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SENSITIVITY ANALYSIS OF DIVERGENCE OF ION BEAM WITH RESPECT TO CHANGES OF SHAPE OF ACCELERATION GRID IN KAUFMAN TYPE ION SOURCES

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Abstract

This paper presents results of simulation for ion extraction from Kaufman type ion source by using CPO 2DS software. For electric potential and field determination the Boundary Element Method (BEM) implemented in CPO 2DS computer program is used. Simulations are made for different accelerator grid shapes. Variations of plasma meniscus shape and the sensitivity of divergence are analyzed in respect to variations of acceleration grid shape by using a finite difference approximation. The objective of the present work is a verification of influence of grid shape variations on beam divergence by numerical experiment. It is shown that a diameter variation of an acceleration grid aperture does not significantly influence on a divergence of ion beam.

Key words: ion source, extraction of ion beam from plasma source, ion beam divergence

1. INTRODUCTION

Ion sources of the Kaufman type are widely used in processes of ion surface modification. One of processes, where Kaufman's type ion source is used in the dual beam ion beam assisted deposition (DB IBAD) process. Surfaces coatings produced by DB IBAD have two advantageous features such as a high adhesion and high density. The method is also used to produce the functionally gradient materials (FGM). These coatings have wide spectrum of application ranging from the machine industry to biomedical implants. The diamond like carbon (DLC) coatings are especially useful in manufacturing of biomedical implants and chemical cells. Development of implantation techniques and their applications in industry processes motivate the investigation of ion source characteristics. A numerical simulation of phenomena occurring in an ion source can significantly help in the evaluation of desirable process parameters for a workpiece surface. The extraction of ion beam from an ion source is dynamically developing subject of research, because ion beam parameters are related to surface parameters. Ion beam optics have been studied for many years for heavy ion fusion [4], space propulsion [6] and for surface modification applications [16]. The review of numerical models of electrical propulsion, which are similar to models of ion sources, can be found in [1]. Many recent publications treat on the problem of ion extraction, but the relation between the divergence and the shape of electrode has not been yet analyzed by using BEM.

2. EXPERIMENT DESCRIPTION

The Kaufman type ion source is modeled by the DB IBAD process, which is schematically shown in figure 1.

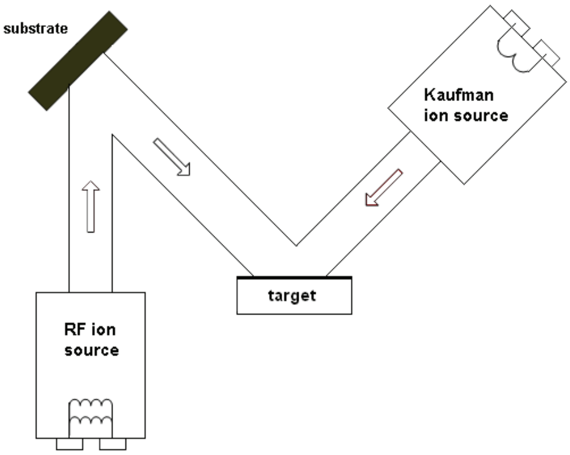

Fig. 1. The scheme of the DB IBAD process [15].

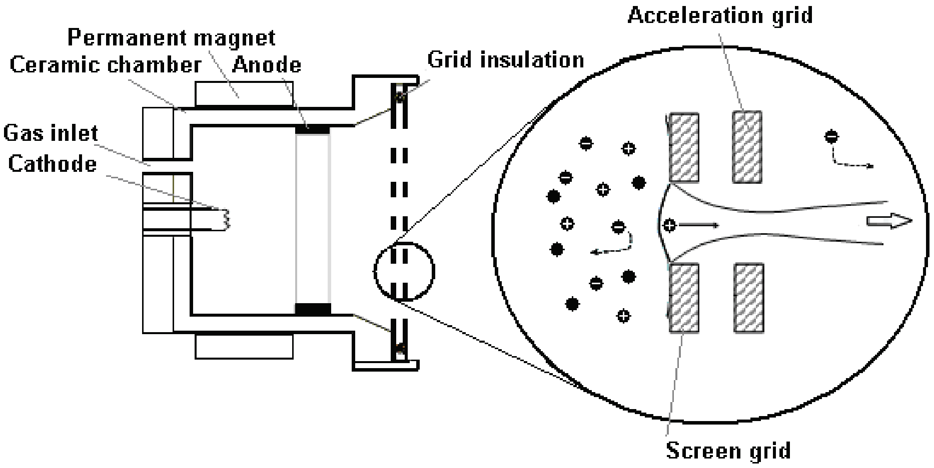

Fig. 2. Schematic diagram of the ion source with enlarged grid zone sector [7].

