Modeling electron beam parameters and plasma interface position in an anode plasma electron gun with hydrogen atmosphere

A Krauze¹, J Virbulis¹ and A Kravtsov²

¹ Center for Processes Analysis and Research Ltd, Zeļļu str. 25, LV-1002 Riga, Latvia
² KEPP EU LLC, Karnikavas str. 5, LV-1034 Riga, Latvia

Abstract. A beam glow discharge based electron gun can be applied as heater for silicon crystal growth systems in which silicon rods are pulled from melt. Impacts of high-energy charged particles cause wear and tear of the gun and generate an additional source of silicon contamination. A steady-state model for electron beam formation has been developed to model the electron gun and optimize its design. Description of the model and first simulation results are presented. It has been shown that the model can simulate dimensions of particle impact areas on the cathode and anode, but further improvements of the model are needed to correctly simulate electron trajectory distribution in the beam and the beam current dependence on the applied gas pressure.

1. Introduction

Silicon (Si) is the most widely used semiconducting material in microelectronics, high-power electronics and solar applications.

Traditional silicon crystal growth methods have limitations that do not allow them to grow large-diameter high-purity Si monocrystals. In the Czochralski method, Si monocrystals are pulled from Si melt in a quartz crucible. Due to crucible material dissolution in the molten Si, impurities are incorporated in grown crystals. Float zone (FZ) method requires high-purity polycrystalline Si feed rods as input material, and needle-eye high-frequency electromagnetic inductors that are used for the feed rod melting make it difficult to increase the diameter of the grown crystals.

An alternative to these systems could be a silicon crystal growth system where a crystal is pulled from a crucible in which the silicon melt is heated by a high-power beam glow discharge based electron gun, see figure 1. Because the beam energy is concentrated on a very small area of the free silicon melt surface, the silicon melt can be heated locally to very high temperatures. This allows to purify the silicon material to a very high degree. On the other hand, such melt heating allows to preserve a layer of solid Si crust between the melt and the crucible, which prevents contaminants from the crucible from entering the crystal. This method therefore can potentially be used to grow both high-purity and very large diameter crystals.

A key issue of electron guns is wear and tear of gun parts (cathode and anode in particular) that is caused by impacts of high-energy charged particles produced inside the guns. Besides increased exploitation costs, such wear also serves as an additional contamination source which must be reduced. One way to reduce the wear and tear is to reduce the particle impact areas. A mathematical model that can describe the working of the electron gun and potentially show the way to optimize it would be very helpful for this purpose.
For this reason a program system for modeling the applied beam glow discharge based electron gun has been developed. The program system simulates 2D axisymmetric EM field distribution in the gun and calculates 3D particle trajectories to model the electron beam formation. The aim of the model development is to obtain a tool that would correctly model the basic working parameters of the gun, especially the dimensions of the ion and electron impact areas on the cathode and anode. In this article, we present the description of the employed mathematical models, their numerical implementation, and the first simulation results.

2. Description of existing software for modeling electron guns

There are several software programs available for modeling electron guns. We will give here a brief description of some of the software.

EGUN/IGUN software package is a set of programs for modeling different aspects of electron guns [1]. EGUN is a 2D electron gun simulation software that calculates relativistic electron trajectories in electric and magnetic fields. It solves Poisson’s equation for the electric potential which is coupled with charge distribution generated by moving electrons. Similarly the magnetic field simulations take into account electron currents. Different modes of electron emissions are considered. IGUN is a related program for positive ion extraction from plasma, which uses a 1D model for the plasma sheath simulations. It seems however that EGUN and IGUN are two separate programs, whereas in our case we have to consider both electron and positive ion trajectories.

Opera FEA Simulation Software [2] is finite element electromagnetic simulation software that can also model electron guns. Similarly to EGUN/IGUN it also takes into account the space-charge and beam current influence on the EM field distributions and particle trajectories. This program contains additional features such as secondary particle emission from surfaces and ionization in the gas volume. A constant-potential plasma surface with constant-rate ion emission is implemented as an ion emission model for the plasma, and the plasma shape is determined iteratively. An example of a simulation of ion extraction from plasma surface can be found in [3].

