



ACTUAL PROBLEMS OF MODERN SCIENCE, EDUCATION AND TRAINING

KHOREZMSCIENCE.UZ





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Section 1. MODERN PROBLEMS OF PHILOLOGY AND LINGUISTICS

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THEORETICAL FOUNDATIONS OF THE COMPARATIVE STUDY OF SCIENCE FICTION WORKS

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Annotatsiya. Mazkur maqolada ilmiy fantastika janrini qiyosiy o'rganishning nazariy-metodologik asoslari tahlil qilinadi. Tadqiqotda ushbu janrning global adabiy hodisa sifatidagi o'rni va turli adabiy an'analarda shakllanish xususiyatlari yoritiladi. Tadqiqot davomida qiyosiy-tipologik yondashuv, struktur-semantik tahlil hamda xronotop modeli asosiy metodologik tayanch sifatida qo'llanadi. Maqolada ingliz va o'zbek adabiyoti materiallari asosida ilmiy fantastikaning o'ziga xos modellari qiyoslanadi. Tahlillar natijasida ingliz adabiyotidagi ilmiy fantastika ko'proq tizimli va texnologik xarakterga egaligi, o'zbek adabiyotida esa ushbu janr ijtimoiy, axloqiy va falsafiy qatlamlar bilan uyg'unlashgan holda namoyon bo'lishi isbotlanadi. Shuningdek, zamonaviy texnologik tafakkur va interdisiplinar yondashuv bilan bog'liq jihatlar tadqiq etiladi. Tadqiqot natijasida ilmiy fantastikani qiyosiy o'rganish janrning universalligi va milliy xususiyatlarini aniqlash, uni jamiyat tafakkuri hamda madaniy jarayonlar bilan bog'liq holda talqin qilish imkonini berishi asoslanadi. Mazkur ish janr nazariyasini tizimli boyitishga xizmat qiladi.

Kalit so'zlar: *ilmiy fantastika, qiyosiy adabiyotshunoslik, janr nazariyasi, qiyosiy-tipologik tahlil, xronotop, ilmiy faraz, badiiy model, ingliz adabiyoti, o'zbek adabiyoti, texnologik tafakkur.*

Аннотация. В данной статье анализируются теоретико-методологические основы сравнительного изучения жанра научной фантастики. В исследовании освещается роль научной фантастики как глобального литературного феномена и особенности её формирования в различных литературных традициях. В качестве основной методологической базы используются сравнительно-типологический подход, структурно-семантический анализ и модель хронотопа. На материале английской и

узбекской литературы выявляются специфические модели научной фантастики. Анализ показывает, что если в английской литературе научная идея носит более системный и технологический характер, то в узбекской литературе она проявляется в гармонии с социальными, этическими и философскими пластами. Также рассматриваются современные направления развития, связанные с технологическим мышлением и междисциплинарным подходом. В результате исследования обосновывается, что сравнительное изучение научной фантастики позволяет определить универсальные и национальные особенности жанра, а также интерпретировать его в тесной связи с общественным сознанием и культурными процессами. Работа вносит вклад в системное обогащение теории жанра.

Ключевые слова: научная фантастика, сравнительное литературоведение, теория жанра, сравнительно-типологический анализ, хронотоп, научная гипотеза, художественная модель, английская литература, узбекская литература.

Abstract. This article analyzes the theoretical and methodological foundations of the comparative study of the science fiction genre. The research explores the role of science fiction as a global literary phenomenon and its formation across diverse literary traditions. The study utilizes comparative-typological approaches, structural-semantic analysis, and the chronotope model as its primary methodological framework. Based on materials from English and Uzbek literature, the article identifies distinct models of science fiction. The analysis demonstrates that while science fiction in English literature tends to be more systematic and technological, in Uzbek literature, it manifests through an integration of social, ethical, and philosophical layers. Furthermore, the study examines modern trends related to technological thinking and interdisciplinary approaches. The findings justify that a comparative study of science fiction enables the identification of both universal and national characteristics of the genre, allowing for its interpretation in relation to social thought and cultural processes.

This research contributes significantly to the systemic enhancement of genre theory.

Key words: *science fiction, comparative literature, genre theory, comparative-typological analysis, chronotope, scientific hypothesis, artistic model, English literature, Uzbek literature, technological thinking.*

Introduction

In the contemporary literary process, science fiction is manifested not only as a literary genre, but also as a complex phenomenon at the intersection of science, philosophy, and social thought. This genre makes it possible to artistically model humanity's perceptions of the future, the consequences of technological progress, and civilizational anxieties. Therefore, studying science fiction within the framework of a single national literature cannot fully reveal its essence; the need arises to study it in a comparative context. Comparative literature serves as an important methodological basis for the study of science fiction. This approach makes it possible to determine how common problems are interpreted in different literary traditions. René Wellek and Austin Warren explain the essence of comparative literature as follows: “Comparative literature is the study of literature beyond the boundaries of any national literature, as well as the study of the relationships between literature and other fields of knowledge. It seeks to identify the connections, similarities, and differences between different literatures.” [12]. This theoretical approach is particularly relevant to science fiction. This is because, by its nature, the genre is transnational, and scientific ideas, technological imagination, and elements of social forecasting interact and converge in different cultures. Therefore, through a comparative study of science fiction, not only the general laws of the genre but also the characteristics of national thought are revealed.

Literature review

In the theoretical interpretation of science fiction, its cognitive function is of particular importance. Darko Suvin writes about this: “Science fiction is a literary genre formed on the basis of the interaction of the elements of estrangement and cognition. Its ‘novum’ is a new phenomenon or relationship that departs from the reality familiar to the author and reader” [11]. This view shows that the essence of science fiction is not

the direct depiction of reality, but a means of understanding it through an alternative model. Thus, its comparative study makes it possible to compare the mechanisms of “reconstructing reality” in different literatures. From this point of view, the aim of this article is to identify the theoretical foundations of the comparative study of the science fiction genre and to systematize its methodological principles and main criteria. The article consistently examines the need for comparative analysis of science fiction, the theoretical views on which it is based, and the methods applied.

Although science fiction has emerged in different literary traditions, common intellectual problems lie at its foundation. The relationship between humans and technology, the social consequences of scientific progress, and perceptions of models of the future develop independently in different cultures. This aspect makes a comparative study of science fiction necessary. In the theoretical interpretation of the genre, its connection with cognition is particularly emphasized. Carl Freedman writes as follows: “Science fiction is a distinctive form of understanding social reality. It shows the existing world in an altered form and expands the possibility of understanding it” [5].

Research Methodology

This approach defines the main task of science fiction. The genre does not directly reflect reality. It creates a new model through a scientific hypothesis. Therefore, comparing how this model is constructed in different literatures is of scholarly significance. In Western literature, science fiction is often expressed through a technological system. In Isaac Asimov’s “I, Robot”, robots are depicted as a system based on strict laws. In this model, the main problem is connected with control and responsibility. In Stanislaw Lem’s novel “Solaris”, however, humans attempt to understand an alien consciousness through scientific knowledge, but this attempt reaches its limits. Here, scientific cognition itself is interpreted as a problem.

In Uzbek literature, science fiction has its own distinctive path of development. In Hojiakbar Shaykhov’s novel “Tutash Olamlar”, the idea of parallel spaces is used as a scientific hypothesis. The work depicts a connection between human consciousness and another world. Although this concept is constructed on the basis of a scientific hypothesis, the philosophical layer is strong in its interpretation. In Tohir Malik’s work

“Chorrahada qolgan odamlar”, a scientific experiment is presented as a factor directly affecting human destiny. Here, the scientific element sets the plot in motion and reveals the problem of social choice. In Mahkam Mahmudov’s work “*Teskari ko‘zlar sayyorasi*”, the moral and social shortcomings of humanity are reflected through a model of another planet. In this work, the fantastic environment functions as a critical means. The social function of science fiction also requires a comparative approach. Fredric Jameson expresses the following view: “Science fiction makes it possible to understand the present indirectly. It shows social systems in an altered form and serves to understand them” [7]. This view connects science fiction with historical thought. By comparing works created in different literatures, the attitudes of societies toward scientific progress and the characteristics of social consciousness can be identified. Science fiction is formed according to a distinctive model in each culture. In Arthur Clarke’s work “*2001: A Space Odyssey*”, human evolution is connected with technological progress. In Uzbek science fiction, however, scientific ideas are often interpreted together with the moral and spiritual state of the individual. In the works of Hojiakbar Shaykhov and Mahkam Mahmudov, social and spiritual problems also come to the forefront alongside scientific hypotheses. As a result, through a comparative study of science fiction, the general directions of the genre’s development, the artistic interpretation of scientific hypotheses, and the models of thought formed in different cultures are identified.

Results and Discussion

A comparative study of science fiction requires a specific methodological foundation, unlike general literary theory. The issue here is not merely placing works side by side, but interpreting them within a unified theoretical field. A comparative approach makes it possible to view a literary phenomenon within a broader system. In the contemporary interpretation of comparative literature, the main focus is placed not on inter-literary relationships, but on their typological similarities. Claudio Guillén writes about this: “Comparative literature studies literary phenomena beyond national boundaries, on the basis of general laws. This field seeks to identify similarities in structure and function, rather than relationships” [6].

This view is important for science fiction. This is because the genre often develops independently not as a result of direct influence, but under similar historical and scientific conditions. Therefore, comparative analysis here is typological rather than genetic in character. One of the main concepts in the theory of science fiction is the “scientific hypothesis.” Darko Suvin explains this concept as follows: “At the center of science fiction stands a new element that differs from ordinary reality. This element serves as the main principle organizing the world of the work” [11].

This “new element” takes different forms in different literatures. In Isaac Asimov’s works, it appears as a technological system. In Stanislav Lem, it becomes a form of consciousness expressing the limits of cognition. In Uzbek literature, in Hojiakbar Shaykhov’s novel “Tutash Olamlar”, this element is presented through the idea of parallel spaces. A comparative approach reveals precisely the essence of these differences. Another important theoretical foundation in the comparative study of the genre is the concept of the chronotope. Mikhail Bakhtin defines the chronotope as follows: “The chronotope is the artistic unity of time and space in a work. The development of events and the movement of the character find their expression in it” [14]. The chronotope is of particular importance in science fiction. This is because the genre often relies on models of alternative space and future time. For example, in the novel “Solaris”, the chronotope of an unknown planet reveals the limits of human consciousness. In “Tutash Olamlar”, reality is expanded through the idea of movement between spaces. By comparing these cases, different interpretations of fantastic space and time can be identified.

Another theoretical direction in the comparative study of science fiction is related to its social function. According to Fredric Jameson, “Science fiction shows social structures in an altered form. Through it, society becomes aware of its possibilities and limitations” [7]. This approach presents science fiction as a product of social thought. Thus, through comparative analysis, the scientific and social views of different societies can be identified. As a result, the comparative study of science fiction is based on the following theoretical foundations: the typological approach, the concept of the scientific hypothesis, the chronotope model, and the principle of social interpretation. These

foundations make it possible to analyze the genre systematically and consistently from a scholarly perspective. It should not be forgotten that in the comparative study of science fiction, the main problem is not the method, but the correct definition of the criteria of analysis. This is because the genre is distinguished not by general literary categories, but by its specific theoretical characteristics. The first criterion is the artistic model of scientific change. Unlike other genres, science fiction places “change” at its center. James Gunn writes about this: “Science fiction depicts changes that affect human life. These changes are connected with scientific or technological discoveries.” When works are compared on the basis of this criterion, their differences become clear. For example, in Isaac Asimov, change occurs through an ordered system. In Mahkam Mahmudov’s work “Teskari ko‘zlar sayyorasi”, however, change is presented through an alien environment and functions as an external assessment of humanity. Here, the scientific element performs a critical function.

The second criterion is the degree to which the scientific hypothesis is connected to reality. This is also the feature that distinguishes science fiction from other types of fantasy. In research, this is explained as follows: “Science fiction constructs the ‘new element’ in a logically grounded manner. This element must be connected to the real world.” At this point, the difference between Uzbek and American literature becomes clear. For example, in A. Asimov, the scientific model has a strict system. In Hojiakbar Shaykhov’s novel “Tutash Olamlar”, although a scientific hypothesis is present, it is more closely integrated with philosophical interpretation. This helps to determine the boundaries of the genre in comparative analysis. The third criterion is the social function of science fiction. Contemporary research considers this to be one of the main functions of the genre. Carl Freedman assesses the theoretical significance of science fiction as follows: “Science fiction is more deeply connected with historical and social thought than other genres.” This view is important for comparative analysis. This is because every work reflects the problems of its own society. For example, in Ray Bradbury’s novel “Fahrenheit 451”, the problems of mass culture and control are central. In Tohir Malik’s work “Chorrahada qolgan odamlar”, the issue of human moral choice is

revealed through a scientific experiment. Both works contain a scientific element, but its social function is different.

