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CALCULATION OF MACROPARTICLE FLOW IN FILTERED VACUUM ARC PLASMA SYSTEMS

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Model of macroparticle behavior inside plasma guiding channels of vacuum arc systems and program for calculation of macroparticle flow in plasma filters (separators) used in vacuum arc film deposition are described. Several magnetic filters have been modeled to compare calculated and experimental data. The capability of the program to optimize filters is demonstrated on example of straight filter. The high compliance degree of calculated and experimental data is shown.

INTRODUCTION

Vacuum arc deposition is one of the most promising and commonly used techniques to produce coatings of different purposes. During several decades the technique plays an important role in such industry branches as engineering, instrument making, electronics, metallurgy, tools production and decorative coatings. However, vacuum arc method has a significant drawback – the presence of macroparticles among the products of cathode erosion. Macroparticles are solid or liquid fragments of cathode material. Their size varies from tenths to several tens of micrometers. After contact with a substrate, macroparticle may stick to it, bounce from it or fall off from it some time after sticking, which in any case leads to the formation of defective coating [1,2]. Therefore the use of vacuum arc method in some cases may be unacceptable or impractical.

There are some well-known ways to suppress the emission of macroparticle phase or to decrease its amount in deposited films. The most common approach in practice is a spatial separation of plasma and macroparticle trajectories. Magnetoelectric plasma filters (separators) are successfully used for this purpose. In such filters plasma streams are guided by magnetic field along curved path from the area of plasma formation (near-cathode space), to the coating deposition area – a workpiece (substrate). At the same time, there must not be a direct line-of-sight between the cathode and the substrate. Macroparticles have low negative (or neutral) charge [1,2] and their mass is much greater then ion mass. As a result, macroparticles are almost not influenced by magnetic and electric fields, used for plasma transport. Therefore their movement paths are representing straight lines. Such spatial separation of the trajectories allows intercepting the flow of macroparticles by plasma duct walls, making the substrate unreachable for macroparticles.

As was shown by practical use of curvilinear filters, an absence of a direct line-of-sight between a cathode and a substrate is necessary but not sufficient condition for removing macroparticles from the plasma. There are some possible scenarios when macroparticle collides with plasma duct walls. The macroparticle may scatter on several smaller parts. Solid macroparticles may also bounce from duct walls, which is especially relevant when graphite cathode is used for films deposition. A third option is also possible – macroparticle may stick to the wall. In first two cases, nothing prevents macroparticle from hitting the substrate after collision with filter walls. Therefore filters are equipped with baffles (fins), which are acting as additional obstacles for macroparticles and as source of additional collisions for them. During collision with baffles and filter walls macroparticle gradually loses its kinetic energy. And after a series of such collisions it eventually sticks to an obstacle.

Thus, the design of an effective filtering system is a challenging task. In addition to providing the "no direct line-of-sight" principle, a designer is forced to rely mainly on his intuition because it is scarcely possible to take into account all cases of macroparticle rebounds (ricochet).

The process of filter designing can be significantly simplified by using specially developed algorithms for macroparticle trajectories calculation. Computer based calculations were made earlier by other authors [1,3]. However, neither program description nor list of tasks it can handle were not provided or referred to. Moreover, the number of calculated filtering systems was very limited. It can be seen from analysis of given results, that used algorithm is able to calculate very small amount of macroparticles (about 180) emitted only from a single point. Any information about geometry construction and calculation result output features the program owns were also not been given. So the task of creating a necessary tool for computer simulation and analysis of filtering features of plasma separators still remains actual.

For the purpose of solving this problem Macroparticle Tracer (MPT) program have been developed. It is able to assist designer to make a qualitative evaluation of filtering abilities of various systems, to significantly simplify the task of designing of such systems and also to define the basic concepts of baffle systems construction. The program is capable to perform a real-time simulation, uses own user-friendly interface and has tools for geometry construction, visualization of problem and results. It also provides a flexible adjustment of problem input and result output.