Charged Particle Optics Software (CPO) is another software for calculation of electrostatic and magnetostatic fields and trajectories of charged particles flying through these fields. CPO uses a boundary element method for the field calculation, see [4].

Reference [5] describes a mathematical model of a beam glow discharge based electron gun which directly corresponds to the type of the gun that is considered in this article. As in all the previous models, it considers modeling a self-consistent electric field distribution coupled with a model for tracking charged particle movement in this field and calculation of the charge distribution. A description of boundary conditions for the electric field on the plasma boundary and condition required for finding its equilibrium shape are also given. Our mathematical model was based on this source.

3. Description of the working principles of the crystal growth facility and the applied electron gun

KEPP EU uses a beam glow discharge based electron gun for heating the free Si melt surface. The gun works by applying high voltage (30 kV) between its cathode and anode, see figure 2. A low-temperature low-ionization plasma is lit in the low-pressure (some Pa) hydrogen working gas near the anode. The positively charged hydrogen gas ions can escape from plasma into the neutral gas between the cathode and plasma. These ions, accelerated by the electric field, hit the cathode surface. As a result, cathode material atoms are released from its surface, and they can contaminate Si material.

The ion hits cause also emission of several secondary electrons. Accelerated by the electric field, they form a narrow beam that travels through a hole in the anode in the direction of the Si melt. Because the beam is larger than the hole, the anode surface is also damaged, and its material also becomes a contaminant. The hole cannot be freely widened because it will increase the gas flow out of the gun chamber and increase Si contamination.

Outside the gun chamber, the beam is affected by a system of electromagnets. Since the optimization of the beam control was not part of this task, only the two electromagnets that were the closest to the anode and could affect the electron trajectories were taken into account in the model.
FIGURE 1. A general scheme of a crystal growth system that uses an electron gun for the Si melt heating.

Heating up of the plasma by the electron beam creates a positive back-feed loop in the system and ensures continuing ion-electron pair generation in the plasma. Typically, the plasma is not at equilibrium, as the electron gas temperature is much higher than ion and neutral gas temperature. The electron gas pressure is balanced by the electric field pressure at the plasma interface which determines its form.

Thus, to obtain a quasi-stationary solution for electron beam formation, several physical models should be coupled together. Electric and magnetic field distributions determine particle trajectories. Particle trajectories determine electric charge distribution which affects the electric field. Finally, the plasma interface determines both the particle trajectories and the electric field distribution. Below we describe an iterative algorithm that couples these models.

4. Modeling the electron beam

4.1. Modeling the EM field

The gun geometry is axisymmetric, therefore it was assumed that the electric and magnetic field distributions in the gun are also axisymmetric.

$\varphi = -30 \text{kV}$ potential is applied to the cathode and its shield, see figure 3. A zero potential $\varphi = 0 \text{V}$ is set on the gun chamber walls and anode. The gun chamber volume can be divided into three different regions with separate properties. The plasma region is partially ionized gas near the anode, and it has electrical conductivity comparable to that of metals. Therefore, it is assumed that the electric field in the plasma is practically zero. The plasma is considered quasi-neutral (i.e. concentrations of electrons and positive ions in it is approximately the same, $n_e \approx n_p$). Nevertheless due to higher electron mobility, it becomes slightly charged, and the plasma potential $\varphi_{\text{plasma}}$ is slightly positive.

