ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Taking into Account Forces of Beam Spatial Charge upon Calculations of Particle Dynamics in Standing-Wave Accelerators.

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ABSTRACT

As technology advances, charged particle beams with high current density become more and more popular. Obtaining of such beams has some peculiar features caused by the influence of inter-particle interaction, so called effect of spatial charge. In practice dynamics calculation of intensive charged particle beams is reduced to solution of non-linear self-consistent problem, involving equations of charged particle motion, the Poisson equation for electric field potential and equation of continuity.

Keywords: spatial charge, dynamics of particles, simulation of physical processes, standing-wave accelerator, microparticle.

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INTRODUCTION

Nowadays the charged particle beams are used in commercial technologies for non-destructive testing, especially for non-destructive quality control of materials (Logatchov, et al., 2006), for processing of various materials, in medicine (Zhang, et al., 2013), in geological exploration, and in scientific researches.

Nearly all important properties of vacuum devices and assemblies, which are applied for production and diagnostics of materials of nuclear power engineering, depend on the processing quality, spatial configuration, as well as on physics of wave processes upon their interaction with electromagnetic fields propagating in various materials (Drozdenko, & Magilin, 2007). Such researches facilitate development of new electrophysical devices for diagnostics and production of materials, improvement of existing and experimental methods of generation and diagnostics of charged particle beams.

Charged particle fluxes are used in numerous electrophysical devices, primarily in cyclic and linear accelerators. Intensive development of accelerative engineering intended for fundamental physical researches in the field of high-energy physics and significant advances in other fields of science and engineering make it possible to apply in practice accelerators in industry and medicine (Zavadtzev, et al., 2011).

The accelerators increase significantly efficiency of commercial production in such fields as radiography, radiation chemistry, sterilization of medical preparations, tools and food stuff, elemental activation analysis (Zavadtsev, et al., 2006). Significant economic benefit is achieved due to application of the accelerators in geology, for radiation survey of wells, in particular.

The accelerative engineering is more and more widely applied in medicine (Volobuev, 2012). X-ray therapy enables combination of comparatively high treatment efficacy with possibility of mass services (Auditore, et al., 2006).

The interest in application of linear electron accelerators in industry and medicine can be attributed to their numerous advantages. The most important are as follows: simplicity of input and output of accelerated particles, which makes it possible to obtain strictly oriented fast electron beams and braking radiation; easy adjustment of dose rate power and intensity; high dose rate power of braking radiation even at comparatively small (up to $10 MeV$) energies of accelerated electrons.

While considering motion of electron beams it is not sufficient to account only for external electromagnetic field created by certain exterior sources. The beam electrons create electric and magnetic self fields, which exert reverse impact on electron motion. Consideration for self consistent fields is required in the case of high density electron beams (Aleksandrov, & Kuzelev, 2007).

The beams are considered to be intensive, if it is impossible to neglect the forces of Coulomb repulsion, created by self spatial charge. Such beams are an active element in electron and ion optical systems and charged particle accelerators, which are widely applied in practice, for instance, for melting and cutting of metals, sputtering and other important practical purposes.

In general case the dynamics of charged particle beams is described self consistent set of equations. Taking into account contemporary issues of physics and engineering of high current beams it is necessary to apply and to develop new mathematical procedures of dynamics simulation of high spatial charge beam. At present the macroparticle method is most widely applied (Bobyleva, 2003).

Numerical simulation of intensive charged particle beams is required upon investigation into the processes in various electrophysical devices. Numerical simulation methods assume development of a mathematical model, numerical algorithms and software packages for implementation of the developed algorithms (Sveshnikov, 2006).

EXPERIMENTAL

Calculation of forces of beam spatial charge by numerical solution of the Poisson equation of two-dimensional grid

While considering the issues of beam dynamics in accelerator at certain current and beam energy it becomes necessary to account for the forces of spatial charge of the beam itself. These forces depend on the charge density and beam configuration should be taken into account in the equations of particle motion at any time and in any location where a particle can exist. Therefore, the preset issue should be solved in approximation of self consistent field, when the electromagnetic forces, which determine the motion of particle flux, depend on the charge density or particle motion.