The fourth criterion is the cognitive function of science fiction. Contemporary research also views this genre as a “form of theoretical thinking.” Science fiction develops in close connection with theory and becomes a means of explaining it. From this criterion, science fiction appears not only as a plot, but as a model of thought. In Uzbek literature, this aspect often manifests itself in a philosophical direction. In the works of Mahkam Mahmudov and Hojiakbar Shaykhov, scientific ideas are interpreted together with the spiritual state of the individual. In English-language literature, however, this is presented more often in a systematic and technological form. The fifth criterion is the relationship between the global and national characteristics of the genre. Contemporary research assesses science fiction as a global phenomenon. Science fiction develops common themes in different cultures. This makes comparative analysis necessary. This is because the same themes find different solutions in different cultures. While technology is central in English-language literature, questions concerning humans and society predominate in Uzbek science fiction. As a result, the main criteria for the comparative study of science fiction are as follows: the model of scientific change, the logic of the scientific hypothesis, social function, the process of cognition, and cultural context. Through these criteria, works are compared not superficially, but at a theoretical level. One of the main issues in the comparative study of science fiction is determining what form it takes in different literary traditions. Here, the issue is not common themes, but the ideological mechanism through which the genre operates. That is, the question is how a scientific idea is transformed into an artistic system, which elements come to the forefront, and which mode of thought becomes dominant. In contemporary research, science fiction is often viewed as a product of cultural thought. Professor John Rieder of the University of Hawaii writes about this: “Science fiction is closely connected with the cultural context that produces its content. Although it is a global genre, it takes a distinctive form in each culture” [9]. This view provides an important basis for comparative analysis. Science fiction does not develop according to a single model. It takes different directions in different literatures. In English literature, science fiction

often relies on a systematic and technological model. For example, in Isaac Asimov's works, scientific ideas are constructed on the basis of strict logic. The robot system obeys clear laws, and through this a model of society is created. In Arthur Clarke's works, science fiction develops on a cosmic scale. Here, technology becomes the main factor in human evolution. In this model, scientific thought occupies a central position. In Uzbek literature, science fiction develops in a different direction. Although a scientific idea is present in Hojiakbar Shaykhov's novel "Tutash Olamlar", it does not become a strict system. In the work, the concept of parallel worlds is connected with the possibilities of human consciousness. In Mahkam Mahmudov's work "Teskari ko'zlar sayyorasi", however, the fantastic space becomes a means of social criticism. Here, the evaluation conveyed through the scientific element is more important than the scientific element itself. Contemporary researchers also note the difference between these two directions. Farah Mendlesohn, a scholar who has analyzed British and American science fiction literature, explains the formation of science fiction as follows: "Science fiction manifests itself in different forms in different cultural environments. Its structure depends on the agreement established with the reader" [8]. This view reveals an important point. Science fiction is shaped not only by the author, but also on the basis of cultural expectations. In English-language literature, the reader expects scientific accuracy. In Uzbek literature, artistic and philosophical interpretation tends to predominate. Another important aspect in identifying the comparative model is the function of the scientific idea. In English-language literature, it often performs the function of forecasting (prediction). A model of the future is constructed, through which humanity's prospects are shown. In Uzbek literature, science fiction is more reflective in character. It functions as a means of understanding not the future, but the existing state of affairs. From this point of view, the views of Adam Roberts, a Cambridge University doctor and science fiction writer, on science fiction are highly relevant. According to the scholar and writer, "Science fiction is one of the main forms of understanding the contemporary world. It is a way of understanding technological culture itself" [10]. This approach gives comparative analysis a new direction. Science fiction is now viewed not only as a literary genre, but also as a form of cultural thought.

On this basis, different literatures are compared. In turn, comparative models of science fiction manifest themselves in two main directions. The first is a systematic and technological model, in which scientific logic is predominant. The second is an artistic and philosophical model, in which scientific ideas are integrated with human problems. By comparing these models, the global and national characteristics of science fiction are identified. As a result of the comparative study of science fiction, it is determined that although this genre relies on the same basic principles in different literary traditions, these are manifested in different artistic models. This difference is seen, above all, in the function of the scientific idea in the work and its place within the artistic system. In some literatures, the scientific hypothesis becomes the central constructive factor of the work, while in other cases it participates as an additional semantic layer.

Conclusion and Recommendations

The results of comparative analysis show two main directions of development of science fiction. In the first direction, the scientific model completely determines the artistic structure, and the plot, system of characters, and conflict are formed precisely on the basis of this model. In the second direction, the scientific element is integrated with other artistic layers and does not separate as an independent system. The second case is more often observed in Uzbek literature; that is, science fiction develops in close connection with social, moral, and psychological problems. This characteristic has also been noted in Uzbek literary studies. Professor Ra'no Ibrahimova evaluates Uzbek fantasy as a broader system and emphasizes that science fiction exists in close connection with other fantastic forms: "The formation and development of fantastic traditions in Uzbek literature is an important phenomenon in the literary process. Fantasy includes not only science fiction, but also adventure, mythological, and folkloric forms." She also specifically notes that the place of the fantastic element in a work is determined by the author's aesthetic position: "The place of fantastic elements in a work depends on the author's worldview, the characteristics of the genre, and the methods of realizing the artistic intention" [16]. This view provides an important methodological conclusion for the comparative study of science fiction. It is necessary to analyze the genre not only within the framework of the scientific model, but also within the general

system of fantastic thought. This, in turn, creates an opportunity to define more precisely the place of science fiction in national literature. The comparative approach produces another important result. Although science fiction develops common themes in different cultures, their interpretation changes depending on historical and social conditions. Therefore, comparative analysis serves to identify, alongside the universality of the genre, its national characteristics as well. In this process, science fiction manifests itself not only as an artistic phenomenon, but also as a product of society's thought.

The prospects for the comparative study of science fiction can continue in several directions. First of all, there is a need to systematically study Uzbek science fiction. Although individual works have been studied in this field, generalizing theoretical studies have not been sufficiently developed. In addition, by expanding comparative analysis with English, American, and other literatures, it is possible to identify the development trends of the genre. Works reflecting contemporary technological problems serve as new material for comparative research. As a result of the comparative study of works in this genre, a new approach can be formed within literary studies. This approach makes it possible to analyze a literary text not as an isolated phenomenon, but in connection with a broader cultural and intellectual process.

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Section 2. MODERN PROBLEMS OF TOURISM AND ECONOMICS

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INNOVATION ACTIVITY AND SCIENTIFIC CAPACITY IN ENTREPRENEURIAL ENTITIES

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Annotatsiya. Ushbu maqolada tadbirkorlik subyektlarida innovatsion faoliyatni rivojlantirish va ilmiy salohiyatdan samarali foydalanish masalalari tadqiq etiladi. Zamonaviy iqtisodiyotda kichik biznes va xususiy tadbirkorlik subyektlarining raqobatbardoshligi nafaqat moliyaviy resurslar va bozor ulushiga, balki yangi bilimlarni yaratish, o'zlashtirish va amaliyotga joriy etish qobiliyatiga ham bog'liq. Tadqiqotning maqsadi tadbirkorlik subyektlarining innovatsion faolligi bilan ularning ilmiy, texnologik, inson kapitali va institutsional salohiyati o'rtasidagi o'zaro bog'liqlikni aniqlashdan iborat. Tadqiqotda tizimli tahlil, qiyosiy tahlil, ilmiy adabiyotlarni umumlashtirish va konseptual yondashuvlardan foydalanildi. Natijalar shuni ko'rsatadiki, malakali kadrlar, ilmiy-tadqiqot infratuzilmasi, moliyalashtirish, raqamli texnologiyalar, intellektual mulkni himoya qilish va oliy ta'lim muassasalari bilan hamkorlik tadbirkorlik subyektlarining innovatsion salohiyatini belgilovchi asosiy omillardir. Ayniqsa, universitet–biznes hamkorligi ilmiy ishlanmalarni tijoratlashtirish, startaplarni shakllantirish va yangi texnologiyalarni ishlab chiqarishga joriy etish uchun muhim institutsional mexanizm sifatida namoyon bo'ladi. Maqolada O'zbekiston sharoitida kichik biznes va xususiy tadbirkorlik subyektlarining ilmiy-innovatsion salohiyatini kuchaytirish bo'yicha amaliy takliflar ishlab chiqilgan. Xulosa sifatida ilm-fan, ta'lim, tadbirkorlik va davlat qo'llab-quvvatlash mexanizmlarining integratsiyasi bilimlarga asoslangan iqtisodiyotga o'tishning muhim sharti ekanligi asoslanadi.

Kalit so'zlar: *innovatsion faoliyat, ilmiy salohiyat, tadbirkorlik, kichik biznes, xususiy tadbirkorlik, innovatsion ekotizim, ilmiy-tadqiqot ishlari, universitet–biznes hamkorligi, tijoratlashtirish, inson kapitali.*

Аннотация. В статье исследуются вопросы развития инновационной деятельности и эффективного использования научного потенциала субъектами предпринимательства. В условиях современной экономики конкурентоспособность малого бизнеса и частного предпринимательства определяется не только финансовыми ресурсами и рыночными позициями, но и способностью создавать, воспринимать, адаптировать и коммерциализировать новые знания. Цель исследования заключается в выявлении взаимосвязи между инновационной активностью предпринимательских субъектов и их научным, технологическим, кадровым и институциональным потенциалом. В работе применены системный и сравнительный анализ, обобщение научной литературы и концептуальный подход. Результаты показывают, что квалифицированные человеческие ресурсы, научно-исследовательская инфраструктура, доступ к финансированию, цифровые технологии, защита интеллектуальной собственности и взаимодействие с высшими учебными заведениями являются ключевыми факторами инновационного развития бизнеса. Особое значение имеет сотрудничество университетов и предприятий, позволяющее коммерциализировать результаты исследований, создавать стартапы и внедрять новые технологии в производство и сферу услуг. В статье сформулированы практические рекомендации по усилению научно-инновационного потенциала малого бизнеса и частного предпринимательства в условиях Узбекистана. Сделан вывод о том, что интеграция науки, образования, предпринимательства и государственных механизмов поддержки является важным условием формирования экономики, основанной на знаниях.

Ключевые слова: инновационная деятельность, научный потенциал, предпринимательство, малый бизнес, частное предпринимательство, инновационная экосистема, научно-исследовательские работы, сотрудничество университета и бизнеса, коммерциализация, человеческий капитал.

Abstract. This article examines the development of innovation activity and the effective use of scientific capacity by entrepreneurial entities, with particular attention to small businesses and private enterprises. In the contemporary economy, business competitiveness depends not only on financial resources and market position but also on the ability to create, absorb, adapt, and commercialize knowledge. The purpose of the study is to identify the relationship between entrepreneurial innovation activity and scientific, technological, human-capital, and institutional capacity. The research applies a systematic and comparative analytical approach, literature synthesis, and conceptual analysis. The findings indicate that qualified human resources, research infrastructure, access to finance, digital technologies, intellectual property protection, and cooperation with higher education institutions are major determinants of innovation performance. University–industry cooperation is particularly important because it can facilitate the commercialization of research results, the creation of startups, technology transfer, and the practical implementation of scientific knowledge. The article develops practical recommendations for strengthening the scientific and innovation capacity of small businesses and private entrepreneurial entities in Uzbekistan. It concludes that closer integration of science, education, entrepreneurship, finance, and public support mechanisms is an important condition for the transition toward a knowledge-based economy and for improving the productivity and competitiveness of entrepreneurial entities.

Key words: *innovation activity, scientific capacity, entrepreneurship, small business, private enterprise, innovation ecosystem, research and development, university–industry cooperation, commercialization, human capital.*

Introduction

The transformation of the global economy has significantly increased the importance of knowledge, innovation, and entrepreneurial initiative. Businesses operate in an environment characterized by technological change, digitalization, globalization, changing consumer expectations, environmental pressures, and increasingly complex forms of competition. Under these conditions, the traditional sources of competitive

advantage—low costs, physical assets, and access to established markets—are increasingly complemented by intangible resources such as knowledge, creativity, technological competence, organizational learning, and research capability.

Entrepreneurial entities, especially small and medium-sized enterprises, occupy a distinctive position within this transformation. Their organizational structures are generally more flexible than those of large corporations, allowing them to respond rapidly to changes in demand, identify market niches, test new ideas, and introduce incremental innovations. At the same time, small businesses commonly face constraints in access to finance, qualified researchers, specialized equipment, research infrastructure, technology, and international knowledge networks. Consequently, the innovation potential of entrepreneurial entities depends not only on their internal capabilities but also on the quality of the external innovation ecosystem., [4]

Innovation should be understood broadly. It includes the introduction of new or significantly improved products and services, production processes, marketing methods, organizational practices, and business models. The OECD and Eurostat's Oslo Manual provides a widely used framework for measuring business innovation and emphasizes that innovation is closely connected with knowledge creation, acquisition, application, and commercialization. For entrepreneurial entities, innovation can therefore range from radical technological breakthroughs to relatively simple but economically meaningful improvements in products, logistics, customer service, management, and digital operations. [1], [9]

Scientific capacity is a critical component of this process. In the context of entrepreneurship, scientific capacity can be defined as the ability of an enterprise or entrepreneurial ecosystem to generate, acquire, absorb, adapt, apply, and disseminate scientific and technological knowledge. It includes human expertise, research competence, organizational learning, technological infrastructure, access to scientific information, financial resources for experimentation, and relationships with universities and research institutions [2].