MACROPARTICLE BEHAVIOR MODEL AND CALCULATION PROBLEM

Simulation of macroparticles rebounds from the walls of plasma duct and baffles (hereinafter "system borders" or simply "borders") a number of assumptions have been made. Macroparticles (hereinafter "particles") are solid spheres with radius tending to zero and represented in calculation as dots. Collision of particle with borders has partially elastic nature. After certain number of collisions the energy of the particle becomes insufficient for the subsequent rebound – such particle is considered to be absorbed by filter. Borders are completely smooth (no roughness) and represented as broken lines. Segments of particle trajectory before and after rebound are forming equal angles with respect to the collided border (angle of incidence is equal to reflection angle). Particles do not collide with each other. Calculations are made in two-dimensional approximation, i.e. in one plane. This plane should be symmetry plane of the system. Particle emission from the working surface of the cathode is equiprobable in any direction. Collisions of particles with borders do not lead to the particle fragmentation (scattering). An influence of magnetic and electric fields, gravity and other forces are not taken into account – particles are always flying along straight paths (between collisions). Used model is very similar to previously used [1,3].

Formulation of particle trajectory calculation (tracing) problem is reduced to the following stages. Definition of system borders: an input of coordinates of all borders (defined as line segments) involved in calculation. Definition of emitter (cathode working surface) and emission direction. Setting tracing parameters, such as: maximum (allowable) number of particle impacts with borders, when the particle is considered to be absorbed by filter due to complete lose of particle energy; the number of emission points and the way their coordinates are being calculated (for example, fixed step between points or their total number); the number of particles flying out from every emission point (by step or total number); and also emission base (starting) angle and its relation (to global coordinate system or to local – with respect to emitter orientation). It is also possible to define absorbing borders, i.e. particle collided this borders will be considered as absorbed by filter regardless of how many collisions this particle has experienced before. Though definition of such borders is not necessary for tracing task setting.

Additional postprocessing tools are added to make simulation results easier to analyze and to lower the load on used computational system. For example, it is possible to display trajectories of only those particles that collided with specified border (or group of borders) or these trajectories can be displayed in other color.

BASIC ALGORITHM

After initial coordinates and directions for all involved in simulation particles have been specified, the program enters calculation mode with the following stages.

1. Calculation of equations coefficients of lines from endpoints coordinates of line segments. These lines describe borders.
2. Determination of equation coefficients of line, which describe initial segment of particle trajectory.
3. Calculation of collision points coordinates for every border.
4. Discarding collision points which do not belong to line segments of corresponding borders.
5. Determination of the collision point which is closest to emission point (or previous collision point).
6. Calculation of equation coefficients of line, describing trajectory segment of particle after rebound:

$$A_{m+1} = 1\,,\ B_{m+1} = \frac{B_m\left(B_n^2 - A_n^2\right) + 2A_nA_mB_n}{A_m\left(A_n^2 - B_n^2\right) + 2A_nB_nB_m}\,,$$

$$C_{m+1} = \frac{2C_n\left(A_nA_m + B_nB_m\right) - C_m\left(A_n^2 + B_n^2\right)}{A_m\left(A_n^2 - B_n^2\right) + 2A_nB_nB_m}\,,$$

where A_m, B_m, C_m − equation coefficients of line of particle trajectory before rebound; A_n, B_n, C_n − equation coefficients of line, which define border.

7. Determination of particle movement direction, based on the definition of the half-planes (regarding the border) calculated collision point and emission point (or previous collision point) belongs to.
8. Repeat of steps 3 − 7 for each segment of the trajectory line until the particle is absorbed by filter.
9. Repeat of steps 2 − 8 for each emitted particle.
10. Display the simulation results in numerical and graphical forms with required postprocessing.

It should be noted, that line segments representing borders and trajectories are treated as lines (through the coefficients of line equation in general form) during calculation process, while coordinates of their endpoints are used instead for storage and display.

During the tracing process some additional calculation may be needed to solve exceptional cases. Description of the algorithms used for these additional calculations is unreasonable in this work; therefore only cases themselves are listed below. The most common among them are: parallelism or coincidence of border and trajectory lines; emitter enclosure by borders (for example, in case of cup-shaped cathode); collision of particle simultaneously with multiple borders in a single point; particle fly out from simulated system if the last one is not closed.

PROGRAM CAPABILITIES

A program for macroparticle tracing, as a tool for filtering systems development, should provide rather flexible way to define a calculation problem. Some cases of simulation may demand exceptional functional, which is not needed in most other cases of filtering system designing. Therefore, when developing MPT, an attempt was made to anticipate the needs of filter designer and thus to create tools capable to satisfy these needs.