The working gas near the cathode, however, is characterized by very low ionization level and by a very strong electric field ($E \approx 10^6 \text{V/m}$) caused by the potential difference between the plasma and walls on the one hand and the cathode and the other hand. This electric field accelerates electrons and positive ions emitted from the cathode and plasma, respectively, so that an electric charge distribution is created in the gas. The charge density is higher near the cathode and plasma surfaces where particle velocities are lower. Thus the electric field in the working gas is modeled by solving a Poisson equation for the electric potential:
\[ \Delta \varphi = - \frac{\rho}{\varepsilon_0} \]  

(1)

where the distribution of the electric charge \( \rho \) is calculated from the particle trajectories.

\[ \nabla \times \left( \nabla \times \vec{H}_\theta \right) = \nabla \times \vec{j}_{r,z} \quad \nabla \times \left( \frac{1}{\mu \varepsilon_0} \nabla \times \vec{A}_\theta \right) = \vec{j}_\theta \]  

(2)

\( \vec{H}_\theta \) and \( \vec{A}_\theta \) are the azimuthal magnetic field and vector potential components, respectively.

The plasma and the working gas is separated by a very thin boundary layer called the plasma sheath. It is an electrically charged layer in which the positive ions are accelerated, and electrons are slowed down to prevent their escape from the plasma. Because the boundary between the plasma sheath and the working gas is not clearly defined, we assume for simplicity that it corresponds to the zero electric potential isoline. For this reason we use \( \varphi = 0 \) V boundary condition on the gas-plasma interface.

The equation for an axisymmetric magnetic field distribution can be split in two separate equations, one for the azimuthal magnetic field component \( \vec{H}_\theta \), and one for the azimuthal magnetic vector potential component \( \vec{A}_\theta \):

\[ \vec{H}_\theta = H_\theta \vec{e}_\theta \] (and similarly \( \vec{A}_\theta \) and \( \vec{j}_\theta \)), and \( \vec{j}_{r,z} = j_r \vec{e}_r + j_z \vec{e}_z \) is a meridional vector.

Although both equations systems can be solved by our model, only \( \vec{A}_\theta \) equation is used in practice, because electromagnet current strength (~1000 A-windings) by far exceed the beam current strength (1-3 A). The simulation area for the magnetic field encompasses the gun and a rectangular area around it. Symmetry boundary condition is applied on rotation axis and natural boundary condition on other boundaries.

The material properties of the ferromagnetic shields of the electromagnets could not have been determined. Simulations have shown that a typical magnetic field strength in the shields is about 0.1-0.3 T. It was decided that a constant permeability \( \mu = 1000 \) would be a good approximation of the shield material. A test simulation with \( \mu = 20 \) showed no significant changes in the particle impact distribution on the cathode or anode surfaces, which was our primary concern.

4.2. Calculation of plasma interface position
The plasma interface must obtain a shape that ensures that the electron gas pressure at the plasma interface is equal to electric field pressure [5]:

![Figure 3. Boundary conditions in electric field simulations.](image-url)
\[ p_E = \frac{\varepsilon_0 E^2}{2} = n_e kT_e \]  

(3)

where \( E_n \) is the normal component of the electric field at the plasma interface, \( n_e \) is electron concentration in the plasma, \( k \) is the Boltzmann constant, and \( T_e \) is electron temperature. Since we do not model the electron concentration and temperature in these simulations, we simply assume a constant \( p_E \) value. Several \( p_E \) values were used in the simulations to obtain a better agreement with experiments.

The following iterative algorithm is applied to find the interface position: first, electric field distribution is calculated, then an equation for interface node shifts \( h_i \) is solved:

\[ h_i + \lambda \frac{\partial^2 h_i}{\partial s^2} = p_E - \frac{\varepsilon_0 E^2}{2} \]  

(4)

where \( \lambda \) is a smoothing factor and \( s \) is interface arc length. The interface nodes are shifted in the normal direction, \( \delta_x = h_i \delta x_i \), where is some parameter. The node on the symmetry axis is shifted in the vertical direction, and the interface cross point with the wall is found by linear continuation of the penultimate segment of the interface.