The forces of beam spatial charge can be determined by the Poisson equation:

$$\Delta\Phi = -4\pi\rho \ (1)$$

and

$$\boldsymbol{E}'_{\rho} = -grad\Phi, (2)$$

where Φ is the potential generated by the charge density ρ, and $\boldsymbol{E}'_{\rho}$ is the field intensity of spatial charge. While solving it is required to know distribution of charge density in the considered region at any time, that is, it becomes necessary to simulate charge particle beam.

While developing the mathematical model it is necessary to account for characteristic features of the considered physical process and accelerator design. For the standing-wave accelerator this is, for instance, a complicated dependence of electromagnetic field on the coordinates in transit channel, comparatively moderate accelerator length, high rate of energy gaining by the particles and associated relativistic effects, fast generation of clusters from charged particles captured into the acceleration process.

Since the spatial period of accelerating structure in initial accelerator portion , as well as amplitude and phase velocity of accelerating harmonics vary along the accelerator length, then the physical processes in such systems should be simulated in adiabatic approximation (Mayorov, 1974). Let us assume that all properties of the simulated system slowly vary in time and as a function of coordinate along accelerator. In such approximation in laboratory coordinates along the axis z it is possible to highlight the region V, restricted by cross sections $z = Z$ and $z = Z + \Lambda$, where Λ is the spatial period of the system. Let us consider that the highlighted region moves along the axis z at the speed equaling to average speed of particles in this region. As a consequence of spatial periodicity of physical processes in the considered system the charged beam can be simulated only in the region V with periodic boundary conditions. On the basis of location of particles it is possible to determine the charge density distribution while considering the motion of a group of closely positioned particles integrated into macroparticles (Potter, 1975). Maintaining the ratio of macroparticle charge to weight the same as of actual physical particles, the motion of macroparticles will be described by the same equations. If cumulative charge of all macroparticles and average density of spatial charge are maintained the same as in the simulated system, then the self field and flux dynamics in the model and in physical system should coincide (Roshal', 1979).

Upon simulation of the flux by coarse particles the pair interactions in the model are sharply distorted, since the impingement frequency increases proportionally to the coefficient of coarsening at zero self size of macroparticles. In our case, while simulating impingement-free flux of charged particles, we will weaken short-range interactions due to the use of macroparticles of finite size. Then, each macroparticle is a "cloud" of spatial charge with the center relatively which the equations of motion are solved. Upon approaching of the "clouds" the interaction force between them increases, however, while penetrating into each other the "clouds" stop interactions between each other which leads to decrease in the short-range interactions.

An important issue upon simulation of charged particles flux in linear accelerator is setting of initial distribution of macroparticles in phase space of coordinate--pulse. It is required to set such initial terms in the model which would agree with actual properties of beam escaping from injector. Let us use "quiet start" approach, when coordinate and macroparticle velocity are set by means of regular procedure, so that charge density distribution in the model and configuration of simulated beam in initial acceleration region are the same as in actual accelerator.

Therefore, mathematical model of charged particle flux is described by macroscopic Maxwell equations, medium and motion equations for actual flux particles. The obtained set of equations is non-linear, since the field of forces of spatial charge, acting on the flux particles, depends on charge density distribution, determined by motion of the particles. Electromagnetic fields acting on the particles in the resonators of complex shape are not expressed in analytical form, they are determined by numeric methods and preset in spreadsheets.

Solution scheme of the set of equation of mathematical model is as follows: electromagnetic fields in overall aperture of transit channel are calculated and set as spreadsheets, then, the distribution of macroscopic charge density on discrete grid is determined at each integration step over time using position of macroparticles. Using the same grid, the Poisson equation is solved with the boundary conditions corresponding to physical interpretation. The obtained solution of the Poisson equation in the grid nodes is interpolated in order to find solution in intermediate points where macroparticles are positioned and the forces of spatial charge acting on them are calculated. While solving the motion equations with the calculated forces we determine the macroparticle position at the next time point and so forth.

