ABSTRACT

of the dissertation for the degree of Doctor of Philosophy (PhD)
in the specialty 6D060400- "Physics"

Shugayeva Tilektes Zhalgasovna

Simulation of dynamics of charged particle beams in static and time-of-flight mass spectrometers

Relevance of the topic. Mass spectrometry is a universal and most accurate method for determining the elemental, chemical and isotopic composition of a substance in an arbitrary aggregate state. Thanks to its wide capabilities, it has found application in a wide variety of fields of science, technology and production. At present, new research methods have also developed, such as chromatography-mass spectrometry, tandem mass spectrometry, etc., which have significantly expanded the possibilities of mass spectrometric analysis. Thus, with the help of chromato-mass spectrometers, the problem of determining the content of dioxin, a toxic pollutant of celluloid production in the Great Canadian Lakes, was solved. Recently, due to the development of soft methods of sample ionization, mass spectrometry has also become an indispensable method of research in the field of so-called "life sciences": proteomics, genomics, biochemistry, pharmacy and medicine. Time-of-flight mass spectrometers are particularly successfully used here.

Thus, the development of new methods for calculating and modeling the physical and instrument characteristics of static and time-of-flight mass spectrometers based on correct physical and mathematical theories and using the increased capabilities of computing technologies that allow us to design and calculate devices with improved analytical capabilities is an urgent task of corpuscular optics and scientific instrumentation.

The methods used in calculating the physical and instrument characteristics of static mass spectrometers: resolution, sensitivity and aberration are traditional methods of corpuscular optics. Corpuscular optics (CO), or, as it is also called, electron or ion optics, arose from the analogy between the propagation of light in transparent media and the movement of charged particles in electric and magnetic fields. CO is the basis of scientific instrumentation, determining the level of scientific and technical development of many experimental research methods and the basic principles underlying the creation of a large number of various corpuscular optical devices and instruments. These are such devices as: cathode ray tubes, scanning and emission electron and ion microscopes, energy and mass spectrometers, various electron-optical converters, accelerators and systems for transporting charged particles, ion-optical channels of transporting complexes for molecular beam epitaxy, etc.

The theoretical basis of CO is classical electrodynamics. In electrodynamics, the motion of charged particles in electric and magnetic fields is determined by the action of the Lorentz force. However, the CO considers not only the motion of individual charged particles, but also the problems associated with the formation of charged particle beams and the control of these flows. First of all, it is worth noting here the problems of separating charged particle beams by mass and energy, which are solved in mass and energy spectroscopy, as well as the problems of beam formation and focusing that arise in electron and ion microscopy. To solve these problems, the CO uses theoretical methods borrowed from light optics; namely, first, the solution of a linear problem or a paraxial approximation is found, and then the theory of aberrations is developed. Moreover, the aberration theory is traditionally constructed using asymptotic series for small parameters characterizing the ion beam. The method of successive approximations used to find aberration coefficients leads to very cumbersome expressions, especially for high-order aberration coefficients. At the same time, it is impossible to determine within the framework of the aberration theory itself, at which values of small parameters characterizing the beam, the chosen approximation works well enough.

Another method that is used in the CO to calculate the physical properties of corpuscular optical systems (COS) is the "central particle method" or otherwise the "axial trajectory method". Here, the axial trajectory along which the "central particle" moves is calculated first, and the trajectories of the remaining ion beam particles are characterized by their deviation from the axial trajectory. This method is described in detail in the second chapter of the dissertation. The second chapter also describes a new method for calculating the COS proposed in the dissertation, based on the use of dimensionless Newton equations and analytical expressions for potentials describing the electric and magnetic fields of the COS.

Experience shows that usually the most significant ideas in CO began with original theoretical works. Here, for example, an approximate direction in mass and energy analysis should be noted, which led to the creation of mass analyzers and energy analyzers similar in their scheme to prismatic light-optical devices. In addition, we note other studies related to the creation of systems with ideal focusing for separating beams of charged particles by energy, as well as analytical work that formed the basis of the Orbitrap mass analyzer.

The aim of the dissertation is to develop methods for modeling the dynamics of charged particle beams in static and time-of-flight mass spectrometers and optimizing their physical and instrument characteristics.

To achieve this goal , the following **main tasks** were formulated:

1. To develop a method for calculating the dynamics of charged particle beams based on the use of dimensionless Newton equations and analytical expressions for potentials describing the electric and magnetic fields of the COS.

2. To obtain analytical expressions for potentials describing electric and magnetic fields of conical prism systems, as well as potentials of transaxial and axisymmetric braids using TFCV methods.

3. Simulation of the dynamics of charged particle beams formed by an ion source using the Monte Carlo method.

4. Perform calculation and optimization of physical and instrument characteristics of a static prismatic mass analyzer with a CSAP and transactional collimator and focusing lenses.

5. To calculate the physical and instrument characteristics of time-of-flight mass analyzers based on the use of dimensionless Newton equations and analytical expressions for the potentials of transaxial and electrostatic fields and optimize their characteristics.

6. To calculate the electron-optical scheme of the microfocus tube using the computer application "FOCUS".

The object of the study is the dynamics of charged particle beams in static and time-of-flight mass spectrometers.

The subject of the study is the physical and instrument characteristics of static and time-of-flight mass spectrometers.