The relationship between innovation activity and scientific capacity is especially relevant for developing economies seeking to diversify their production structure and

move toward higher-value economic activities. A country can import advanced technologies, but sustainable technological development also requires the domestic ability to absorb, adapt, improve, and eventually generate knowledge. This makes the interaction between businesses, universities, research institutions, investors, and public organizations a central issue in innovation policy [3].

In Uzbekistan, the expansion of private entrepreneurship and the modernization of the economy create new opportunities for developing innovation-oriented businesses. Small enterprises can contribute to employment creation, regional development, digital transformation, and the introduction of new products and services. However, their contribution to innovation can be strengthened if they gain better access to scientific expertise, research infrastructure, financing, technology-transfer mechanisms, and qualified human resources [9].

The purpose of this study is to analyze the role of innovation activity and scientific capacity in entrepreneurial entities and to identify the principal factors that determine their development. The study focuses particularly on small businesses and private enterprises and considers how cooperation with universities and research institutions can support innovation and commercialization [5].

The research addresses four questions: (1) How are innovation activity and scientific capacity connected within entrepreneurial entities? (2) Which factors determine the scientific capacity of small businesses? (3) How can university–industry cooperation stimulate innovation? and (4) Which institutional and financial mechanisms can improve the commercialization of scientific knowledge? [4], [9].

Research Methodology

The study employs a qualitative analytical methodology based on the systematic examination and synthesis of theoretical and empirical literature on entrepreneurship, innovation, scientific capacity, knowledge-based development, and university–industry relations. The methodological approach is designed to identify mechanisms and relationships rather than to estimate a statistical causal model. The evidence base includes academic literature and institutional publications dealing with innovation systems, entrepreneurial capabilities, research and development, human capital,

technology transfer, and small-business development. The theoretical foundations include Schumpeter's theory of entrepreneurial innovation, the national innovation systems approach, the knowledge-based view of the firm, and the Triple Helix model of university–industry–government relations [9].

For analytical purposes, scientific capacity is divided into five interconnected dimensions. The first is human scientific capacity, including education, professional qualifications, analytical skills, creativity, research competence, and technological literacy. The second is organizational capacity, meaning the ability to manage knowledge, organize experimentation, conduct innovation projects, and integrate research results into business processes. The third is technological capacity, including access to digital tools, laboratories, production technologies, specialized equipment, and technical infrastructure [7].

The fourth dimension is financial capacity. Innovation projects require resources for research, experimentation, prototyping, testing, intellectual property protection, market validation, and commercialization. The fifth dimension is networking capacity, which reflects the ability of enterprises to cooperate with universities, research organizations, investors, technology providers, government agencies, and other firms.

The research uses systematic comparison to distinguish internal and external determinants of innovation. Internal determinants include management quality, entrepreneurial orientation, employee competencies, organizational culture, financial resources, digital capabilities, and willingness to experiment. External determinants include the regulatory environment, research infrastructure, access to finance, intellectual property protection, university–industry relationships, innovation support programs, and market conditions [8].

The conceptual framework assumes that scientific capacity and innovation activity reinforce each other. A business with stronger research and absorptive capacity is more capable of identifying technological opportunities and implementing new solutions. At the same time, innovation activity creates new demand for skills, research, technology, and external knowledge. The study therefore treats innovation as an organizational capability embedded within a broader institutional ecosystem [4].

Results and Discussion

The analysis shows that innovation is most effective when it becomes a continuous strategic capability rather than an occasional response to competitive pressure. Entrepreneurial entities that systematically monitor markets, experiment with new solutions, collect customer feedback, and invest in learning are better positioned to adapt to technological and market changes. Product innovation involves the creation or substantial improvement of goods and services. Process innovation concerns production, logistics, distribution, or service-delivery methods. Organizational innovation may involve new management systems, human-resource practices, internal communication structures, or knowledge-management approaches. Marketing innovation includes new approaches to pricing, promotion, customer segmentation, branding, and digital engagement. These forms frequently overlap and can reinforce each other [9]. For small businesses, innovation is often incremental. A firm may introduce digital accounting, automate a production stage, redesign packaging, develop an online sales channel, use data analytics, or establish a new delivery system. Such changes may not constitute radical technological breakthroughs, but they can generate productivity improvements, cost reductions, better customer experience, and stronger market positioning [6]. Human capital is the foundation of scientific and innovation capacity. Entrepreneurs and employees need the ability to identify problems, formulate solutions, analyze information, use technologies, conduct experiments, and interpret results. Scientific capacity is therefore not limited to the employment of researchers; it also involves the ability of ordinary business personnel to absorb and apply new knowledge [4]. Continuous professional development is particularly important for small businesses. Short training courses can be useful, but sustainable capacity requires lifelong learning, internships, participation in research projects, interaction with experts, and access to current scientific and technological information. Universities can contribute by offering executive education, applied research programs, student internships, innovation competitions, and entrepreneurship education [7]. An important finding is that the scientific capacity of a small business can be extended through external networks. A firm does not need to establish a large internal R&D department to become innovation-

oriented. It can contract research services, cooperate with university laboratories, employ academic consultants, participate in joint projects, license technologies, or join innovation clusters [4]. University–industry cooperation emerges as one of the most important mechanisms for strengthening entrepreneurial innovation. Universities possess scientific expertise, laboratories, researchers, students, and access to international knowledge networks. Businesses possess practical knowledge of customer needs, market conditions, production processes, and commercialization. Combining these capabilities can reduce the distance between scientific research and market application [3]. Cooperation may take the form of joint research projects, contract research, consulting, student internships, joint laboratories, technology-transfer agreements, patent development, business incubators, startup acceleration, and co-designed educational programs. Such cooperation is particularly valuable for small businesses because it allows them to access expertise and infrastructure that would be expensive to maintain internally [7]. However, sustainable cooperation requires institutional mechanisms. Universities need technology-transfer offices, intellectual property support, clear commercialization procedures, innovation centers, and incentives for academics to cooperate with businesses. Enterprises need mechanisms for communicating technological problems and research needs to universities. Public institutions can facilitate these relationships by supporting joint projects and reducing administrative barriers[7]. Financing is a major constraint on entrepreneurial innovation. Research, prototyping, testing, equipment, software, certification, intellectual property protection, and market introduction require investment. Small enterprises may find it difficult to obtain conventional loans because innovative projects often have uncertain returns and limited collateral [8]. A diversified financing system is therefore necessary. Potential instruments include competitive grants, innovation vouchers, preferential loans, venture capital, business-angel investment, crowdfunding, public–private partnerships, and co-financing schemes. Grants are especially relevant at early research and experimentation stages, while venture capital can be important for scalable technology-based startups. The effectiveness of innovation finance depends on transparent selection criteria, professional evaluation, monitoring of outcomes, and

opportunities for follow-on financing. Financing should also be combined with mentoring and technical support, because capital alone cannot compensate for weaknesses in human or organizational capacity [3]. Digital technologies have changed the accessibility and speed of innovation. Cloud computing, artificial intelligence, data analytics, digital platforms, automation, and online collaboration tools allow small businesses to perform activities that previously required substantial physical infrastructure. Digitalization can therefore reduce some barriers to experimentation and market entry. At the same time, digital transformation increases demand for new competencies. Entrepreneurs need digital literacy, data-analysis skills, cybersecurity awareness, and the ability to evaluate emerging technologies. Digital tools are most valuable when they are integrated into broader organizational learning and innovation strategies rather than adopted simply as isolated technologies [4]. Recent official statistics provide additional evidence of the relevance of innovation capacity to entrepreneurial development in Uzbekistan. The National Statistics Committee reports that the number of enterprises and organizations implementing innovations was 1,835 in 2024, while the number of implemented innovations reached 5,521. The reported volume of scientific research and development amounted to 1,603,040.1 million soums in 2024. These indicators should be interpreted carefully because statistical coverage and methodology may change over time, but they demonstrate the scale of innovation and R&D activity recorded in the national statistical system [3]. International benchmarking also shows a continuing improvement in Uzbekistan's innovation position. According to WIPO, Uzbekistan ranked 83rd in the Global Innovation Index 2024 and 79th in the 2025 edition. The 2025 profile indicates that innovation inputs ranked 69th while innovation outputs ranked 92nd, suggesting a gap between resources entering the innovation system and the outputs generated from them [10]. Recent research by economists and researchers working in Uzbekistan supports the importance of human capital, finance, digitalization, infrastructure, and management capabilities. Boboyeva's 2025 study identifies owners' experience and employees' knowledge and skills as important factors affecting the innovativeness of small businesses in Uzbekistan. Samadov's research at Tashkent State University of Economics examines

the export potential of small businesses and private entrepreneurship using econometric analysis. Rizayeva examines e-commerce platforms and marketplaces as channels for small-business development and technology adoption. Botirova's work addresses entrepreneurial infrastructure, including incubators, technology parks, venture funds, innovation centers, and public–private partnerships. Abduvoxidov's recent study highlights regional disparities, limited finance, and insufficient innovation-support mechanisms in the Uzbek business environment. Mavrulov's 2026 assessment uses 2021–2025 data to examine the development dynamics of small-business entities in Uzbekistan. These studies provide a recent national research base for interpreting the relationship between entrepreneurship, innovation, and scientific capacity [10].

Results and Discussion

The results confirm the close relationship between entrepreneurial innovation and scientific capacity. Schumpeter's theory emphasizes the entrepreneur as an agent of economic change who introduces new combinations of products, technologies, markets, and organizational forms. In contemporary knowledge economies, however, the entrepreneur increasingly depends on distributed sources of knowledge rather than relying exclusively on individual creativity.

The national innovation systems perspective provides a broader explanation. Innovation emerges from interactions among firms, universities, research institutions, government agencies, financial organizations, and other actors. The performance of an individual enterprise is therefore partly determined by the quality of its surrounding ecosystem. This is particularly relevant to small businesses, which generally possess fewer internal resources than large corporations [9]. The Triple Helix model further emphasizes the interaction of university, industry, and government. Each actor performs a different but complementary role. Universities generate and disseminate knowledge; businesses transform knowledge into products and services; and government establishes rules, infrastructure, incentives, and public support. Effective innovation ecosystems emerge when these functions overlap constructively [9]. For Uzbekistan, these findings suggest that innovation policy should not focus exclusively on large enterprises or high-technology sectors. Small businesses should be systematically integrated into innovation

programs, university partnerships, technology-transfer networks, and regional clusters. This can increase the practical relevance of academic research and simultaneously improve the technological capabilities of businesses [9]. One important challenge is the commercialization gap. Scientific publications and patents do not automatically generate economic value. A research result becomes economically significant when it is transformed into a product, process, service, or business model that solves a real problem. Technology-transfer offices, incubators, accelerators, intellectual property services, and university spin-offs can help close this gap [9]. Another challenge is organizational culture. Innovation requires experimentation, learning from unsuccessful attempts, and sharing knowledge. If employees perceive that failure will always be punished, they may avoid proposing new ideas. Innovation-oriented management should therefore encourage responsible experimentation, continuous improvement, interdisciplinary collaboration, and recognition of employee contributions to innovation [9]. Human capital policy is equally important. Universities should develop students' entrepreneurial and research competencies, while businesses should create opportunities for internships, applied research, and continuous professional development. Young researchers can become a bridge between academic knowledge and entrepreneurial practice when appropriate incentives and institutional channels exist [9]. The analysis also indicates that government support should be systemic rather than fragmented. A grant program may have limited impact if firms cannot access qualified personnel. University laboratories may remain underused if there are no mechanisms for cooperation with businesses. Similarly, technology startups may struggle to scale if intellectual property procedures, investment mechanisms, or market access are weak. An integrated policy should therefore connect education, research, entrepreneurship, finance, technology, intellectual property, and markets [8]. Based on the findings, an effective entrepreneurial innovation ecosystem can be represented as a mutually reinforcing chain: knowledge creation → knowledge transfer → experimentation → commercialization → market expansion → reinvestment in research and innovation. Strengthening each link increases the probability that scientific knowledge will generate measurable economic and social value [7].