Two ion sources, used in the DB IBAD process, are placed in the high vacuum chamber. The ion beam generated by Radio Frequency (RF) ion source impinges ions on substrate and knocks out carbon atoms. A part of carbon atoms flux is deposited on the target, where carbon atoms are impinged by the second argon ion beam from the Kaufman type ion source. These carbon atoms deposited on substrate surface create a thin film. A surface modified in this process (DLC) has the special properties: enhanced wear resistance, low friction factor, high corrosion resistance and good oxidation resistance. Other materials can also be used to produce chemical cells with special properties, e.g. such that are tissue-friendly biomedical implants. The Kaufman type ion source is the central element of the system and has two different rooms: discharge chamber and grid zone. Such division is convenient, because various physical phenomena occur in these rooms. It also helps in the ion source simulation. The scheme of ion source is shown in figure 2. The ion source consists of the following parts: ceramic chamber, heated cathode emitting electrons, anode, permanent magnets enforcing the helical electron trajectory in discharge chamber, and extraction system. The extraction system is composed of a screen and an acceleration grid. Gas is supplied by a gas inlet. Output parameters of the ion source depend on potentials of two grids: acceleration and screen grid, as well as on parameters of plasma generated in discharge chamber.

3. MATHEMATICAL MODEL OF ION EXTRACTION SYSTEM AND SOLUTION METHOD

Ion extraction is simulated for such a system, which is composed of two grids, each of 0.5 mm thick. Computer simulation is prepared for the single aperture in the two and half dimensional coordinate system, i.e. for the case of the cylindrical symmetry. The variable parameter in the simulation is the diameter of acceleration grid aperture and the objective are variations of the plasma meniscus.

The mathematical model of ion gun consists of Poisson's equation, the equation of motion for a single charged particle in electromagnetic field, and equations describing formation of plasma meniscus. The boundary element method (BEM) is chosen for the problem solution. BEM was firstly used for electrostatic lenses simulation in [11]. Following this approach it is possible to solve the electrostatic optics problem with quite good accuracy. Relatively low computational costs and good numerical accuracy are the main advantages of BEM method [3]. The method has obviously some disadvantages such as the problem with a solution of non-linear problems and the unfeasibility of formulation of some problems, but nevertheless, it does not have a great influence on divergence sensitivity analysis. The model is coded in CPO software and is successfully used for the solution of space charge electrostatic problems, which are widely presented in [14].

3.1. Model description

The first equation of the model is the Poisson's equation, which describes the distribution of the electric field potential and is given by

$$\nabla^2\varphi = -\frac{\rho}{\varepsilon} \tag{1}$$

where φ is the electric field potential, ρ is the charge density, and ε is the permittivity, which is expressed by

$$\frac{\partial^2\varphi}{\partial r^2} + \frac{1}{r}\frac{\partial\varphi}{\partial r} + \frac{\partial^2\varphi}{\partial z^2} = -\frac{\rho}{\varepsilon} \tag{2}$$

in the system of cylindrical coordinates, where r and z are cylindrical coordinates.

The intensity of electrical field is defined by

$$\mathbf{E} = -\nabla\varphi\,, \tag{3}$$

where $\mathbf{E}$ is the vector of electric field.

A plasma meniscus is evaluated by using the energy conservation law with the assumption, that a work of electrical field made on the distance equal to the Debye length is equal to the electron thermal energy. Due to the comparison of these two quantities, it is possible to evaluate the magnitude of electric field, which results in an ion extraction. This assumption was verified in Kovaleski's work [10].

The Debye length is formulated by:

$$\lambda_D = \sqrt{\frac{\varepsilon k T_e}{e^2 n_e}} \tag{4}$$

where λ_D is the Debye length, k is the Boltzmann constant, T_e is electron temperature, e is electron charge, and n_e is electron density.

The work done by electric field on the Debye length, called also as the electric field work is given by

$$W = eE\lambda_D \tag{5}$$

where W is the electric field work and E is the magnitude of electric field.

The comparison of the work and energy leads to the equation for the magnitude of an electrical field, which is the boundary for the plasma meniscus:

$$E = \frac{kT_e}{e\lambda_D}\,. \tag{6}$$

The current of extracted ions from the ion source is confined by space charge in the similar way as the electron current generated by heated cathode. That is why Child-Langmuir [2] equation is commonly used to calculate maximum ion source current. Child-Langmuir law is a simplified theoretical model used with electrode flatness assumption. Read and Bowring showed numerical current simulation for heated cathode for various shapes [12].