One of the most important areas in particle tracing task is the setting of emission. At the stage of emission centers creation (the points on cathode working surface macroparticles will "fly from" during simulation) it is possible to set their total number or, for example, specify their offset, i.e. distance between them. When the emission centers have been set, an amount of particles per emission center must be specified. The amount can be defined the same ways as in case of emission centers, i.e. by total number or by angular step. Because it is not possible (expedient) to calculate every possible direction of emitted particle, it is often handy to have an opportunity to set up the orientation of the particles bunch. This can be made by specifying base (starting) emission angle. So every direction of particles (in the bunch associated with emission center) will be calculated with relation to this base angle. In addition, base angle can be set in global coordinate system, or in local – relative to emitter.

Allowable number of collisions (see above) with system borders can be set to any number. The only limitation is the performance of computer system used for simulation. It is especially vital when comparing different filters, which are well-designed and optimized. Using small allowable number of impacts will give barely noticeable difference between simulation results. Described situation is also applicable to emission settings (high or low). The higher the amount of emitted particles, the more reliable results can be obtained. Emission is also limited only by computer performance.

For detailed analysis of a separator it is often important to know its filtering abilities at different allowable number of collisions. For example, the same filtering degree at different maximum allowable particle impacts may indicate nonoptimality of the separator construction (in particular – location and shape of used baffles). Detailed examination may reveal "weak points" of the filtering system, when minor modification to its design leads to significant filtering abilities gain. Mentioned above procedures are greatly simplified with visualization of said dependencies by means of graphs. Furthermore, graphs can provide additional data on filters with the same final results, but having different intermediate ones.

Week dependence of filtering degree from allowable impacts number is typical for separators of open architecture. In this case particle bouncing from vacuum chamber walls is not considered. But the chamber definitely has certain dimensions and construction, thus its exclusion from simulation is rather questionable. Such situation will be shown and discussed below.

One of the most useful features of the developed program is to perform real-time calculation and results display. Using this mode one can change separator architecture and obtain results simultaneously. For example, changing baffles orientation and see the result changes during the rotation. This mode is also can be used as "single-particle emission scanning". Both cases allow designer to rapidly find a construction close to optimal one.

MPT has its own visualization means of calculated system geometry and calculation results. They incorporate several types of viewport pan and scaling; tuning such settings as color, lineweight, transparency and linetypes (solid, dashed, etc.) for grids, borders, trajectories, snaps and snap tracking lines.

Solving every tracing task starts from geometry definition of the system simulated. In order to provide ease of program use, speedup calculation task formulation and provide independence from third-party software, MPT features its own vector graphics editor. The editor itself has standard for such editors tools, the main ones are: drawing/modifying, rotating, copying, moving, mirroring, scaling, array copying, lengthening, trimming and extending of lines (borders) or group of lines, and also measurement of angles and distances. Each of listed tools has additional options, which can modify behavior of the tools. For convenient and easy construction of complex geometric objects the program has some support functions: snap to various object parts and tracking of the snaps. Viewport of the program supports two independent tunable grids to simplify navigation and drawing.

Results data can be obtained for each border both in absolute values – as number of collided particles, and in relative values – as a filtration degree for the border. Filtration degree is a number of collided particles normalized to emission and expressed as a percentage:

$$Filtration\,degree = \left(1 - \frac{Unfiltered\ particles}{Emitted\ particles}\right) \cdot 100\ .$$

Such approach allows evaluation of practical significance of each baffle or plasma duct wall and economic feasibility of their manufacturing. If simulation revealed that one of the baffles have very little collisions count (or have none at all), then manufacturing of this baffle and installation of it in real filter are meaningless, therefore it only increases final cost and complexity of the filter.

Clarity of the results is sharply decreased in case of filter simulation with high emission (lots of particles) setting, because the most part of the calculated system will be filled with a single color, corresponding to trajectory display setting. That is, particle trajectories become indistinguishable and moreover, displaying a large number of lines significantly loads graphical core of the computer used. To resolve this issue MPT provides the following measures. It is possible to display only trajectories which collided with the substrate. In general, it can be any of the borders or a group of them. But if there are enough computer resources, mentioned trajectories can be displayed in another color. This method unambiguously emphasizes the trajectories of most interest without losing the integrity of the picture. For the detailed separator analyzing, it is often needed to view trajectories of specific particles. For example, in the vicinity of some baffles, in order to determine whether designer's idea worked or not. MPT provides such ability: any individual trajectory can be highlighted.

