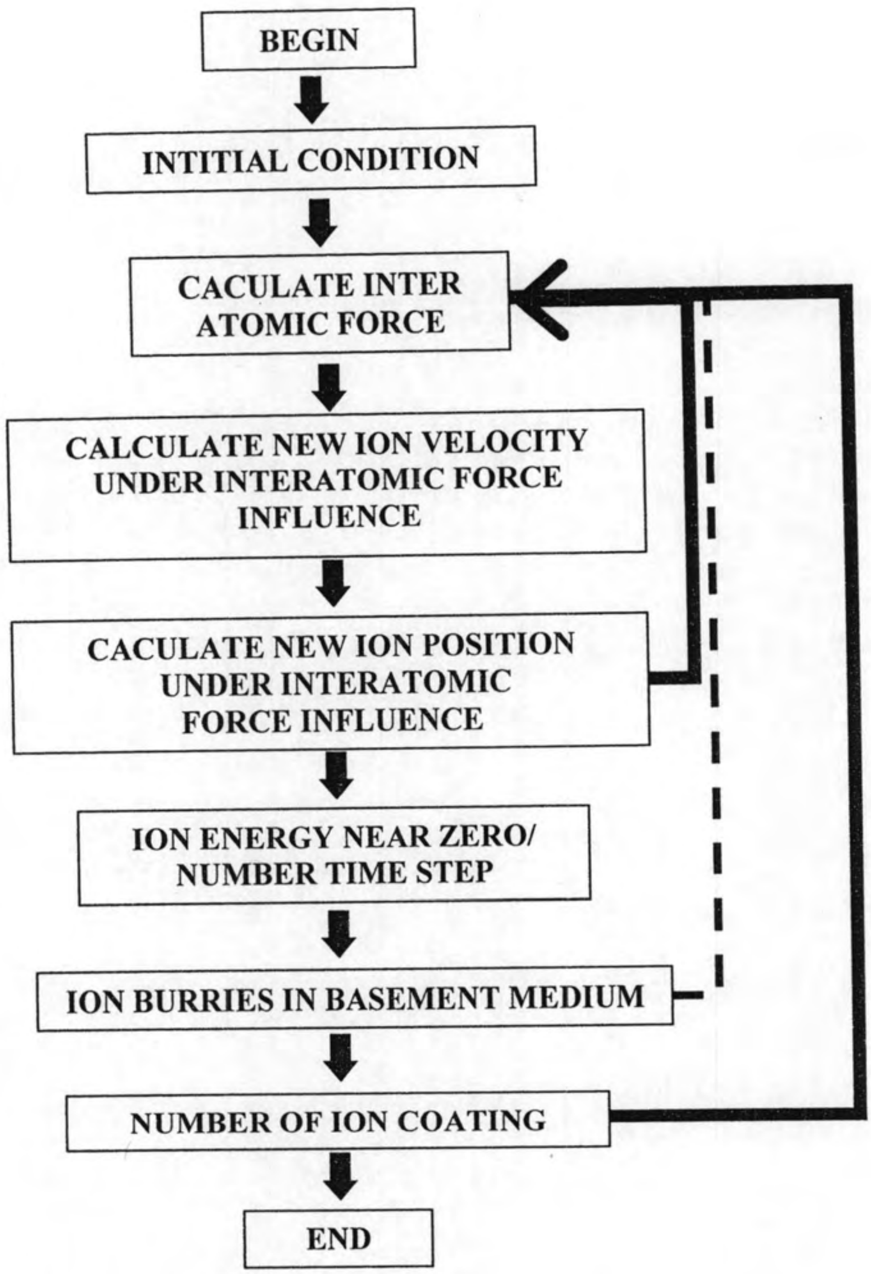

Fig. 3.6 Flow chart of ion coating calculation