4.3. Modeling particle trajectories and charge distribution

A predefined number of ion trajectories is calculated by integrating the Newton’s equations

\[ m \ddot{\vec{r}} = q(\vec{E} + \vec{v} \times \vec{B}) \]  

(5)

with 4th order Runge-Kutta method. It is assumed that emitted ions were protons. In [5], the Bohm’s speed is used to determine the ion emission current density \( j_p \) from the plasma surface:

\[ j_p = n_e \sqrt{\frac{2kT_e}{m_p}} \]  

(6)

where \( m_p \) is the mass of a positive ion. Assuming a homogeneous distribution of the electron temperature and ion concentration, a homogeneous emission rate for the ions can be used. The initial positions of the ion trajectories are chosen by randomly picking interface meridional segments and positions on them according to surface area represented by the segment. Zero velocity is used as initial condition. Each trajectory corresponds to part of the total ion current:

\[ I_p = \frac{I_{\text{ion}}}{N} \]  

(7)

where \( I_{\text{ion}} \) is predefined ion current strength, and \( N \) is the number of the ion trajectories.

| Table 1. Secondary electron emission coefficient for H\(^+\) hits on Al surface at 250\(^\circ\)C, [6]. |
|-----------------------------------|--------|--------|--------|--------|
| Kinetic energy, keV              | 9.9    | 20.12  | 30.2   | 41.08  |
| \( \kappa \)                    | 0.69   | 0.98   | 1.17   | 1.27   |

When an ion hits the cathode, an electron trajectory is generated with electron current \( I_e = -\kappa I_p \), where \( \kappa \) is the number of emitted secondary electrons. Initially we used \( \kappa \) from [6], table 1, however, the efficiency of the gun (~90%) suggests that \( \kappa \) is much larger, and simulations with \( \kappa = 9 \) where also performed. Electron trajectories are calculated until they hit any part of the gun elements or boundary of the simulation area.
Table 2. Cross sections for hydrogen ionization. [7]. Values for H$_2$ are doubled values for H.

| Kinetic energy, keV | 9.4  | 11.4 | 13.4 | 15.4 | 18.4 | 22.4 | 26.4 | 32.4 |
|-------------------|------|------|------|------|------|------|------|------|
| $\sigma$ for H, Å$^2$ | 0.162 | 0.245 | 0.331 | 0.438 | 0.569 | 0.779 | 1.053 | 1.227 |
| $\sigma$ for H$_2$, Å$^2$ | 0.324 | 0.490 | 0.662 | 0.876 | 1.138 | 1.558 | 2.106 | 2.454 |

We were also concerned with ion-electron pair generation in the neutral gas due to ionization by fast moving ions. For this reason, an ionization effect was implemented. During a time step, an ion travels a distance $l$. Its kinetic energy determines the reaction cross section $\sigma$, table 2, and reaction probability $\Gamma = 1 - e^{-n\sigma t}$, where $n$ is the gas particle concentration calculated from a given gas pressure $p$. If a reaction occurs, a pair of ion and electron trajectories is generated with currents $I_p$ and $-I_p$.

The electric charge density for a mesh node is calculated by determining time $\Delta t$ spent by each trajectory in the node neighborhood $S$. Charges $I_{p,e}\Delta t$ are added to the total node charge, and later it is divided by the 3D volume $V$ obtained by rotating $S$, see figure 4.

**Figure 4.** A node neighborhood area $S$ in 2D meridional plane can be rotated around the symmetry axis to obtain the associated 3D charge distribution volume $V$.

5. Numerical implementation

Triangular meshes for discretization of the electric and magnetic field equations were generated with a mesh generation program gmsh [8]. A single mesh for both electric and magnetic fields is created, figure 5. For the electric field simulations, only part of the whole mesh is used.

**Figure 5.** Example of 2D triangular mesh generated by gmsh.

**Figure 6.** A block scheme of the main iteration cycle for the electron beam simulation.
The equations were discretized using a finite element program getdp [9]. Both gmsh and getdp use special text input files, which are generated by a special python language script, which also calls gmsh to generate the mesh.