Display of calculated dependencies graphs is realized in a separate from system geometry and trajectories space. Functions of calculation and display of graphs are incorporating sizing, scaling, positioning, curves and axes visual settings adjusting, etc. A single graph, as a simulation result, includes curves for all borders of the system. The curves are tuned independently from each other. The same applies to graphs. But graphs also can inherit visual settings from other graphs and be created using adjustable templates.

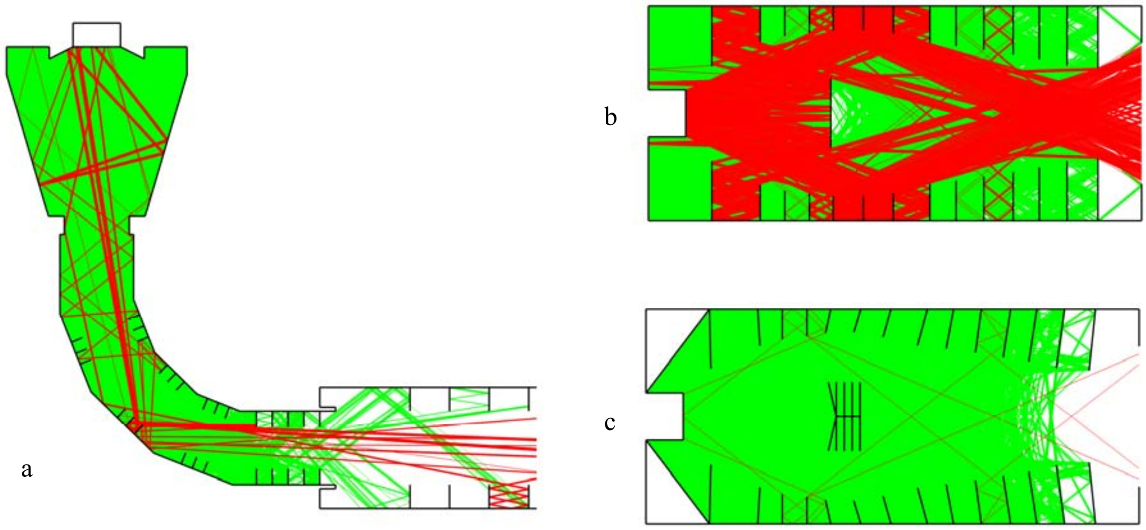

Fig. 1. Schematic representation of macroparticle tracing results for classical toroidal filter [3] (a), straight filter [3] (b) and optimized straight filter (c). Number of emitted macroparticles is about 9900, distance between emission centers is 0.6 mm, angular step – 1.8° and particles don't bounce from substrate. Green – filtered particles, red – unfiltered

CALCULATION RESULTS

Using the developed program some previously known filtering systems were simulated. Data on the filtering abilities of the systems were obtained experimentally by corresponding authors. These systems include classical curvilinear filter in a quarter torus form [3], straight filter with a disc in front of cathode [3] and open architecture filter with 60 degrees bend angle [4] in several variations described below. Optimization of baffles of straight filter was also performed, as an example.

Toroidal and straight filters simulation results are presented in Fig. 1,a,b. Particle emission was set in such way as to clearly demonstrate the difference of filtering abilities of the separators. As it can be seen from the figure, toroidal filter shows much better results as compared to straight one. Filtering degree of toroidal filter is approximately 12 times higher. This difference is qualitatively agrees with experimentally obtained data [3] (Table. 1).

Optimization of straight filter was made by means of insignificant variation of its baffles angles. This allows do decrease the amount of unfiltered macroparticles approximately in 65 times. Having such baffle design the filter should be capable to provide 5.5 times higher filtering degree than toroidal one (Fig. 1c and Table. 1) if macroparticles are not capable to bounce more than 11 times.

For more complex analysis of toroidal and straight filters emission was increased by 100 times. Calculation was performed for different macroparticle energy values, represented as number of allowable impacts (see above). The results are shown in Fig. 2. Both filters demonstrate good filtering of particles that bounce no more than 4 times. Macroparticles bouncing 6 times still nearly do not leave toroidal separator.