The next equation of the mathematical model is the equation of motion for single charged particle in electromagnetic field given by

$$\frac{d\boldsymbol{v}}{dt} = \frac{q}{m}[\boldsymbol{E} + \boldsymbol{v}\times\boldsymbol{B}]\,, \tag{7}$$

where $\boldsymbol{v}$ is a particle velocity, q is a particle charge, m is a particle mass, and $\boldsymbol{B}$ is the magnetic induction.

For non-relativistic velocities, the influence a particle motion on the magnetic field can be neglected. Therefore, an influence of the magnetic field is not taken into account in this paper. Unfortunately, it is not possible the to model extraction by molecular dynamics in reasonable time because of the order of particle number magnitude ranging up to $1\cdot10^{18}m^{-3}$. Modelling of motion is facilitated by using the concept of super-particles, whose charge and mass are multiplied by a particular factor. The multiplication factor is determined by the current assigned to a single super-particle. Based on the super-particle current, it is useful to determine the charge by

$$q = i\cdot s/v\,, \tag{8}$$

where i is the super-particle current, s is the time step, and v is the magnitude of a particle velocity.

The charge of each particle is used to model the Coulomb interactions among super particles.

The influence of the space charge is evaluated by using the space charge tube method (SCTM) [13] implemented in CPO 2DS software.

3.2. Boundary and initial conditions

The initial condition is specified for the plasma meniscus, where initial velocity of argon ions is assumed to be zero.

Boundary conditions for shape and location of plasma meniscus are specified by potentials on surfaces on both electrodes. These conditions are control parameters for the Kaufman type ion source. Voltages are taken as zero for the screen grid and -

1.5 kV for the acceleration grid. A plasma meniscus boundary is assumed to be a surface for which the magnitude of electrical field is determined by equation (6). The magnitude of electrical field for the plasma meniscus is calculated for electron density equal to ion density $n_i = n_e = 1 \cdot 10^{18} m^{-3}$ and electron temperature is assumed at $T_e = 1\ eV$. The magnitude of electrical field for the plasma meniscus is $134328\ \frac{V}{m}$.

The plasma meniscus is approximated by a circular sector.

3.3. Solution method

The most important issue for ion extraction simulations is a proper setting of the initial and boundary conditions [16]. Firstly, the plasma meniscus surface is calculated on the basis of the magnitude of electrical field. In figure 3, the contour of electrical field, evaluated by CPO 2DS software, is presented. CPO 2DS solves the Poisson's equation by using BEM.

The principles of BEM can be easily explained. The real charges appear on electrode surfaces for each physical system with conducting electrodes and the difference of electrical potential between them. The charges will remain unchanged, if no leakage occurs even when the source voltage is disconnected. These surface charges are sources of the potential and all fields in the system. In BEM method, electrodes are represented by these charges. The system of electrodes may not be closed and no mesh is required.

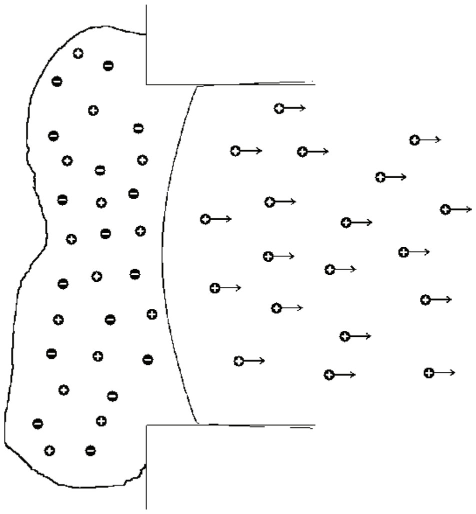

Fig. 3. *Electric field contour which determines plasma meniscus.*

Trajectories of charged particles were computed by using CPO 2DS software according to the following steps:

1) Poisson's equation with BEM,
2) Electric field by potential differentiation,
3) Plasma meniscus with scheme shown in boundary conditions section ,
4) Plasma meniscus with the "cathode" option in CPO 2DS,
5) Equation of motion for each single particle,
6) Coulomb forces among ions,
7) Crossing points among particles and test planes.

4. DIVERGENCE CALCULATIONS

The divergence of ion beam is calculated by using the following relation

$$Divergence = 2arctg\left(\frac{R_f - R_i}{l}\right), \tag{9}$$

where R_f is the trajectory radius of the ion beam at final point, R_i is the trajectory radius of the ion beam at initial point, l is the distance between points.

The final and initial points are placed on the test planes. The radius is taken for the most divergent particles as shown in figure (4).