Conclusion and Recommendations

The study demonstrates that innovation activity and scientific capacity are mutually reinforcing foundations of entrepreneurial competitiveness. For small businesses and private enterprises, innovation depends not only on financial resources but also on human capital, organizational learning, technological infrastructure, external knowledge, networking, and institutional support. Scientific capacity should be understood broadly as the ability to create, acquire, absorb, adapt, and apply knowledge. Small businesses can strengthen this capacity through cooperation with universities and research institutions instead of relying exclusively on internal R&D. Such cooperation can provide access to laboratories, researchers, students, scientific information, technology-transfer services, and international networks. University–industry cooperation should therefore become an integral element of entrepreneurial development. Joint research projects, internships, technology-transfer agreements, innovation centers, incubators, and startup programs can help convert scientific knowledge into commercially viable solutions. The financing system should also be diversified. Grants, innovation vouchers, preferential loans, venture investment, business-angel financing, and public–private partnerships can address different stages of the innovation cycle. Financial support should be accompanied by mentoring, research expertise, and commercialization assistance. For Uzbekistan, strengthening the innovation capacity of small businesses can contribute to economic diversification, productivity growth, digital transformation, higher-value employment, and stronger integration into international markets. Regional innovation ecosystems connecting universities, research institutions, businesses, investors, and government organizations can provide an effective institutional foundation for this process. Future empirical research should test the conceptual relationships identified in this study using firm-level data from Uzbekistan. Potential indicators include R&D expenditure, number of innovation projects, patents, technology adoption, cooperation agreements with universities, employee qualifications, access to innovation finance, and productivity. Such evidence would allow researchers and policymakers to identify which instruments have the strongest relationship with entrepreneurial innovation performance.

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Section 3. MODERN PROBLEMS OF TECHNICAL SCIENCES

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RESEARCH ON OBTAINING CALCIUM CHLORATE THROUGH COMPLEX PROCESSING OF BY-PRODUCTS OF POTASSIUM SULPHATE PRODUCTION AT LLC "SOGDA KIMYO ZAVOD"

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Annotatsiya: Maqolada MCHJ «Sogda kimyo zavod»da kaliy sulfat ishlab chiqarish jarayonida hosil boʻladigan ikkilamchi mahsulot – kalsiy xloridni qayta ishlash orqali yuqori qoʻshimcha qiymatga ega kalsiy gipoxlorit va kalsiy xlorat olish imkoniyatlari oʻrganilgan. Konversiya jarayonida «Navoiyazot» AJ kaustik soda sexida hosil boʻladigan natriy gipoxlorit eritmasidan foydalanildi. Kalsiy xlorid namunalari IQ-spektroskopiya, XRD va XRF usullari yordamida tahlil qilinib, uning yuqori tozalik darajasiga ega ekanligi aniqlandi. SHuningdek, harorat va reaksiya davomiyligining konversiya jarayoniga taʼsiri baholanib, kalsiy gipoxlorit hamda kalsiy xlorat hosil boʻlishining maqbul texnologik sharoitlari aniqlandi.

Kalit soʻzlar: kalsiy xlorid, kalsiy gipoxlorit, kalsiy xlorat, natriy gipoxlorit, konversiya, ikkilamchi mahsulot, kaliy sulfat.

Аннотация: В статье исследуются возможности получения высокоценных продуктов переработки хлорида кальция, побочного продукта, образующегося при производстве сульфата калия на ООО «Согда Кимё Завод». В процессе переработки использовался раствор гипохлорита натрия, производимый в цехе каустической соды АО «Навоязот». Образцы хлорида кальция были проанализированы методами ИК-спектроскопии, рентгеновской дифракции и рентгенофлуоресцентного анализа, и было установлено, что они обладают высокой степенью чистоты. Кроме того, была оценена роль температуры и продолжительности реакции в процессе переработки, а также определены оптимальные технологические условия образования гипохлорита кальция и хлората кальция.

Ключевые слова: хлорид кальция, гипохлорит кальция, хлорат кальция, гипохлорит натрия, переработка, побочный продукт, сульфат калия.

Abstract: The article studies the possibilities of obtaining calcium hypochlorite and calcium chlorate with high added value by processing calcium chloride, a secondary product formed during the production of potassium sulfate at LLC "Sogda Kimyo Zavod". The conversion process used sodium hypochlorite solution produced at the caustic soda plant of JSC "Navoiyazot". Calcium chloride samples were analyzed using IR spectroscopy, XRD and XRF methods, and it was found that it has a high level of purity. In addition, the effect of temperature and reaction duration on the conversion process was evaluated, and optimal technological conditions for the formation of calcium hypochlorite and calcium chlorate were determined.

Key words: *calcium chloride, calcium hypochlorite, calcium chlorate, sodium hypochlorite, conversion, secondary product, potassium sulfate.*

Introduction

In the modern chemical industry, the processing of by-products generated during production processes is considered an important direction for the efficient use of resources, reduction of waste volumes, and production of value-added products. The physicochemical regularities of aqueous systems involving sodium hypochlorite, sodium chlorate, as well as chlorates of alkali and alkaline-earth metals have been studied, and technological processes based on these systems have been proposed. Currently, the integrated processing of local raw materials and secondary products in the chemical industry is one of the important directions for the efficient use of resources, reduction of waste, and production of high value-added products. In particular, obtaining import-substituting products through the processing of industrial waste not only increases economic efficiency, but also serves environmental protection.

The conversion of hypochlorite into chlorate is of great importance in the processing of chlorine-containing components of by-products. During the industrial production of sodium hypochlorite, NaClO and NaCl are formed as a result of the interaction of chlorine with an alkali solution:



In subsequent disproportionation processes, chlorate ions are formed, which provides an opportunity to obtain a stable product through their separation and crystallization.

The Sogda Kimyo Zavod LLC, operating in the Navoi region, produces 230 tons of potassium sulfate per day. In this process, approximately 120 tons of calcium chloride are formed as a secondary product. The fact that a large part of this product is not fully utilized in production requires the improvement of its processing technologies.

Therefore, the synthesis of new types of products based on calcium chloride, including calcium hypochlorite and calcium chlorate, is of urgent scientific and practical importance. This study investigated the possibility of obtaining calcium hypochlorite and calcium chlorate by converting calcium chloride with sodium hypochlorite solution produced at the caustic soda plant of Navoiyazot JSC. The physicochemical laws of the process were analyzed and the main technological parameters ensuring product quality were evaluated.

Literature review

Previous studies have mainly focused on the solubility, phase equilibria, crystallization behavior, and physicochemical properties of calcium, magnesium, and sodium chlorate systems, as well as on the preparation and agrochemical application of chlorate-based defoliant [2–5, 7, 8]. These studies have demonstrated that the composition of aqueous chlorate systems, temperature, concentration, and reaction time have a significant influence on phase formation, solubility, crystallization, and product quality. In particular, understanding the phase behavior of chlorate-containing solutions is important for developing efficient separation and crystallization technologies.

Considerable attention has also been devoted to the chemical transformations of hypochlorites in aqueous solutions. Hypochlorites are relatively unstable compounds and can undergo disproportionation reactions, particularly at elevated temperatures and under different pH conditions. During this process, hypochlorite ions can be converted into chloride and chlorate ions. The overall transformation can be represented by the following reaction:



The rate and extent of this transformation depend on several factors, including temperature, hypochlorite concentration, alkalinity, reaction time, and the presence of metal ions. Understanding these parameters is important for controlling the formation of chlorate-containing products and increasing their yield. Calcium hypochlorite is an important chlorine-containing compound that is widely used as a disinfectant, bleaching agent, and source of active chlorine. Calcium chlorate, in turn, has different physicochemical properties and can be considered a potentially useful component of agricultural formulations, including defoliant systems. However, the controlled conversion of calcium hypochlorite into calcium chlorate in systems containing calcium chloride and sodium hypochlorite has received comparatively little attention.

Research Methodology

The objects of research were calcium chloride, which is formed during the production of potassium sulfate at Sogda Chemical Plant LLC, and a 15% sodium hypochlorite solution produced at the caustic soda plant of Navoiyazot JSC. The chemical

composition and purity of calcium chloride were determined using infrared spectroscopy (FTIR), X-ray phase analysis (XRD), and X-ray fluorescence analysis (XRF).

Conversion experiments were conducted in laboratory conditions. In this, calcium chloride was reacted with sodium hypochlorite solution at temperatures ranging from 60–100 °C for various times to study the formation of calcium hypochlorite and calcium chlorate. The resulting products were evaluated by spectral and physicochemical analyses. In the initial stage of the study, the chemical composition and physicochemical properties of a calcium chloride sample formed during the production of potassium sulfate were studied using modern instrumental analysis methods. Fourier transform infrared spectroscopy (FTIR) was used to identify the functional groups of the sample, X-ray phase analysis (XRD) to assess the crystal structure, and X-ray fluorescence analysis (XRF) to determine the elemental composition.

Results and Discussion

The IR spectrum of the calcium chloride sample was recorded in the region of 4000–500 cm^{-1} (Fig. 1). The broad absorption line observed in the spectrum around 3440 cm^{-1} corresponds to the valence vibrations of the O–H group and indicates the presence of water molecules adsorbed in the crystal lattice due to the high hygroscopic nature of the sample. The absorption maximum observed at 1640 cm^{-1} is explained by the deformation vibrations of water molecules. In the low-frequency part of the spectrum, at about 750 cm^{-1} , an intense absorption maximum characteristic of Ca–Cl bonds was observed. This peak is the main spectral feature confirming the formation of calcium chloride. At the same time, the absence of absorption bands characteristic of organic compounds indicated that the sample had a high degree of purity.

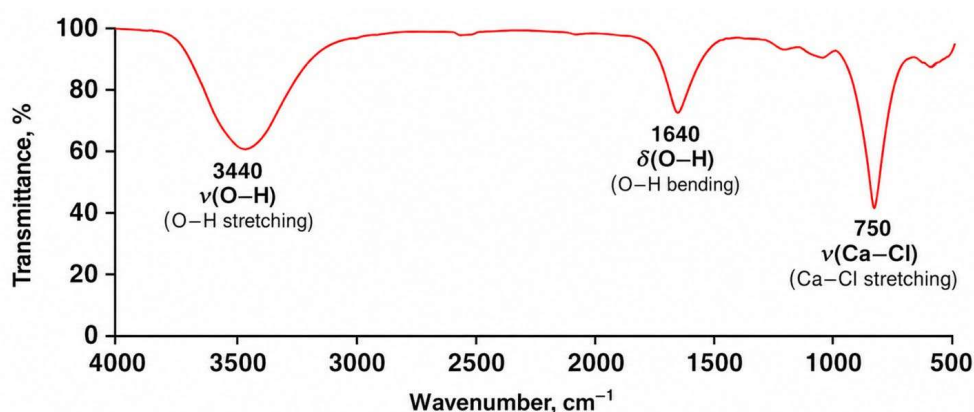


Figure 1. IR spectrum of a calcium chloride sample.

The diffraction peaks obtained in the X-ray phase analysis of calcium chloride samples (Figure 2) were found to be in good agreement with the standard data of JCPDS 85-1461, confirming that the main crystal phase of the sample is calcium chloride.

According to the results of X-ray fluorescence analysis, the chlorine content of the sample was 63.58%, and the calcium content was 36.21%. The content of impurities

was found to be no more than 0.21%. The results showed that calcium chloride has a high purity and can be used as an effective raw material for the subsequent conversion process. For the conversion process, a 15% sodium hypochlorite solution produced at the caustic soda plant of Navoiyazot JSC was used.

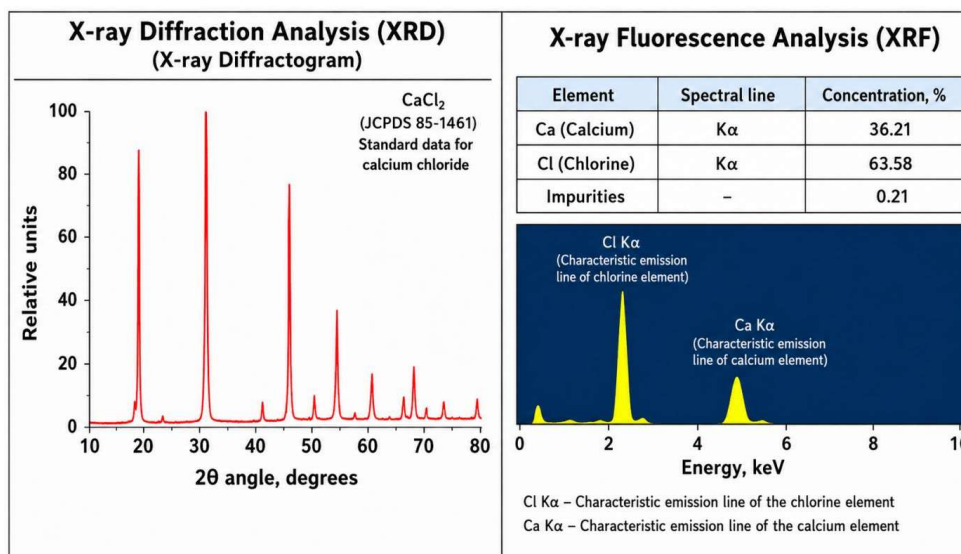
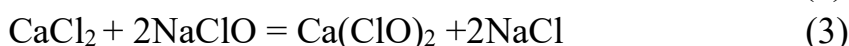


Figure 2. XRD and XRF analyses of a calcium chloride sample.