Research methods. Dimensionless Newton equations and analytical expressions for potentials describing electric and magnetic fields of static and time-of-flight mass spectrometers obtained using TFCV methods were used to simulate the dynamics of charged particle beams. When modeling the dynamics of charged particle beams, numerical integration of a system of differential equations was carried out using a computer program in the VBA language implementing the four-point Adams method with automatic selection of the integration step. The acceleration points for the Adams method were found using the Krylov method of successive approaches. The initial conditions for charged particles escaping from the ion source were determined using the Monte Carlo method. Numerical calculation of the EOS of the microfocus tube was carried out using the computer application "FOCUS".

The scientific novelty lies in the fact that in the work for the first time:

1. A mathematical and computer model of the dynamics of charged particle beams has been created based on the numerical integration of dimensionless Newton equations for a charged particle in electric and magnetic fields described by dimensionless scalar potentials.

2. Analytical expressions for potentials describing electric and magnetic fields of conical prism systems, as well as analytical expressions for potentials of transaxial and axisymmetric braids using TFCV methods are obtained.

3. Methods for solving boundary problems of electrostatics for the Laplace equation using methods of the theory of functions of a complex variable (TFCV) have been tested. The adequacy of the obtained analytical expressions for the potential is ensured by the correctness of the mathematical methods used.

4. A three-electrode transaxial lens in anamorphic mode is calculated, which reduces the energy of the ion beam, which is used as a collimator lens before entering the CSAP.

5. Chromatic aberrations of CSAP, as well as axisymmetric and transaxial electrostatic mirrors are investigated and ways to optimize the instrument characteristics of time-of-flight mass analyzers are determined.

6. An electron-optical scheme of a microfocus tube has been developed and numerically investigated, providing acceleration of the electron flow and its transportation from the emission region to the focus point with a 10-fold compression of the cross-section radius.

Theoretical and practical significance of the results. The results of the dissertation are mainly theoretical. The scientific significance of the work lies in the development of analytical and computer methods for calculating and optimizing the physical and instrument characteristics of static and time-of-flight mass analyzers based on two-dimensional, conical, as well as axisymmetric and transaxial electrostatic systems by modeling the dynamics of charged particle beams.

The main provisions submitted for defense

1. Numerical solutions of exact dimensionless differential equations of motion of charged particles in electric and magnetic fields of the studied corpuscular-optical systems, analytical expressions for the potentials of which were found in the work, allow us to take into account the distribution of ions in the source by coordinates and departure angles, as well as by energies and masses, and contain corrections for aberrations.

2. In a static prism mass spectrometer with a cone-shaped achromatic prism and transaxial lenses, modeling of a mass doublet with $\gamma=0$ and $\gamma=1/20000$ showed that a mass resolution of 20,000 is achieved, and at half-height peaks of 40,000, which is 8 times more in comparison with the resolution of the Matsuda mass spectrometer with almost identical device dimensions and ion parameters the source.

3. As a result of reflection of charged particles flying out of a point source located in the middle plane of a three-electrode transaxial mirror, energy and spatial time-of-flight focusing of the ion beam is achieved, and in a time-of-flight mass spectrometer based on an axisymmetric cylindrical mirror for a mass doublet with a relative difference in masses $\gamma = 1/4000$, a resolution of 4000 is achieved at 50% of the peak height.

The reliability and validity of the scientific statements, results and conclusions formulated in the dissertation work is confirmed by the use of proven physical theories and methods and the absolute consistency of the results obtained with the fundamental provisions of corpuscular optics, as well as by the correctness of the analytical and numerical mathematical methods used, comparison with the results of numerical modeling for some test cases and agreement with the results obtained by others by the authors.

The connection of the topic of the dissertation with the plans of scientific works. The results of the dissertation work were used in the preparation of project documents with grant funding from the Ministry of Internal Affairs of the Republic of Kazakhstan for fundamental research in the field of natural sciences "Modeling the influence of edge fields in the design and calculation of grid-free energy and mass analyzers of charged particles" (No. AP09258546, 2021-2023).

The author's personal contribution of the author lies in the fact that the author participated in the development of programs and numerical calculations of the physical and instrumental characteristics of static and time-of-flight mass analyzers based on two-dimensional, conical, transaxial and axisymmetric electrostatic systems using algorithms and an application package created using the Monte- Carlo. The participation of scientific consultants consists in setting tasks and discussing the results obtained.

Approbation of the study. The main results of the work were reported and discussed at the following conferences and seminars:

–International Scientific and Practical Conference "Actual problems of analysis, differential equations and algebra" (Astana, October 16-19, 2019);

– The Ninth Congress of the All-Russian Mass Spectrometric Society, the 8th All–Russian Conference with international participation "Mass Spectrometry and its applied problems" (Moscow, October 14-18, 2019);

–XV International Scientific and Practical Conference "Youth, Science and Innovation" (Aktobe, April 12, 2019);

–III International Scientific Forum "Nuclear Science and Technology", (Almaty, September 20-24, 2021).

Publication of research results. According to the results of the research presented in the dissertation, 12 scientific papers have been published, including 4 articles in rating scientific journals indexed in the Web of Science and Scopus database; 1 article in the journal recommended by the Committee for Quality Assurance in Education and Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan; 7 publications in other scientific journals and materials of international conferences.

The structure and scope of the dissertation. In accordance with the specific purpose and objectives of the study, the dissertation work consists of an introduction, five sections, a conclusion, a list of sources used. The numbering of formulas is two-digit: the first number means the number of the section, the second - the own number of the formula, graphics, figures, tables, formulas within the subsection. The total volume of the dissertation is 111 pages, 5 tables, 46 figures and a bibliography containing 115 titles.