Calculation and experimental results

	Chamber present	Emitted particles	Unfiltered particles	Filtration degree, %	Macroparticles density [3,4], cm^{-2}	Measured ratio	Calculated ratio
Torus [3]	–	998706	4097	99.59	$1\cdot10^{6}$	1	1
Straight [3]	–	999000	48827	95.11	$16\cdot10^{6}$	16	11.92
Straight (opt.)	–	999000	752	99.92	–	–	0.18
Open (rectangles) [4]	No	999000	110724	88.92	$4.3\cdot10^{6}$	10.75	4.88
	Yes	999000	222714	77.71			2.62
Open (triangles) [4]	No	999000	22679	97.73	$0.4\cdot10^{6}$	1	1
	Yes	999000	85124	91.48			1
Open (squares)	No	999000	37932	96.20	–	–	1.67
	Yes	999000	198967	80.08			2.34
Open (rotated squares)	No	999000	21749	97.82	–	–	0.96
	Yes	999000	90852	90.91			1.07

Allowable number of impacts is 10, distance between emission points is 20 µm for open type filters and 53 µm for rest, angular step is 0.18 degrees. "Chamber present" means that the spiral duct and the substrate of the system were enclosed in chamber with dimensions 800×800 mm. Measured and calculated ratios are for comparison of filters inside of their own group. Closed filters are compared to the toroidal filter, open filters – to the filter with triangular cross-section of solenoid turns

Meanwhile initial (not optimized) straight filter loses filtering abilities to a considerable extent. As the energy of emitted macroparticles continues to grow, filtering degree of both filters continues to fall. Such a trend is more pronounced in straight filter what makes toroidal one more preferable in the areas where maximum plasma filtering degree is needed.

The optimization of straight filter baffles makes it able to compete with toroidal filter on condition that particles can bounce from separator wall less than 12 times. An amount of particles, unfiltered by both optimized straight filter and its unoptimized version, undergoes increase for macroparticles with higher energies. It should be stated, that in practice actual number of particle rebounds is 9 or less [1, 3]. From this point of view, straight filter with modified baffle system has the best filtering performance among three examined above separators. It is obvious, that baffles optimization of the toroidal separator will increase its filtering abilities, and they will be greater than the straight one obtained due to optimization.

Architecture of the open type filters with 60 degrees bending is reconstructed from the data specified in work [4]. In order to understand determinant factors of their design (according to filtering) – is it a cross-section of plasma guiding solenoid turns or their orientation, two more design modifications were simulated. Cross-section of the solenoid was chosen to be a square with 10 mm edge size. First modification has these squares directed to the filter curvature center by one of the edges, second modification – by one of the corners. Hereinafter, second modification will be referenced as rotated square filter.

In addition, all considered open type filters were calculated twice. The first calculation was made to determine the value of the conception used. Therefore macroparticles left the spiral plasma duct was considered as absorbed by filter. In practice, the filters must have some kind of vacuum chamber, which they are encapsulated in. Thus the second calculation takes into account macroparticles rebounds from chamber walls. It should be noted, that the simulation result are strongly dependent from the accuracy of separator design reproduction. Authors of the work [4] have not provided any data about the filter enclosure. It means that more significant difference between calculated and experimental data should be expected. It was assumed that vacuum chamber is 800×800 mm in size, and the plasma source used was reconstructed from given schematic figure.

Fig. 3 presents calculation results for filters of open architecture with rectangular and triangular section of spiral plasma duct turns. Numerical data is shown in Table. As depicted in Fig. 3, the number of unfiltered macroparticles reaches its maximum at 2 − 3 rebounds value if vacuum chamber is not present (ignored). Thereafter number of unfiltered particles remains nearly the same. It is due to impossibility of macroparticles to return back inside filter space by means of bouncing from chamber walls. Being inside closed system, most macroparticles will finally get to the substrate after a certain number of rebounds. That's the reason why the amount of particles monotonically increases if the chamber is present. The last case is more likely from the practical point of view.