The high content of active chlorine in this solution and its good solubility in water make it an effective reagent for carrying out conversion reactions with calcium chloride. SEM analysis showed that the sodium hypochlorite particles were mainly composed of well-formed crystals of micron size (Figure 3). The relatively well-developed crystal structure and high dispersion of the particles confirm their high reactivity in subsequent chemical reactions.



XRD and XRF analysis showed that the sample was composed of high-purity sodium hypochlorite (Figure 4). In order to obtain high-value-added products from calcium chloride, which is formed during the production of potassium sulfate, the process of converting it with sodium hypochlorite was studied. A 15% sodium hypochlorite solution produced at the caustic soda plant of Navoiyazot JSC was used as a reagent. This approach allows for the comprehensive processing of secondary products generated at two enterprises and serves to reduce the amount of waste. The conversion process is based on the following basic chemical reactions: To carry out these reactions (3 and 4) was carried out in laboratory conditions. For this, 10 g of calcium chloride and 250 ml of 15% sodium hypochlorite solution were loaded into a three-neck reactor, and the mixture was stirred at temperatures of 60, 80, and 100 °C for 30–120 minutes. The

effect of temperature and time on the degree of conversion was studied during the process.

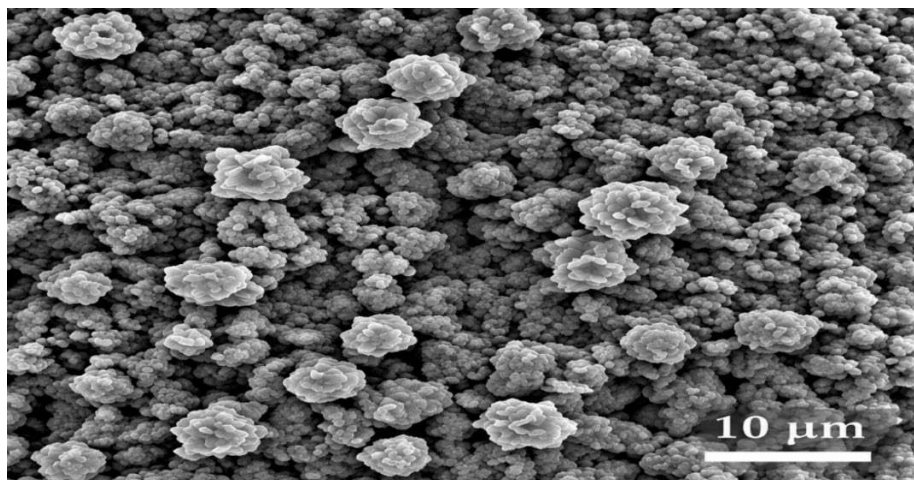


Figure 3. SEM image of sodium hypochlorite samples.

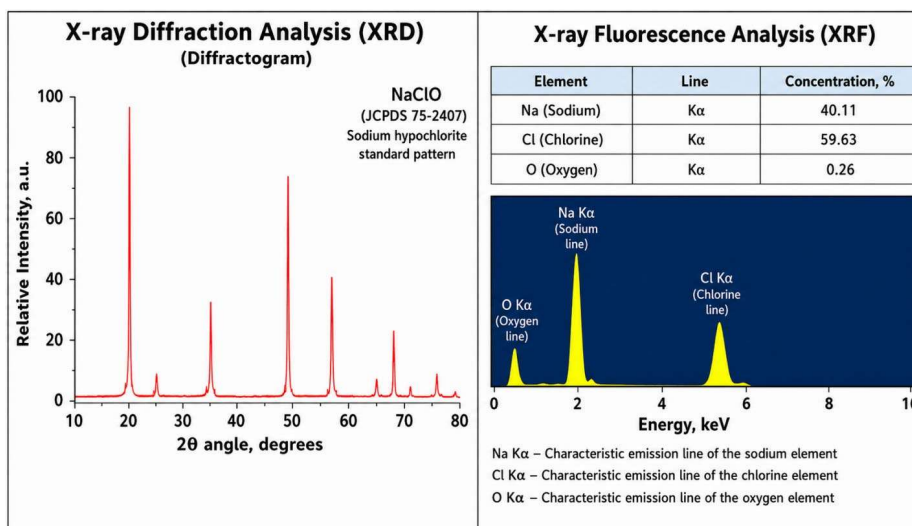


Figure 4. XRD and XRF analyses of sodium hypochlorite.

According to the results obtained, the formation of calcium hypochlorite and calcium chlorate accelerated with increasing temperature and reaction time. While the reaction was relatively slow at 60 °C, the conversion rate reached high values at 80 °C. At 100 °C, the efficiency of chlorate formation decreased due to the accelerated decomposition of hypochlorite. This is explained by the decrease in the stability of hypochlorite at high temperatures (Table 1). As can be seen from the data in Table 1, when the reaction time reached 90–120 minutes, the disproportionation of calcium hypochlorite increased and the amount of calcium chlorate formed increased. This process was also confirmed by the results of IR-spectroscopic analysis (Figure 5). While the solid product obtained in the initial stages was characteristic of calcium hypochlorite, as the reaction time increased, spectral features belonging to calcium chlorate became dominant.

Table 1. Conversion analysis results of calcium chloride and sodium hypochlorite at temperatures of 60-100 °C and time of 30-120 minutes.

Temperature °C	Time (τ), min.	ClO_3^{2-} %	Ca^{2+} %	Density g/ml	Light refraction	pH	Viscosity m^2/s
60	30	4.85	5.0	1.141	1.372	10	0.98
	60	5.2	5.4	1.145	1.380	10	1.14
	90	8.7	7.9	1.230	1.383	11	1.32
	120	9.23	15.1	1.230	1.385	11	1.39
80	30	5.46	8.23	1.205	1.377	10	0.99
	60	5.8	12.78	1.210	1.38	8	1.28
	90	7.11	14.63	1.230	1.383	8	1.286
	120	7.5	16.0	1.233	1.386	8	1.315
100	30	3.67	9.86	1.14	1.379	7	0.998
	60	4.08	13.78	1.158	1.387	7	1.276
	90	4.5	15.3	1.165	1.388	6	1.288
	100	5.8	16.7	1.234	1.39	5	1.317

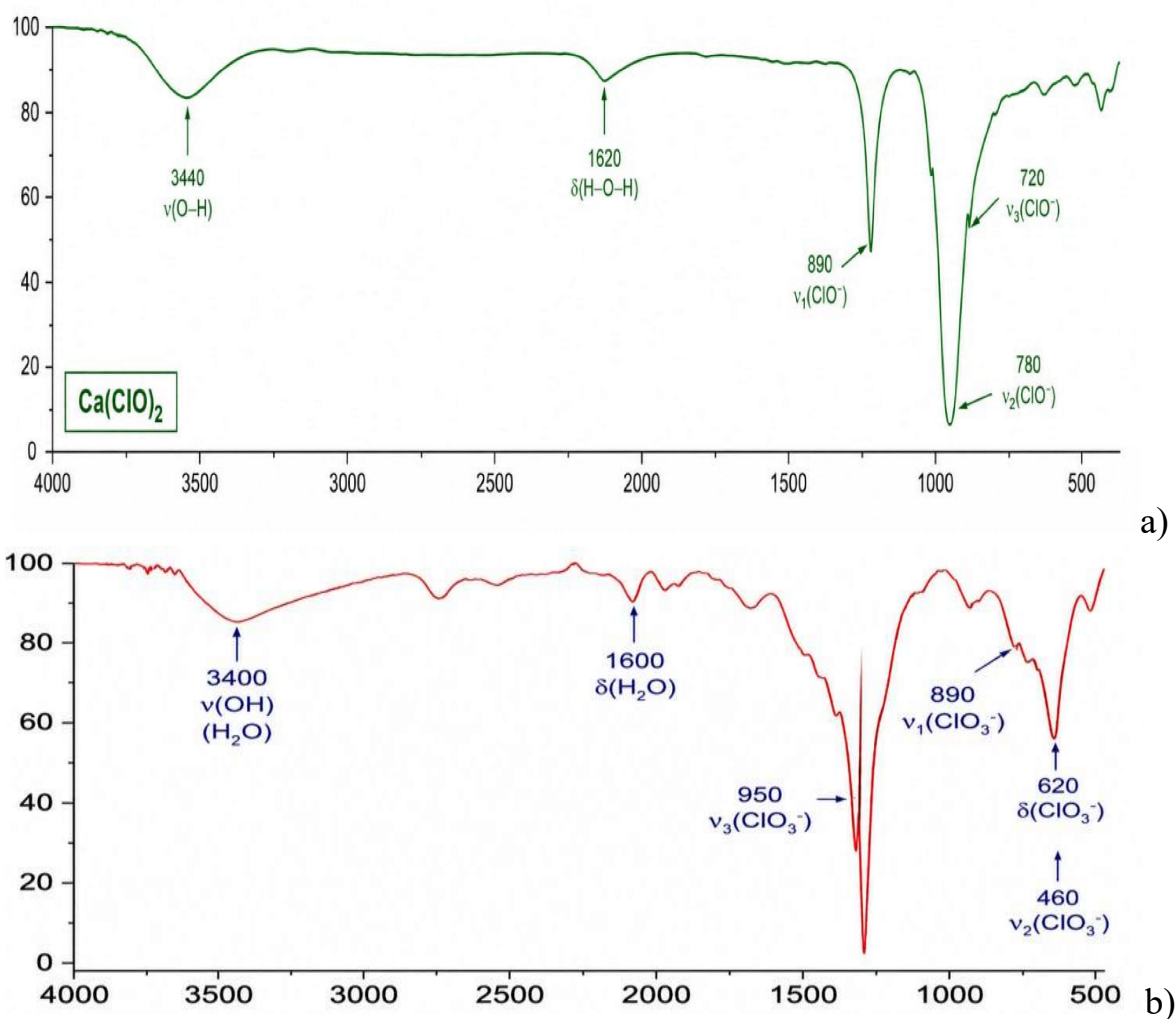


Figure 5. IR spectra of a) $\text{Ca}(\text{ClO})_2$ and b) $\text{Ca}(\text{ClO}_3)_2$

Conclusion and Recommendations

In conclusion, the conversion of the process of obtaining calcium hypochlorite and chlorate based on calcium chloride and sodium hypochlorite produced at Sogda Kimyo Zavod LLC was studied at a temperature of 60 - 100°C for 30 - 120 minutes, and the formation of hypochlorite at the initial stage and chlorate at the subsequent stage was determined by chemical and IR spectroscopic analyses. Technological indicators are being studied to develop the technology of the resulting calcium hypochlorite and chlorates.

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UDC: 004:556.3

A BIG-DATA-BASED THEORETICAL AND MATHEMATICAL MODEL FOR ASSESSING AND MANAGING GROUNDWATER MONITORING IN THE ZARAFSHAN RIVER VALLEY, SAMARKAND REGION

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Annotatsiya. Ushbu tadqiqot Samarqand viloyatidagi Zarafshon daryosi vodiysining oltita gidrogeologik konida yer osti suvlari monitoringi va boshqaruvini qo'llab-quvvatlashga mo'ljallangan Big Data asosidagi axborot tizimining nazariy-matematik modelini taklif etadi. Mavjud yig'ma suv balansi tenglamasi konlarning turlicha oziqlanish mexanizmlarini hisobga oluvchi indekslangan modelga, so'ngra konlararo gidravlik bog'lanishlarni ifodalovchi dinamik differensial tenglamalar tizimiga kengaytiriladi. Sensor o'lchovlarini model prognozi bilan birlashtirish uchun Kalman filtri, ma'lumotlar sifati, suv balansi og'ishi va anomaliya signalini birlashtiruvchi Regional Water Security Index (RWSI), xatolar tarqalishi modeli va cheklangan monitoring resurslarini optimallashtirish masalasi ishlab chiqiladi. Tadqiqot asosan nazariy va raqamli tahlilga asoslangan; ToF sensorining nashr etilgan dala sinovi ma'lumotlari Kalman filtri parametrlarini illustrativ kalibrlash uchun qo'llanadi. Natijalar konlarni tabiiy va irrigatsion oziqlanish ustunligiga ko'ra tasniflash, konlararo dinamik bog'lanishlarni tavsiflash va monitoring resurslarini taqsimlash mezonini shakllantirish imkonini beradi.

Kalit so'zlar: Zarafshon daryosi vodiysi, Samarqand viloyati, Big Data, dinamik suv balansi, Kalman filtri, Regional Water Security Index, gidrogeologik monitoring, optimallashtirish.