The sensitivity analysis answers the question, which of input parameters of the model has the most significant influence on output parameters. In many cases, such analysis could point which parameter can be neglected in the model. The sensitivity analysis can be conducted in the simplest way by perturbation of one of input parameters and observing the result after restarting calculations. This method is called the finite difference method or sometimes, the brute force method [17].

The difference approximation method is based on the following equation:

$$\frac{\partial y}{\partial r} = \frac{r_{av}}{y_{av}} \frac{y(r+\Delta r) - y(r)}{\Delta r}, \tag{10}$$

where r is a radius of aperture in the acceleration grid, Δr is the 10% variation of the radius r, y is the divergence, r_{av} is an average radius, and y_{av} is an average divergence.

5. SENSITIVITY ANALYSIS

Average radii and divergence are calculated by using formulas:

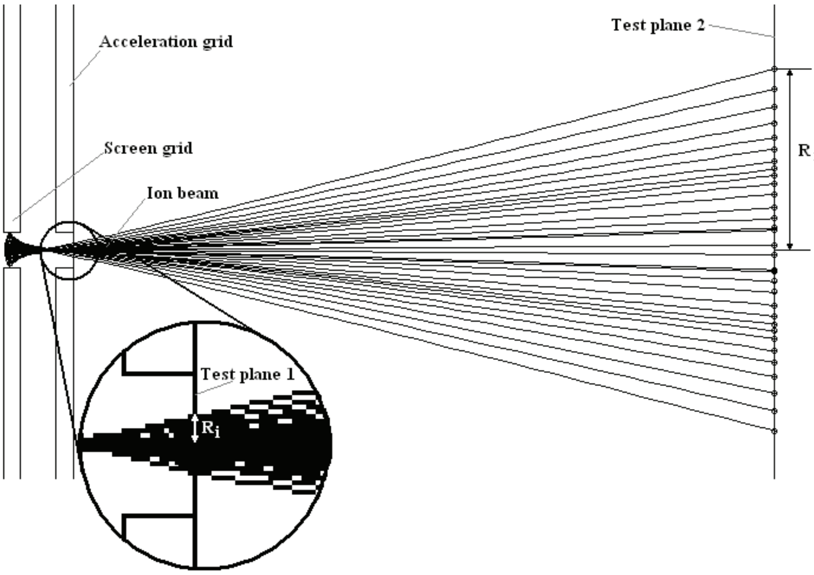

Fig. 4. Simulated ion beam in CPO 2DS with test planes [18].

$$r_{av} = \frac{r + (r + \Delta r)}{2}, \tag{11}$$

$$y_{av} = \frac{y(r) + y(r + \Delta r)}{2}, \tag{12}$$

This method of sensitivity analysis is widely used for many problems ranging from the simulation of nano-coating fracture [7] to modelling of aortic valves [8]. This kind of analysis is often used for a structural optimization of biomedical implants.

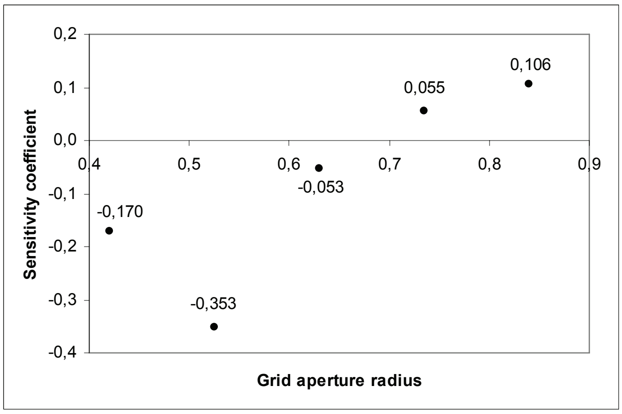

Fig. 5. Results of the sensitivity analysis for variations of acceleration grid aperture.

6. RESULTS

Simulations were made for five different radiuses of acceleration grid aperture ranging from 4 to 8 millimeters. Each radius is amplified by 10%. Figure 5 shows results obtained for the sensitivity analysis. It can be seen that for grid aperture radius below 0.7 the sensitivity coefficient is negative. That means that the divergence is decreasing in this range. Coefficients are positive for aperture radiuses above 0.7. The coefficient increases for the radius range from 0.5 to 0.9 and changing a sign between 0.6 and 0.8.