Determination of spatial beam charge field in the laboratory coordinates is as follows. Two-dimensional rectangular grid in cylindrical coordinates r, z is applied onto selected region of spatial periodicity V. We assume that the particle flux is axially symmetrical, thus, the potential Φ and volumetric density ρ as a function of φ is neglected. We assume that this grid moves synchronically with the particle flux and its velocity with regard to the laboratory coordinates us β_z. Then, at any time the static problem of potential determination can be solved using the Poisson equation.

Five-point differential approximation of Eq. (1) on two-dimensional rectangular grid r, z is as follows (Molokovsky, & Sushkov, 2005):

$$\frac{1}{h_r^2}\left(\Phi_{i+1,j} - 2\Phi_{i,j} + \Phi_{i-1,j}\right) + \frac{1}{r_{i,j}}\left(\Phi_{i+1,j} - \Phi_{i,j}\right) + \frac{1}{h_z^2}\left(\Phi_{i,j+1} - 2\Phi_{i,j} + \Phi_{i,j-1}\right) = 4\pi\rho_{i,j}\,. (3)$$

In Eq. (3) $0 < i < I; 0 < j < J; I + 1$ and $J + 1$ is the number of nodes in the coordinates r, z; h_r and h_z are the grid increments in the coordinates r, z; $\rho_{i,j}$ and $\Phi_{i,j}$ is the preset distribution of charge density and unknown potential in the grid nodes, respectively; $r_{i,j}$ is the distance to the considered point.

Let us assume that the particle beam travels in round waveguide, then the boundary conditions for Eq. (3) can be written as follows:

$\Phi|_{r=a} = 0$, where a is the radius of transit channel,
$\Phi|_z = \Phi|_{z+\Lambda}$, where Λ is the beam spatial period,
$d\Phi/_{dr}|_{r=0} = 0$ on the axis of transit channel.

The set of Eq. (3) is solved as proposed elsewhere (Hockney, 1970), where discrete Fourier transformation of potential and density of spatial charge in the longitudinal coordinate z is applied.

$$\Phi_{i,j} = \frac{1}{2}\hat{\Phi}_i^c(0) + \frac{1}{2}\hat{\Phi}_i^c\left(J/_2\right) + \sum_{k=1}^{J/2-1}\left\{\hat{\Phi}_i^c(k)\cos\frac{2\pi kj}{J} + \hat{\Phi}_i^s(k)\sin\frac{2\pi kj}{J}\right\}, (4)$$

$$\rho_{i,j} = \frac{1}{2}\rho_i^c(0) + \frac{1}{2}\hat{\rho}_i^c\left(J/_2\right) + \sum_{k=1}^{J/2-1}\left\{\hat{\rho}_i^c(k)\cos\frac{2\pi kj}{J} + \hat{\rho}_i^s(k)\sin\frac{2\pi kj}{J}\right\}, (5)$$

where

$$\hat{\rho}_i^c(k) = \frac{2}{J}\sum_{k=1}^{J/2-1}\rho_{i,j}\cos\frac{2\pi kj}{J};\ \hat{\rho}_i^s(k) = \frac{2}{J}\sum_{k=1}^{J/2-1}\rho_{i,j}\sin\frac{2\pi kj}{J}$$

for all $0 \le k \le J$.

Substituting Eq. (4) and Eq. (5) into Eq. (3) for each Fourier harmonics k we obtain tri-diagonal matrix equation with respect to unknown vector $\{\widehat{\Phi}_i(k)\}$, which is solved by sweep method (Potter, 1975). After Fourier analysis in the coordinate z, we determine all required values of potential $\Phi_{i,j}$ in each grid node.