![Figure 7](image7.png)  ![Figure 8](image8.png)

**Figure 7.** Calculated ion particle trajectories (top) and impact density distribution on the cathode (bottom). $p_E = 0.01\, \text{Pa}$, $p = 1.5\, \text{Pa}$, $I_{ion} = 0.1\, \text{A}$.

**Figure 8.** Calculated electron trajectories. $p_E = 0.01\, \text{Pa}$, $p = 1.5\, \text{Pa}$, $I_{ion} = 0.1\, \text{A}$.

The main iteration cycle as well as the particle trajectory and plasma interface models are implemented in the main program written in C++. The block scheme of the main iteration cycle that couples all models together can be seen in figure 6. The program reads its input parameters from a text file and can be run in two modes: the main mode and preparation mode, which allows to calculate an initial plasma interface position by iteratively calculating the electric field distribution without particle trajectories.

6. Simulation results

Considering large secondary electron emission, a small ion current strength was chosen (0.1 A). Due to uncertainty about the actual electron gas concentration and temperature, several different electron gas pressure values were tested, form very low ($p_E = 0.01\, \text{Pa}$) to very high ($p_E = 1.8\, \text{Pa}$).

The calculation results with $p_E = 0.01\, \text{Pa}$ showed a very small ion impact area on the cathode (~8 mm in diameter), and a narrow electron beam, see figures 7 and 8. However, experimental observations, figure 9, show that impact area can be as large as 60 mm in diameter.

Simulations with larger electron gas pressure have showed that the calculated plasma interface shifts upwards when $p_E$ is increased, see figure 10. As a result, the ion emission spreads over larger cathode area. The best agreement with the experimental results is obtained for $p_E = 1.8\, \text{Pa}$, see figure 11.

A significant part of electrons hits the anode. Measured by the spike in the electron impact distribution, see figures 12 and 13, the affected area has diameter between 30 and 40 mm, which approximately corresponds to dimensions observed in experiments (~30-35 mm).
Due to electron current losses on the anode, the calculate gun efficiency rate is very low (~0.24 for \( p_E = 0.6 \) Pa and ~0.13 for \( p_E = 1.8 \) Pa. This suggests that there might be an inhomogeneous ion emission distribution on the plasma interface, in which the emission maximum is centered on the symmetry axis. Such an emission distribution could be caused by the interaction between the plasma and the electron beam. This effect could be modeled by using, for example, bell-shaped ion emission distributions instead of homogeneous emission rates. The electron gas pressure distribution on the plasma interface also can be modeled as a bell-shaped function. Due strong plasma shape dependence on the electron gas pressure, there is also a need to relate it to the applied working gas pressure and generated beam current strength.

7. Conclusions
A 2D quasi-stationary model for electron beam formation in a beam glow discharge based electron gun has been developed and tested. The model includes 2D axisymmetric steady-state modules for electric and magnetic field simulations and for calculation of 3D ion and electron trajectories.

Simulations have shown that the model is able to model the basic properties of the electron beam, such as dimensions of particle impact areas on the cathode and anode. However, further improvements have to be introduced in order to model correctly electron trajectory distribution in the beam, and the beam current dependence on the applied gas pressure.

8. References
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Figure 9. Example of a cathode surface that have been bombarded by ions. The impact area diameter is ~60 mm.

Figure 10. Dependence of the plasma interface shape on the applied electron gas pressure. \( p = 1.5 \) Pa, \( I_{ion} = 0.1 \) A.
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**Figure 11.** Dependence of the radial distribution of ion impact density on the cathode on the applied electron gas pressure. $p = 1.5 \text{ Pa}, \ I_{\text{ion}} = 0.1 \text{ A}.$
Figure 12. Radial distribution of electron impacts on the anode for $p_E = 0.6 \text{ Pa}$, $p = 1.5 \text{ Pa}$, $I_{\text{ion}} = 0.1 \text{ A}$.

Figure 13. Radial distribution of electron impacts on the anode for $p_E = 1.8 \text{ Pa}$, $p = 1.5 \text{ Pa}$, $I_{\text{ion}} = 0.1 \text{ A}$.

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