Quality of plasma filtering provided by the discussed in this work separators both calculated and measured is given in Table. The separators can be rated by their particle filtering degree in a following order. Optimized straight separator offers the best filtration. After it, in descending order are toroidal, initial straight, and open type ones. Inside the group of open architecture filters sequence is as follows: with triangular, square and rectangular cross-section of solenoid turns. Measured ratio of unfiltered particles for toroidal and straight filters equals 16, while calculated using MPT ratio is about 12. Simulation data on open type filters allows one to unambiguously assert that the choice of triangular section of plasma duct solenoid turns is optimal. This fact is also confirmed by authors of experimental studies of the filters [4]. As it has been stated above, due to inaccuracies of open filters design reconstruction, a substantial difference between calculated and experimentally obtained data is observed.

The use of rectangular and square cross-sections in open type filter design provides nearly the same filtering quality. The same situation is observed if calculation data on triangular and rotated square filters are compared. It is evident that the key role in such filters plays the orientation of solenoid turns, not their cross-section alone.

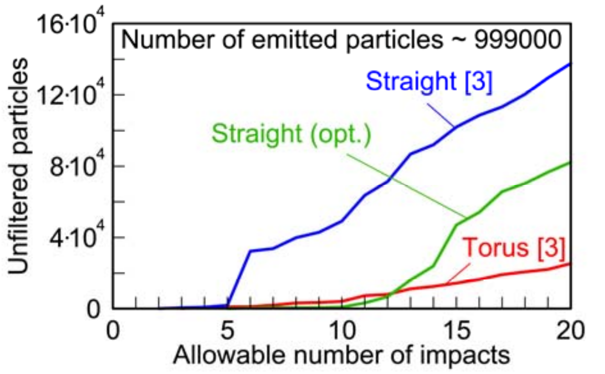

Fig. 2. Dependence of the number of macroparticles at filter output on the allowable number of impacts. Distance between emission centers is 53 µm, angular step – 0.18° and particles don't bounce from substrate

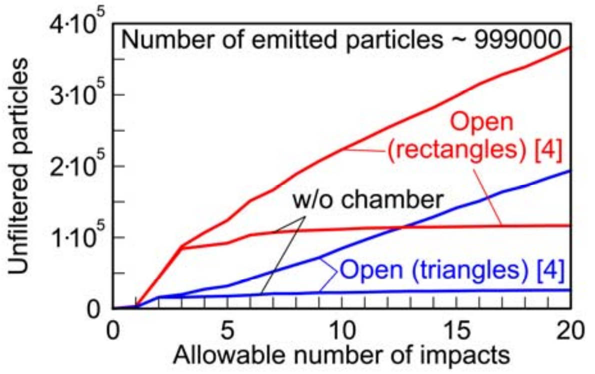

Fig. 3. Dependence of the number of macroparticles at filter output on the allowable number of impacts. Distance between emission centers is 22 µm, angular step – 0.18° and particles don't bounce from substrate

CONCLUSION

This work showed that the developed MPT program is capable to do a qualitative comparison of filtering abilities of different separators. It was demonstrated, that using this program one can successfully create a new filter designs and also optimize the known ones. The results of the performed simulations are substantially correlating with the experimentally obtained data.

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РАСЧЁТ ПОТОКА МАКРОЧАСТИЦ В СИСТЕМАХ ФИЛЬТРОВАННОЙ ВАКУУМНО-ДУГОВОЙ ПЛАЗМЫ

Д.С. Аксёнов

Представлены модель, алгоритм работы и возможности программы для расчёта и оптимизации плазменных фильтров (сепараторов), используемых в вакуумно-дуговом осаждении покрытий. Промоделировано несколько магнитных фильтров для сопоставления расчётных и экспериментальных данных. Продемонстрирована возможность оптимизации одного из фильтров с помощью разработанной программы. Показана высокая степень соответствия расчётных данных экспериментальным.

РОЗРАХУНОК ПОТОКУ МАКРОЧАСТИНОК У СИСТЕМАХ ФІЛЬТРОВАНОЇ ВАКУУМНО-ДУГОВОЇ ПЛАЗМИ

Д.С. Аксьонов

Наведено модель, алгоритм роботи та можливості програми для розрахунку та оптимізації плазмових фільтрів (сепараторів), які використовуються у вакуумно-дуговому осадженні покриттів. Промодельовані декілька магнітних фільтрів для порівняння розрахункових та експериментальних даних. Продемонстрована можливість оптимізації одного з фільтрів за допомогою розробленої програми. Показано високий ступінь відповідності розрахункових даних експериментальним.