Аннотация. В статье предложена теоретико-математическая модель информационной системы на основе технологий больших данных для мониторинга и управления подземными водами шести гидрогеологических месторождений долины реки Зарафшан в Самаркандской области. Агрегированное уравнение водного баланса расширено до индексированной модели, учитывающей различия в источниках питания месторождений, а затем до системы динамических дифференциальных уравнений, описывающих гидравлическую связь между ними. Для объединения измерений датчиков с модельным прогнозом предложен фильтр Калмана; дополнительно сформированы региональный индекс водной безопасности (RWSI), модель распространения ошибок и задача оптимального распределения ограниченных ресурсов мониторинга. Исследование носит преимущественно теоретический и численный характер; опубликованные результаты полевых испытанийToF-датчика использованы только для иллюстративной калибровки параметров фильтра Калмана. Полученные результаты позволяют теоретически классифицировать месторождения по доминирующим источникам питания, описать их динамическую взаимосвязь и сформулировать критерий распределения ресурсов мониторинга.

Ключевые слова: *долина реки Зарафшан, Самаркандская область, большие данные, динамический водный баланс, фильтр Калмана, региональный индекс водной безопасности, гидрогеологический мониторинг, оптимизация.*

Abstract. This study proposes a theoretical and mathematical model of a Big-Data-based information system for monitoring and managing groundwater across six hydrogeological deposits in the Zarafshan River valley, Samarkand Region, Uzbekistan. The conventional aggregated water-balance equation is first indexed to reflect differences in recharge mechanisms and then extended to a coupled system of dynamic differential equations that represents hydraulic connectivity among deposits. A Kalman filter is formulated to fuse sensor observations with model forecasts, while a Regional Water Security Index (RWSI) integrates data

quality, water-balance deviation, and anomaly signals. An error-propagation model and a constrained optimization problem are further introduced to support the allocation of limited monitoring resources. The study is primarily theoretical and numerical; published field-test results for a time-of-flight (ToF) groundwater-level sensor are used only for an illustrative calibration of the measurement-error variance. The results provide a formal classification of deposits according to dominant recharge mechanisms, characterize inter-deposit dynamic coupling, and establish a theoretical criterion for prioritizing monitoring resources. The proposed framework provides a basis for subsequent empirical calibration with long-term observations.

Key words: *Zarafshan River valley, Samarkand Region, Big Data, dynamic water balance, Kalman filter, Regional Water Security Index, groundwater monitoring, resource optimization.*

Introduction

The groundwater system of the Zarafshan River valley in Samarkand Region occupies an intermountain depression bounded by the Nurata and Gobjuntau ranges to the north and the Karatepa and Ziaetdin–Zirabulak ranges to the south. From a geological and geomorphological perspective, the system is divided into six hydrogeological deposits: Northern foothill, Southern foothill, Right Bulungur, Left Samarkand, Zarafshan, and Ulus [6]. These units are not merely geographic subdivisions; their groundwater regimes are controlled by different recharge mechanisms. The foothill deposits are expected to depend more strongly on natural precipitation–infiltration recharge, whereas the riverside deposits are influenced by irrigation return flow and river infiltration. A key methodological problem is that aggregated monitoring can obscure deposit-specific changes: deterioration in one unit may be masked by stability in another.

Several applied studies have introduced modern measurement and monitoring technologies in the region, including non-invasive subsurface scanning [7], automated monitoring stations [8], and GIS-based observation networks [4]. These contributions improve data acquisition and visualization, but they do not provide a unified

mathematical framework that represents the distinct recharge regimes and hydraulic interactions of all six deposits. A numerical geofiltration model was previously developed for regional aquifers of the Fergana Valley [22]; however, the present study addresses a different system-level problem by integrating multiple hydrogeological units, sensor-data assimilation, a composite security index, and monitoring-resource optimization within one information-system framework.

This study develops a theoretical and mathematical model layer for a five-layer Big Data information-system architecture previously proposed by the authors. The objective is not to claim completed real-time monitoring of the Zarafshan system, but to formalize the dynamic relationships among the six deposits and evaluate the theoretical properties of the proposed framework, including stability, sensitivity to measurement uncertainty, and resource-allocation optimality. The main methodological contributions are: (1) an indexed water-balance formulation extended to a coupled dynamic system with inter-deposit hydraulic connectivity; (2) a state-space Kalman-filter formulation for fusing sensor observations with model forecasts; (3) a Regional Water Security Index (RWSI) combining data quality, balance deviation, and anomaly evidence, together with an uncertainty-propagation formulation; and (4) a constrained optimization formulation for allocating limited monitoring resources among deposits. These contributions are presented as a theoretical framework and require deposit-specific empirical calibration before operational deployment.

Literature Review

The hydrogeological structure of the Zarafshan valley has been investigated in a range of geological, hydrogeological, and monitoring studies. Earlier works established the geological and tectonic basis of the region, whereas more recent studies have addressed geoinformation technologies, automated monitoring, and hydrogeochemical characterization [1–9]. These studies provide important observational and technological foundations, but the available literature does not yet offer a unified mathematical formulation that simultaneously represents the different recharge mechanisms and hydraulic interactions among the six deposits considered here. The present work

therefore focuses on the mathematical integration of these components rather than on introducing a new physical law.

Technology-oriented studies—including non-invasive scanning [7], automated monitoring [8], GIS-based design [4], remote data transmission from observation wells [2, 3], and geoportal development [5]—strengthen the measurement and communication infrastructure. For the analytical layer, groundwater-flow calculations commonly rely on Darcy's law [15] and Theis-type solutions [16], while spatial interpolation may use geostatistical methods [17] and model performance is evaluated using established statistical criteria [18, 19]. The contribution of the present study is to connect these established tools within a single multi-deposit information-system model. The literature review also indicates the need for additional international references on groundwater data assimilation, uncertainty quantification, and digital hydrogeological monitoring.

Research Methodology

Study area. The study area is the groundwater system of the Zarafshan River valley within Samarkand Region, Uzbekistan. The valley forms an intermontane depression with a complex geological structure and contains six hydrogeological deposits considered in this study (Table 1).

Table 1. Groundwater deposits of the Zarafshan River valley [6]

Deposit	Location
Northern foothill	Southern slope of the Nurata Mountains, Gobduntau upland
Southern foothill	Northern slopes of the Zarafshan and Ziaetdin-Zirabulak mountains
Right bank (Bulungur)	Right bank of the Zarafshan River
Left bank (Samarkand)	Left bank of the Zarafshan River
Zarafshan	Central part of the river valley
Ulus	Western part of the valley

Climatic conditions. The long-term mean annual precipitation is reported as 331 mm/year, while the mean air temperature is 12.9°C at Samarkand and 13.1°C at Kattakurgan. Approximately 70% of annual precipitation occurs during the winter–

spring period, and precipitation increases with elevation at an estimated gradient of 34 mm per 100 m [9]. The elevation is represented by the following linear approximation:

$$P(h) = P_0 + k \cdot h \quad (1)$$

where $P(h)$ is annual precipitation at elevation h , P_0 is the precipitation reference at the valley floor, and k is the estimated altitudinal precipitation gradient (approximately 0.34 mm/m) [9]. Because P_0 varies spatially across the valley, equation (1) should be interpreted as a local linear approximation rather than as a universal regional relationship.

Hydrological conditions: the Zarafshan River has glacier–snow recharge; the ratio of July–September runoff to March–June runoff ranges from 1.1 to 2.9, the glacial flood accounts for 44.7–64.0% of the annual runoff and the snowmelt flood for 21.8–45.1% [9]. *Irrigation conditions:* the total irrigated area within the region is 398.3 thousand hectares (across the Bulungur, Urgut, Nurabad and Tayloq districts), and changes in the irrigation regime have altered the volume of water supply by 15–65% [9].

Deposit-indexed water balance equation.

The aggregated water-balance formulation implicitly treats the six deposits as equivalent. However, the available hydrogeological evidence indicates substantial differences in recharge mechanisms [9]. To represent these differences, an indexed balance equation is formulated for each deposit i ($i = 1, \dots, 6$):

$$\Delta S_i = \alpha_i Q_{irr,i} + \beta_i Q_{riv,i} + \gamma_i Q_{field,i} - Q_{evap,i} - Q_{out,i} \quad (2)$$

where ΔS_i is the change in groundwater storage in deposit i ; $\alpha_i, \beta_i, \gamma_i \in [0, 1]$ are source-contribution coefficients for irrigation-network infiltration, river infiltration, and infiltration from irrigated fields, respectively; $Q_{irr,i}$, $Q_{riv,i}$ and $Q_{field,i}$ are the corresponding inflow volumes; $Q_{evap,i}$ and $Q_{out,i}$ represent evaporation and outflow losses. The coefficients $\alpha_i, \beta_i \rightarrow 0$ should be estimated from deposit-specific observations rather than assumed to be identical across the region within 0.45–0.90 [9].

Equation (2) is a static balance and does not explicitly represent temporal evolution or hydraulic exchange among deposits. It is therefore extended to a coupled dynamic system:

$$\frac{dS_i(t)}{dt} = \sum_{j=1}^6 a_{ij}S_j(t) + b_i u_i(t) \quad (3)$$

where $S_i(t)$ is groundwater storage in deposit i , a_{ij} is the hydraulic-connectivity coefficient from deposit j to deposit i , and $b_i u_i(t)$ represents the aggregate external forcing for deposit i . For $i \neq j$, a_{ij} can be related to lateral hydraulic conductance derived from Darcy's law; for $i = j$, the diagonal term represents net self-drainage or internal loss. In vector form, the system is $dS/dt = AS(t) + Bu(t)$, where $A \in \mathbb{R}^N$ is the connectivity matrix. Under the linear time-invariant assumption, the system is asymptotically stable if all eigenvalues of A have negative real parts. This is a theoretical stability criterion and does not by itself establish that the real aquifer system is stable.

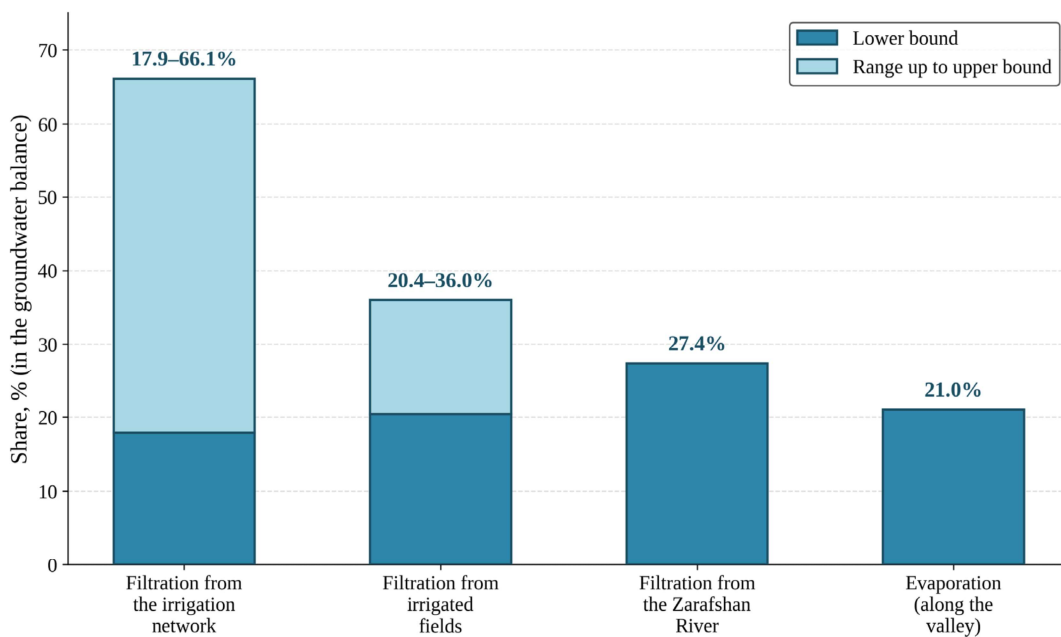


Figure 1. Component shares of the groundwater balance of the Zarafshan River valley (aggregated over the region, [9]).

To connect the precipitation–elevation relationship in equation (1) with groundwater storage, a dimensionless natural-recharge coefficient is introduced as:

$$\mu_i = \frac{\Delta S_i}{A_i P(h_i)} \quad (4)$$

where μ_i is the dimensionless natural-recharge coefficient, A_i is the effective recharge area of deposit i , and h_i is its representative elevation. Including A_i is necessary for dimensional consistency because ΔS_i is a volume whereas $P(h_i)$ is a length. The coefficient μ_i can subsequently be estimated from long-term observations.

Technical chain of the information system. Technical chain of the information system. Submersible water-level sensors and electrical-conductivity (EC) sensors are assumed to be installed in observation wells and connected to remote transmission units based on microcontrollers and GSM/GPRS communication [2]. Measurements are transmitted using MQTT to a central broker and then forwarded to Apache Kafka and Apache Spark for distributed stream processing. This architecture is motivated by the need for low-power communication at remote observation wells. A related sensor-and-telemetry configuration has been tested at 32 observation wells in the Chirchiq groundwater deposit [20]. The ToF sensor results reported in [21] are used here only to define a plausible order of magnitude for measurement uncertainty; they are not presented as measurements from the Zarafshan study area.

