CHAPTER V

Conclusion

5.1 Plasma Source Ion Implantation

The electrical pulse bias certainly affects the ion density distribution and the ion energy. The ion energy depends on the pulse bias. The time period of the electrical pulse dose not affect in the ion flux of the ion field when the frequency of the pulse bias is higher that the plasma frequency. From the periodic boundary condition, the Debye Shield effect did not significant then gave the result in the over estimate of the ion flux.

5.2 Ion Implantation

The ion range in the crystalline medium can be evaluated by this model, the molecular dynamic simulation. In comparison, the result of this model is consistent with the standard TRIM/SRIM model. Furthermore, the research found that the lattice type of the medium and the ion energy have an effect on the ion distribution and range in the medium. The accuracy and the precision of the calculation can be increased by the adjusting of $\boldsymbol{\varepsilon}$ parameter in LJ potential represented the ion energy in the equilibrium state, the decreasing of the dwell time in each time step and the increasing of the ion number.

5.3 Ion Coating

This simulation can be used to describe the model of the ion coating on the target in term of the trajectory, energy and velocity. The layers of the coated material were divided by the ion range and the ions distribution was used to describe the component of those layers. The simulation model of this study reduced the simulation time reasonable but still maintained the accuracy of the calculation. The accuracy and the precision of the calculation can be increased by the adjusting of $\boldsymbol{\varepsilon}$ parameter in LJ potential represented the ion energy in the equilibrium state, the adjusting of $\boldsymbol{K}$ value, the decreasing of the dwell time in each time step and the increasing of the ion number. The molecular dynamic simulation of the coating process is applicable for imagine the probability density function of the ion concentration. Furthermore the function also can be employed to derive the probability density function in macro-scale by Monte-Carlo calculation. The study can be used to change the depth of the mixed layer zone and to design the ion intensity in the coating layer zone by the ion energy adjusting. Nevertheless the time used to create the mixed layer zone and the coating layer zone are calculated by this study.

Since the simulations showed the coating process, the study results were satisfy and completed through the objectives. The simulations could be used to describe the creation mechanism of the mixed layer zone in crystalline materials. Moreover the creation times and the ion densities were obtained by applied with this simulation.

In this study only one ion was assumed to travel through the medium at a particular time, this resulted in the under estimation of the interaction between incoming ions. At the same time, as the atoms were assumed to stay inert, effect of the motions and interactions were also neglected. The study also reduced the simulation time by simulation a small system. To improve the accuracy, it was necessary to investigate the further how the size of the system affected the simulation. The periodic boundary condition was suitable for this study but might not be suitable in the other conditions. Moreover, the more accurate result could be accomplished with the more additional factors.

For the further study, the simulation should be study about the evaluation of the ion density in the mixed and coating layer zone when increasing the sufficient amount of ions.

Finally, the study could be applied for the material industries. One of the applications was the creation and estimation of the coating thickness and time.