Starting from known distribution of potential $\Phi_{i,j}$ in the considered region V we can easily proceed to field intensity of spatial charge $\boldsymbol{E}'_\rho$ using Eq. (2). In order to apply this equation we should determine the potential derivatives in the coordinates z and r.

Attempting to eliminate the influence of calculation errors, related with the grid discretization, time and space in mathematical model, numerical differentiation of potential preset in the grid is performed with local smoothing by means of the least square method. If in the vicinity of angle (j, i) the tabulated function $\Phi(z, r)$ is approximated by the polynomial

$$\Phi^0(\xi, \eta) = a + b\xi + c\boldsymbol{\eta} + d\xi\eta + e\xi^2 + f\eta^2,$$

where $\xi = {}^{z - z_i}/_{h_z}, \eta = {}^{r - r_i}/_{h_r}$, then the potential derivatives can be expressed via the polynomial derivatives as follows:

$$\frac{\partial\Phi}{\partial z} = \frac{1}{h_z}\frac{\partial\Phi^0}{\partial\xi} = \frac{1}{h_z}(b + d\eta + 2e\xi), \frac{\partial\Phi}{\partial r} = \frac{1}{h_r}\frac{\partial\Phi^0}{\partial\eta} = \frac{1}{h_r}(c + d\xi + 2f\eta). (6)$$

Therefore, using Eq. (2) with accounting for Eq. (6) it is possible to determine the field intensity of spatial charge in any point of the considered region V. Since the fields $E'_{\rho z}$ and $E'_{\rho r}$ are determined in self coordinates, then, passing to the laboratory coordinates, the equations of particle are solved on the basis of transformations for the fields (24)

$$E_{\rho z} = E'_{\rho z};\ E'_{\rho r} = \gamma E'_{\rho r};\ H_\varphi = \beta_z E'_{\rho r},$$

where γ is the Lorentz factor.

Calculation error of spatial charge forces is determined by test calculation of increase in electron beam radius under the action of spatial charge forces upon drift in free space. The disagreement does not exceed 1%.

Approximation of clusters of accelerated particles by uniformly charged ellipsoid of rotation

While designing accelerators of charged particles with the aim of determination of optimum beam motion, it is required to consider numerous variants, hence, at the stage of searching for optimum variant it would be reasonable to apply more ordinary model of charged beam. Such model can be successfully presented by uniformly charged ellipsoid of rotation, which approximates particle clusters of arbitrary shape (Vlasov, 1965). Since the rate of energy gaining by the beam in standing-wave accelerators and generation of particle clusters occur in fact in the first resonator, then application of this ordinary model is appropriate.

Let us consider that the accelerated particles move along the accelerator axis in the form of separate clusters, following each other at equal distances Λ (Λ is the beam spatial period). Since the cluster length is approximately 0.15Λ, then the interaction between the clusters can be neglected. Let us assume that each particle cluster is a uniformly charged ellipsoid of rotation with the axis coinciding with the accelerator axis. Then the forces acting on separate electron from such cluster in laboratory cylindrical coordinates can be determined as follows (Akhiezer, et al., 1962):

$$F_r = 4\pi e(1 - \beta_c^2)M_r r\rho, F_z = 4\pi e\rho M_z(z - Z),$$

where e is the electron charge, β_c is the relative velocity of cluster center, r is the particle deviation from the accelerator axis, ρ is the volumetric charge density in the laboratory coordinates, M_r and M_z are shape coefficients in accompanying coordinates, Z is the coordinate of the cluster center.

For ellipsoid with transversal half-axis R_M and longitudinal half-axis a_z the cluster shape coefficients are described as follows:

$$M_r = \frac{1-M_z}{2} = \frac{1}{2} - \frac{1-l^2}{2l^3}\left(\frac{1}{2}ln\frac{1+l}{1-l} - l\right),$$

where $l = \sqrt{1 - \frac{R_M^2}{a_z^2}(1-\beta_c^2)}$.