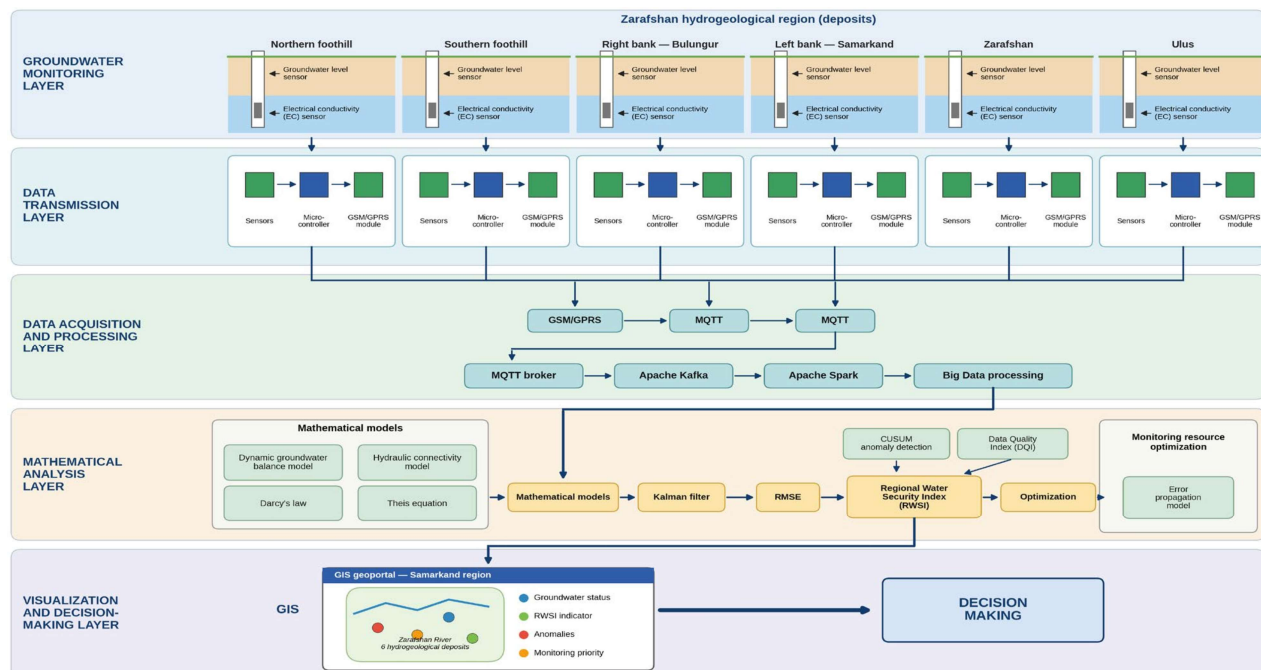


Figure 2. Conceptual architecture of the system for assessing and managing hydrogeological processes based on Big Data technologies (case of the Zarafshan River valley).

In the storage layer, each hydrogeological deposit is represented as a spatial entity in a PostGIS database. This organization allows the coefficients α_i , β_i , γ_i , and μ_i to be

estimated and updated separately for each deposit. The visualization layer presents all six deposits in a GIS-based geoportal together with the estimated indicators.

The proposed information system uses a five-layer architecture integrating IoT, Big Data processing, mathematical modeling, and GIS visualization. The architecture covers the chain from field measurement to data transmission, stream processing, mathematical analysis, and decision support. Its purpose is to provide a formal computational framework in which deposit-specific observations can be incorporated into regional groundwater assessment. The first layer represents groundwater monitoring at the six deposits using water-level and EC sensors. The second layer provides data transmission through microcontrollers and GSM/GPRS modules. The third layer performs data acquisition and stream processing using MQTT, Apache Kafka, and Apache Spark. The fourth layer is the mathematical-analysis layer, where the dynamic water-balance model, Darcy-based hydraulic relationships, anomaly detection, and Kalman data assimilation are applied. The fifth layer provides GIS visualization and decision support. CUSUM is used for change detection, while RMSE is used for forecast-error assessment.

The outputs of the mathematical-analysis layer are summarized by the Data Quality Index (DQI) and the Regional Water Security Index (RWSI). These indicators feed the uncertainty-propagation analysis and the monitoring-resource optimization problem. The final visualization layer displays the resulting indicators and anomaly signals in a GIS geoportal.

Hydraulic and statistical apparatus. The filtration parameters of each deposit are estimated using the classical Darcy's law [15]:

$$v = -K \frac{dh}{dl} \quad (5)$$

where b is the saturated aquifer thickness, S_y is the specific yield, and S_s is the specific storage coefficient. The drawdown induced by pumping is represented using the Theis solution [16]:

$$T = K \cdot b, \quad S = S_y + S_s \cdot b \quad (6)$$

where b is the saturated thickness of the aquifer, S_y is the specific yield and S_s is the specific storage. The drawdown during pumping is predicted by the Theis equation [16]:

$$s(r, t) = \frac{Q}{4\pi T} W(u), \quad u = \frac{r^2 S}{4Tt} \quad (7)$$

For spatial interpolation of groundwater levels between observation points, the semivariogram is defined as:

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [z(x_i) - z(x_i + h)]^2 \quad (8)$$

where $N(h)$ is the number of point pairs separated by lag distance h and $z(x_i)$ is the observed groundwater level at location x_i . Inverse distance weighting (IDW) is considered as an alternative interpolation method:

$$\hat{z}(x_0) = \sum_{i=1}^n \omega_i z(x_i), \quad \omega_i = \frac{d_i^{-p}}{\sum_{j=1}^n d_j^{-p}} \quad (9)$$

For early detection of persistent shifts in monitored variables, a one-sided CUSUM procedure is applied. An alarm is generated when C_t exceeds the predefined threshold C_{cr} :

$$C_t = \max(0, C_{t-1} + (x_t - m_0) - \kappa) \quad (10)$$

where x_t is the current observation, m_0 is the baseline mean, and κ is the reference (sensitivity) parameter. The Data Quality Index (DQI) is defined as a weighted mean of completeness, accuracy, timeliness, and consistency:

$$DQI = \frac{\lambda_1 Com + \lambda_2 Acc + \lambda_3 Tim + \lambda_4 Con}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \quad (11)$$

where Com , Acc , Tim , and $Con \in [0, 1]$ denote completeness, accuracy, timeliness, and consistency, respectively, and $\lambda_1, \dots, \lambda_4$ are non-negative weights. The forecast error is evaluated using the root mean square error (RMSE):

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (12)$$

where $\hat{y}_i$ and y_i are predicted and observed values, respectively, and n is the number of observations. For time-series applications, the test set must be separated chronologically from the training data to avoid temporal leakage.

Regional Water Security Index, real-time assessment and resource optimization.

To combine data quality, water-balance deviation, and anomaly evidence into a single decision-support indicator, the Regional Water Security Index (RWSI) is defined as:

$$RWSI_i = w_1(1 - DQI_i) + w_2 \frac{|\Delta S_i|}{\Delta S_{\max}} + w_3 \min\left(1, \frac{C_i}{C_{cr}}\right) \quad (13)$$

where $w_1, \dots, w_3$ are non-negative weights satisfying $w_1 + w_2 + w_3 = 1$; $\Delta S_{\max}$ is a reference maximum absolute balance deviation; and C_{cr} is the CUSUM alarm threshold. The index is scaled to $[0, 1]$ under the stated normalization. Higher RWSI values indicate greater theoretical instability or monitoring concern; the index should be interpreted only after its weights and reference scales have been empirically calibrated.

Computing the RWSI in real time requires an estimate of the current storage state. Because the dynamic model provides a forecast while sensor observations contain measurement error, a discrete state-space Kalman filter is used to combine them. For the six-deposit coupled system, the full covariance-matrix formulation is preferable to a scalar approximation.

$$F = I + A\Delta t, \quad B_d = B\Delta t$$

$$\hat{S}_{i,k}^- = \hat{S}_{i,k-1} + \Delta t \left(\sum_{j=1}^6 a_{ij} \hat{S}_{j,k-1} + b_i u_{i,k-1} \right), \quad P_{i,k}^- = (1 + a_{ii}\Delta t)^2 P_{i,k-1} + q_i$$

where q_i is the six-dimensional storage-state vector, $F = I + A\Delta t$ is the first-order discrete transition matrix, $B_d = B\Delta t$ is the discretized input matrix, and $u_{i,k-1}$ is the external forcing vector.

The prediction-error covariance is propagated as:

$$\hat{S}_{i,k} = \hat{S}_{i,k}^- + K_{i,k}(z_{i,k} - \hat{S}_{i,k}^-) \quad (15)$$

The Kalman gain and state-update equations are then:

$$K_{i,k} = \frac{P_{i,k}^-}{P_{i,k}^- + R_i}, \quad P_{i,k} = (1 - K_{i,k})P_{i,k}^- \quad (16)$$

where P_{k-} is the predicted covariance matrix, Q is the process-noise covariance, H is the observation matrix, R is the measurement-noise covariance, and z_k is the vector of sensor observations. This matrix formulation explicitly preserves the coupling among deposits and avoids treating the six-state system as six independent scalar filters.

To illustrate the magnitude of the measurement-noise term, the published ToF sensor in [21] reported an MAE of 0.048 m over a 12-month field test. If the

measurement error is approximately Gaussian with zero mean, its variance can be approximated by $R \approx (\pi/2) \cdot \text{MAE}^2 \approx 0.0036 \text{ m}^2$. Assuming, for illustration, a predicted variance of $P^- \approx 0.01 \text{ m}^2$ in a scalar component, the corresponding scalar Kalman gain is approximately 0.73. This calculation is illustrative rather than a calibration of the Zarafshan system; deposit-specific R values should be estimated from the actual sensors deployed in the study area.

The numerical example therefore indicates that, under the assumed variances, approximately 73% of the scalar update weight is assigned to the measurement and 27% to the model forecast. The result is sensitive to the assumed forecast and measurement-error variances, which should be estimated empirically in the operational system. The 99.4% detection rate reported in [21] may provide a reference for sensor completeness, but it should not be directly transferred to the DQI of the Zarafshan network without local validation. The robustness of the RWSI with respect to errors in its input quantities (including the variance $P_{i,k}$ inherited from the Kalman filter) is assessed using the law of error propagation (assuming independent errors):

$$R \approx (\pi/2) \text{MAE}^2 \approx 0.0036 \text{ m}^2, \quad K \approx 0.01/(0.01 + 0.0036) \approx 0.73 \quad (17)$$

where $\sigma^2(\Delta S)$ is the variance of the balance change, $\partial(\Delta S)/\partial Q_m$ is the sensitivity of the balance to source m , and $\sigma^2(Q_m)$ is the corresponding measurement-error variance. Under the independent-error assumption, the source contributions are additive. Because the partial derivatives are α_i , β_i , or γ_i for the corresponding inflow terms, measurement errors in sources with large contribution coefficients can dominate the uncertainty of ΔS_i . To support practical decision-making, the allocation of a limited monitoring budget is formulated as a constrained optimization problem:

$$\begin{aligned} \min \sum_{i=1}^6 RWSI_i(x_i), \quad \sum_{i=1}^6 c_i x_i \leq B, \quad x_i \geq 0 \\ \sigma^2(\Delta S) = \sum_m \left(\frac{\partial(\Delta S)}{\partial Q_m} \right)^2 \cdot \sigma^2(Q_m) \end{aligned} \quad (18)$$

where x_i is the monitoring resource allocated to deposit i (e.g., the number of additional sensors or measurement frequency), c_i is the unit cost, and B is the total available budget.

If $RWSI_i(x_i)$ is decreasing and convex, the problem is convex. Under these assumptions, the Karush–Kuhn–Tucker conditions imply that the marginal reduction in regional risk per unit cost is equal across all deposits receiving positive allocations.