7. CONCLUSIONS

A process for singly charged argon ions, extracted from the Kaufman type ion source, is evaluated by using CPO 2DS program. The ion extraction is described by the Poisson equation describing an electrostatic field and a spatial distribution of the potential of this field is evaluated by the Boundary Element Method (BEM) imbedded into CPO 2DS. The electrical field intensity, evaluated on the basis of such distribution, is used for plasma meniscus calculations. This meniscus is defined because it can be imagined as a thermal cathode emitting argon ions, and therefore, the thermal cathode module is implemented in the BEM program. The meniscus is determined as a surface in two and half dimensions with the intensity of the electrical field equal to 134 V/mm. Ions leaving the meniscus area are accelerated and their interactions are accounted by using the space charge tube method. The meniscus shape, dimensions and curvature are related to the diameter of accelerator's grid.

Finally, the divergence of ion beam is calculated on the basis of the formula 9 where two radii and the distance between two control cross-sections of the ion cone. This is illustrated in figure 4.

The plasma meniscus shape related mainly to plasma temperature and the Debye's length, is not significantly dependent on the diameter of the acceleration grid aperture. That can be seen from our sensitivity analysis of the divergence.

The next step of investigations should be directed into numerical experiments with different diameters of screening grid aperture, and various plasma parameters.

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ANALIZA WRAŻLIWOŚCI DYWERGENCJI WIĄZKI JONOWEJ NA ZMIANY KSZTAŁTU SIATKI PRZYSPIESZAJĄCEJ W ŹRÓDŁACH JONÓW TYPU KAUFMANA

Streszczenie

Źródła jonów typu Kaufmana znajdują zastosowanie w procesach jonowej modyfikacji powierzchni. W perspektywie rozwoju technik implantacji jonowej na potrzeby przemysłu, między innymi produkcji implantów biomedycznych, narzędzi skrawających i tnących jak również powłok bioaktywnych, zauważa się potrzebę badań symulacyjnych układów sterowania maszyn do implantacji jonów. Źródła jonów są podstawowym elementem systemów do napylania jonowego i ich automatyczne sterowanie ze wspomaganiem komputerowym jest aktualnym problemem dla konstruktorów obrabiarek do nano-obróbki powierzchni. Niestety, tylko niewielka grupa prac badawczych dotyczy modelowania źródeł jonów używanych w procesach inżynierii powierzchni. Zagadnienia związane z modelowaniem źródeł jonów mogą być obiektem przyszłych badań. W analizie budowy oraz opisie zjawisk fizycznych występujących w źródłach jonów pomocny jest podział źródła jonów na dwie strefy: strefę komory wyładowczej oraz strefę siatek. Modelowanie zjawisk fizycznych zachodzących w źródłach jonów jest znacznie łatwiejsze po rozdzieleniu tych dwóch obszarów. W strefie siatek źródła jonów następuje sformowanie oraz przyspieszenie wiązki jonowej. Parametry wyjściowe źródeł jonów: energia oraz kształt wiązki jonowej, zależą głównie od parametrów siatek przyspieszającej i ekranującej. Na energię wiązki jonowej mają wpływ wielkości potencjałów elektrycznych przyłożonych do siatek. Rozkład przestrzenny wiązki jonowej zależy od kształtu siatek. Geometria siatki ekranującej i przyspieszającej zmienia się na skutek erozji siatek wywołanej uderzeniami jonów o siatki. Analiza wpływu zmian kształtu siatek na właściwości strumienia jonów stanowi ważny praktyczny problem dla użytkowników i projektantów źródeł jonów.

Symulacja komputerowa ekstrakcji strumienia jonów stanowi nieocenioną pomoc w projektowaniu oraz analizie systemów optyki jonowej. Pozwala na oszczędność wynikająca ze zmniejszenia kosztów analizy oraz szczegółowe badanie procesów fizycznych zachodzących podczas pracy źródła. Dotychczas stworzono wiele programów komputerowych do projektowania układów optyki jonowej, jednak porównanie otrzymanych wyników prowadzi do wniosku, że największą dokładnością odznaczają się programy wykorzystujące Metodę Elementów Brzegowych.

Przedmiotem pracy jest analiza numeryczna wpływu kształtu siatek na rozkład pola elektromagnetycznego oraz na trajektorię cząstek naładowanych w kaufmanowskich źródłach jonów używanych w procesach jonowej implantacji powierzchni. W pracy przedstawiono wyniki dotyczące wpływu wielkości promienia otworu siatki przyśpieszającej na dywergencje wiązki jonów. Wyniki otrzymano używając programu CPO firmy CPO Ltd. Program bazujący na Metodzie Elementów Brzegowych pozwala na obliczanie trajektorii jonów z uwzględnieniem rozkładu przestrzennego ładunku oraz określenie wpływu oddziaływań kulombowskich na rozkład przestrzenny wiązki jonowej.

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