If the current of accelerated particles in the pulse is I, then the volumetric charge density can be determined as follows:

$$\rho = \frac{I\lambda}{c}\frac{3}{4\pi R_M^2 a_z},$$

where c is the velocity of light, λ is the generator wavelength.
In relative coordinates dimensionless components of intensity of electric fields acting on an arbitrary particle with coordinates (ξ, η) are written as follows:

$$A_\xi^Q = 1.76 \times 10^{-4}\frac{M_z}{\eta_{max}^2 \Delta\xi_{max}} I(\xi - \xi_c), A_\eta^Q = 1.76 \times 10^{-4}\frac{M_r(1-\beta_c^2)}{\eta_{max}^2 \Delta\xi_{max}} I\eta,$$

where: $\eta = \frac{r}{\lambda}$; $\xi = \frac{z}{\lambda}$; $\Delta\xi_{max} = \frac{a_z}{\lambda}$; $\eta_{max} = \frac{R_M}{\lambda}$; $A_\xi^Q = \frac{e\lambda}{m_0 c^2}E_{\rho z}$; $A_\eta^Q = \frac{e\lambda}{m_0 c^2}E_{\rho r}$.

Upon acceleration the sizes of particle cluster vary, mutual position of particles varies, hence, the forces of spatial charge acting on the particles also vary. At any time, knowing coordinates of particles in the cluster, it is possible to determine half-axes and center of ellipsoid. With this aim the motion equations of all particles are integrated simultaneously. Initially, the particle combination uniformly distributed along r and z is preset and the motion equations of all particles up to the accelerator end are integrated without accounting for forces of spatial charge. The particles not included into the acceleration performance are not taken into account, thus, at the accelerator input there are only the particles in the acceleration performance. These particles determine the initial cluster sizes. Knowing pulse current and sizes of approximating ellipsoid, at each time integration step it is possible to calculate forces of spatial charge acting on each particle.

At certain ratio of transversal to longitudinal half-axes of ellipsoid the path of particle in the ellipsoid center and at the distance of $r = R_M$ to the axis will coincide with the continuous beam envelope. Prior to calculations of continuous beam dynamics it is required to select ellipsoid half-axes on the basis of test problem of beam divergence in drift space under the action of forces of spatial charge. As follows from the calculations, at $I = 1A$ and $\frac{a_z}{R_M} = 10$ the calculation error does not exceed 5%.

RESULTS

The forces of spatial charge upon calculation of electron dynamics were accounted using two procedures for the case study of two-resonator standing-wave accelerator with the energy of $1\, MeV$ and the current up to $500\, mA$ in the pulse. While providing radial motion of electrons, compact design of the accelerator prevents the use of conventional and well proven magnetic coils of aluminum foil. The problem of electron beam focusing was solved by means of two small focusing coils made of copper tubes. Cooling water flows inside the tube, which enables passing of high currents via winding and obtaining of the required reserve of magnetic field intensity in the accelerator axis.

The circuit of injecting, accelerating and focusing systems of the accelerator is comprised of electron injector, injector lens, drift, two accelerating resonators and two focusing coils on both sides of accelerating unit. The injector lens is armored, wound by copper wire, and makes it possible to achieve the magnetic field intensity in the axis up to $1000\ Oe$. Power supply to the injector lens and each focusing coil is independent, which makes it possible to vary relative distribution of external magnetic field along the accelerator axis in wide range.

The accelerating system is comprised of two identical hollow cylindrical resonators with the intensity of accelerating electric field of $200\ kV/cm$ at nominal current load. The resonators are not interconnected and supplied by high-frequency energy via three-decibel directional coupler, which determines the phase shift between the resonator fields. The injector is and electron gun with nearly parallel beam, energy of $40\ keV$ and current up to $5\ A$ in pulse.

Final results obtained by means of approximation of particle cluster by uniformly charged ellipsoid of rotation are illustrated in Fig. 1 in the form of beam envelope along accelerator (Curve 1). Dashed line depicts relative intensity distribution of magnetic field in the accelerator axis.

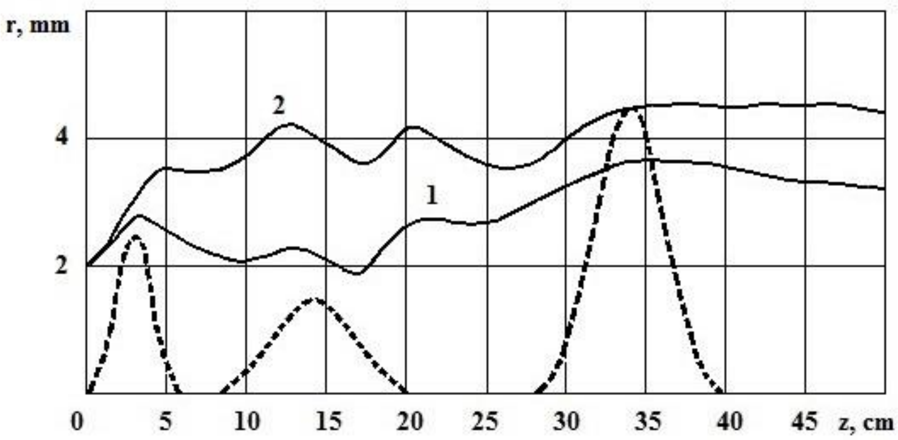

Fig. 1. Beam envelope of overall accelerator. Curve (1) is obtained by approximation of particle cluster by uniformly charged ellipsoid of rotation, curve (2) – by numerical solution of the Poisson equations. The dashed line depicts relative intensity distribution of external magnetic field in the accelerator axis.

The estimation method of the forces of spatial charge on the basis of simulation of particle cluster by uniformly charged ellipsoid of rotation is characterized by certain disadvantages, which lead to difference between the calculations of radial motion of particles and actual physical interpretation of beam motion in accelerator. From this point of view more accurate is the method of accounting for forces of spatial charge based on numerical solution of differential Poisson equation on rectangular grid. Using this method, radial dynamics of particles was calculated in the same accelerator with experimentally measured distribution of external magnetic field. The calculations were performed with the model comprised of 50 coarse particles on the 32×16 grid. The obtained results are illustrated in Fig. 1 (curve 2).

DISCUSSION

The estimation method of the forces of spatial charge on the basis of simulation of particle cluster by uniformly charged ellipsoid of rotation is characterized by certain disadvantages, which lead to difference between the calculations of radial motion of particles and actual physical interpretation of beam motion in accelerator. From this point of view more accurate is the method of accounting for forces of spatial charge based on numerical solution of differential Poisson equation on rectangular grid.

While comparing calculation data obtained by the two various method of estimation of forces of spatial charge, it can be seen that the highest difference corresponds to the accelerator region where continuous particle beam moves. It is obvious that approximation of such beam by ellipsoid of rotation does not correspond to actual physical interpretation exactly in this point. After beam grouping into clusters both methods provide similar results.

The calculation results demonstrate that decrease in injection current improves the state of harness wiring and leads to decrease in the beam output radius, herewith the minimum corresponds to $0.2\ A$. At lower current the beam is refocused which leads to certain increase in its radius.

CONCLUSIONS

The major conclusion derived from the obtained data is that under the acquired values of magnetic field intensities of focusing elements the wiring harness is possible along overall accelerator, herewith, the output beam diameter will not exceed $8 \div 9\ mm$, and the divergence is close to zero. These conclusions agree well with experimental data obtained at operating accelerator. The diameter of beam output spot does not exceed $8\ mm$, and the beam itself can be transported in vacuum without noticeable increase in its diameter.

Taking into account increasing interest in intensive beam linear accelerator for application purposes, we are planning to continue the researches in the field of calculations of radial dynamics of charged particle fluxes with high density of spatial charge.

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