Results and Discussion

The theoretical analysis of equation (2) suggests two broad recharge regimes. The Northern and Southern foothill deposits are expected to be more strongly influenced by natural recharge; under $\alpha_i, \beta_i \rightarrow 0$, their balance approaches $\Delta S_i \approx \gamma_i Q_{\text{field},i} - Q_{\text{evap},i} - Q_{\text{out},i}$, subject to the limitations of the underlying assumptions. The Bulungur, Samarkand, Zarafshan, and Ulus deposits are expected to be more strongly influenced by irrigation and river infiltration and may exhibit stronger inter-deposit coupling through the Zarafshan River. The regional source shares reported in [9] can be used as initial bounds, but deposit-specific values of $\alpha_i, \beta_i, \gamma_i, \mu_i$, and a_{ij} require calibration using long-term observations. The uncertainty-propagation analysis indicates that, in irrigation-dominated deposits, errors in measurements with large source-contribution coefficients can make a substantial contribution to $\sigma^2(\Delta S)$. The Kalman filter provides a principled mechanism for weighting observations according to their estimated uncertainty. Consequently, improving the accuracy of high-contribution inflow measurements is theoretically expected to provide greater benefit to the RWSI than improving measurements of low-contribution sources, subject to the actual covariance structure of the system. The limiting behavior of the RWSI follows directly from its normalization: if DQI approaches 1, $|\Delta S_i|$ approaches 0, and the CUSUM signal remains well below the alarm threshold, then $RWSI_i$ approaches 0. Conversely, poor data quality, large balance deviation, and a strong anomaly signal drive the index toward 1. Illustrative thresholds such as $RWSI < 0.3$, $0.3\text{--}0.6$, and > 0.6 may be used for exploratory visualization, but these thresholds are not validated decision boundaries and should not be presented as operational criteria before empirical calibration. Relative to the regional studies summarized in Table 2, the principal contribution of this work is the integration of deposit-specific water balance, inter-deposit hydraulic coupling, state estimation, uncertainty assessment, and monitoring-resource optimization in a single mathematical framework. The distinction between theoretical formulation and empirical

validation is essential: the present article establishes the model structure and analytical consequences, whereas parameter calibration and operational validation remain future tasks. Practical significance. The proposed framework provides an explicit mathematical criterion for prioritizing monitoring resources among hydrogeological deposits. Limitations. The coefficients α_i , β_i , γ_i , μ_i , and a_{ij} , the weights w_1 , w_2 , w_3 , and the RWSI reference scales are not empirically calibrated for all six deposits in the present study. The ToF example in [21] concerns a different field deployment and is used only to illustrate uncertainty propagation.

Table 2. Comparison of regional approaches

Study	Scope
Normamatov, Abdullayev [7]	One district (Nurabad); scanning equipment, no model
Mardiyev, To‘rayeva [8]	Automated monitoring; differences between deposits not considered
Khabibullayev et al. [4]	GIS-based design; no balance equation
This study Six deposits: coupled dynamic system + Kalman filter + RWSI + constrained optimization	Six deposits: dynamic system + Kalman filter + RWSI + optimization (18 models)

Future work should estimate all deposit-specific parameters from long-term observations, validate the full Kalman filter with the actual sensor network, test the sensitivity of the RWSI to alternative weighting schemes, and compare the proposed framework with established groundwater-assimilation and uncertainty-quantification methods.

Conclusion and Recommendations

A theoretical and mathematical Big-Data-based information-system model has been formulated for groundwater management in the Zarafshan River valley, Samarkand Region. The conventional water-balance equation was extended to a deposit-indexed formulation and then to a coupled dynamic system representing hydraulic connectivity among six hydrogeological deposits. A full state-space Kalman-filter formulation was introduced to combine model forecasts with noisy sensor observations, while the

Regional Water Security Index (RWSI), its uncertainty-propagation model, and a constrained monitoring-resource optimization problem provide a decision-support layer. A numerical illustration based on published ToF sensor performance gives a scalar Kalman gain of approximately 0.73 under the stated variance assumptions; this value is illustrative and not a site-specific calibration. The theoretical analysis distinguishes deposits by dominant recharge mechanisms and identifies how source-contribution coefficients affect uncertainty. The framework provides a basis for subsequent empirical calibration and operational validation using long-term Zarafshan groundwater observations.

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COMPARATIVE ANALYSIS OF HIGH-PURITY SELENIUM RECOVERY TECHNOLOGIES: EFFICIENCY AND ENVIRONMENTAL ASPECTS

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Annotatsiya. Selen yarimo'tkazgichli qurilmalar, fotoelektrik tizimlar, shisha ishlab chiqarish, metallurgiya va kataliz sohalarida keng qo'llaniladigan, texnologik jihatdan muhim element hisoblanadi. Selen birlamchi mineral konlardan kamdan-kam olinishi sababli uning sanoat miqyosidagi ishlab chiqarilishi, asosan, mis, qo'rg'oshin-rux va boshqa polimetall xomashyolarni qayta ishlash bilan bog'liq. Ushbu tadqiqotda ilgari e'lon qilingan tajribaviy va texnologik ma'lumotlar asosida selenni vakuum sharoitida tozalash samaradorligi baholangan hamda natijalar adabiyotlarda keltirilgan muqobil gidrometallurgik ajratib olish usullari bilan taqqoslangan. Selenning tozalik darajasi, aralashmalarni chiqarib tashlash samaradorligi, ajratib olish darajasi, ishchi bosim, harorat, jarayon davomiyligi va energiya sarfiga alohida e'tibor qaratilgan. Tahlil qilingan ma'lumotlarga ko'ra, vakuumda tozalash natijasida selen miqdori 99,4% dan 99,992% gacha oshgan. Bu mutlaq hisobda 0,592 foiz punktiga va nisbiy hisobda taxminan 0,596% ga o'sishni tashkil etadi. Aralashmalarning umumiy konsentratsiyasi 2 997,38 ppmw dan 79,08 ppmw dan past qiymatgacha kamaygan. Bu aralashmalarni chiqarib tashlash samaradorligi kamida 97,36% ni, tozalash koeffitsiyenti esa kamida taxminan 37,9 ni tashkil etganini ko'rsatadi.

Kalit so'zlar: selen, vakuum distillatsiyasi, selenni tozalash, aralashmalarni chiqarib tashlash, tozalash koeffitsiyenti, selenni ajratib olish, yuqori tozalikdagi selen, energiya sarfi, gidrometallurgiya, qiyosiy tahlil.

Аннотация. Селен является технологически важным элементом, широко применяемым в полупроводниковых устройствах, фотоэлектрических системах, производстве стекла, металлургии и катализе.

Поскольку селен редко получают из первичных минеральных месторождений, его промышленное производство преимущественно связано с переработкой медного, свинцово-цинкового и другого полиметаллического сырья. В настоящем исследовании на основе ранее опубликованных экспериментальных и технологических данных оценена эффективность вакуумной очистки селена, а полученные результаты сопоставлены с альтернативными гидрометаллургическими способами его извлечения, описанными в литературе. Особое внимание уделено чистоте селена, удалению примесей, степени извлечения, рабочему давлению, температуре, продолжительности процесса и энергопотреблению. Анализируемые данные показывают, что вакуумная очистка позволила повысить содержание селена с 99,4 до 99,992%, что соответствует абсолютному увеличению на 0,592 процентного пункта и относительному увеличению приблизительно на 0,596%. Суммарная концентрация примесей снизилась с 2 997,38 ppmw до уровня ниже 79,08 ppmw, что соответствует эффективности удаления примесей не менее 97,36% и минимальному коэффициенту очистки приблизительно 37,9.

Ключевые слова: селен, вакуумная дистилляция, очистка селена, удаление примесей, коэффициент очистки, извлечение селена, высокочистый селен, энергопотребление, гидрометаллургия, сравнительный анализ.

Abstract. Selenium is a technologically important element widely used in semiconductor devices, photoelectric systems, glass production, metallurgy, and catalyst applications. Because selenium is rarely obtained from primary mineral deposits, its industrial production is mainly associated with the processing of copper, lead-zinc, and other polymetallic raw materials. This study evaluates the purification performance of vacuum-based selenium processing using previously reported experimental and technological data and benchmarks the results against alternative hydrometallurgical selenium recovery routes described in the literature. Particular attention is given to selenium purity, impurity removal, recovery, operating pressure, temperature, processing duration, and energy consumption. The

analyzed data show that vacuum purification increased selenium content from 99.4% to 99.992%, corresponding to an absolute increase of 0.592 percentage points and a relative increase of approximately 0.596%. The total impurity concentration decreased from 2,997.38 ppmw to below 79.08 ppmw, corresponding to an impurity removal efficiency of at least 97.36% and a minimum purification factor of approximately 37.9.

Keywords: selenium, vacuum distillation, selenium purification, impurity removal, purification factor, selenium recovery, high-purity selenium, energy consumption, hydrometallurgy, comparative analysis.

Introduction

Selenium is an important technological element with applications in semiconductor electronics, photoelectric devices, electro-photographic systems, glass manufacturing, metallurgy, and catalyst production. Selenium compounds are also used in the preparation of selenides and phosphors. The combination of its electrical, optical, and chemical properties makes high-purity selenium particularly valuable for advanced technological applications [1]. Although approximately 40 selenium-containing minerals have been identified, selenium is rarely recovered from dedicated primary deposits. The principal industrial sources of selenium are therefore associated with the processing of copper, copper-nickel, and lead-zinc concentrates. Copper electrorefining anode slimes represent one of the important secondary sources because selenium is concentrated during the metallurgical treatment of copper-bearing materials [1, 2].

Because selenium is recovered almost entirely as a byproduct of copper electrorefining, both the scale and the geographic distribution of its production are closely linked to the copper industry. China alone accounted for close to half of the estimated global refined selenium output in 2024 [8], which underlines the practical relevance of purification technologies that can be implemented efficiently wherever copper-refining capacity exists, including emerging producing regions such as Central Asia. Selenium recovery from secondary metallurgical resources is complicated by the presence of accompanying elements such as copper, lead, iron, arsenic, tellurium, mercury, silver, and gold. Consequently, selenium purification requires a process

capable of separating selenium from these accompanying components while maintaining high recovery. Thermal and electrochemical methods have been investigated for selenium recovery, while vacuum distillation provides a route based on differences in volatility between selenium and less volatile components [3–10].

Recent advancements in sustainable pyrometallurgy emphasize that vacuum distillation routes provide superior environmental compliance compared to traditional hydrometallurgical extraction, effectively avoiding acid-intensive wastewater generation while achieving high recovery rates for critical elements [6–8]. A recent comprehensive review has similarly emphasized that oxidation-reduction methods, vacuum distillation, zone melting, and hydrogenation each play complementary roles in meeting increasingly stringent purity requirements for high-technology applications, and that research interest in selenium and tellurium purification has grown accordingly across these different pathways [10].

Research Methodology

1. Research Design. This study was conducted as a comparative analytical evaluation of previously reported experimental and technological data related to vacuum-based selenium recovery and purification, supplemented by independently reported hydrometallurgical selenium recovery data used for benchmarking purposes. The analysis focused primarily on vacuum treatment of selenium-containing metallurgical materials and crude selenium.

The investigated parameters included initial and final selenium purity, total impurity concentration, selenium recovery, direct yield, operating temperature, pressure, processing duration, and energy consumption. The numerical values used in the analysis were obtained from the reported data and were not treated as newly generated experimental measurements.

2. Evaluation Parameters. The purification performance was evaluated using selenium enrichment, impurity removal efficiency, purification factor, selenium recovery or direct yield, and energy consumption. The relative increase in selenium concentration was calculated from the difference between the final and initial selenium contents relative to the initial selenium content. Impurity removal efficiency was calculated from the

reduction in total impurity concentration relative to the initial impurity concentration. Because the final impurity concentration was reported as below 79.08 ppmw, 79.08 ppmw was used as the upper-limit value for the calculation; consequently, the calculated impurity removal represents a minimum value. The purification factor was determined as the ratio of the initial impurity concentration to the upper-limit final impurity concentration. Energy consumption was additionally converted from kilowatt-hours per tonne to kilowatt-hours per kilogram to provide a more direct technological measure.

Results and Discussion

1. Selenium Enrichment during Vacuum Purification. The analyzed vacuum purification data demonstrate a substantial increase in selenium concentration. Crude metallurgical selenium containing 99.4% Se was purified to 99.992% Se after triple consecutive vacuum distillation [5].

The absolute increase in selenium concentration was calculated as 0.592 percentage points, while the relative increase with respect to the initial selenium concentration was approximately 0.596%. Although the numerical increase in selenium concentration appears relatively small because the initial material already contained a high proportion of selenium, the change is technologically significant in the context of high-purity selenium production, where even small reductions in impurity content can substantially improve the final product quality.

2. Comparative Technological Characteristics. The principal reported and calculated characteristics of the investigated vacuum-based selenium purification processes are summarized in Table 1. The results demonstrate that the purification performance of vacuum treatment can be described through several complementary parameters. The highest reported selenium purity was 99.992% [5], while the calculated impurity removal efficiency was at least 97.36% [5].

The minimum purification factor of 37.9 further indicates the substantial reduction of accompanying impurities [5]. At the same time, the reported recovery and direct-yield values show that high selenium recovery can be achieved under appropriate technological conditions [4, 6].

Table 1. Comparative characteristics of selenium recovery and purification technologies

Parameter	Selenium sludge treatment	Triple vacuum distillation	Industrial vacuum process
Initial selenium content	—	99.4%	—
Final selenium purity	98.68%	99.992%	>98.0%
Selenium recovery/direct yield	90.76%	—	>96.5%
Initial total impurities	—	2,997.38 ppmw	—
Final total impurities	—	<79.08 ppmw	—
Minimum impurity removal	—	≥97.36%	—
Minimum purification factor	—	≥37.9	—
Temperature	693 K	~523 K	—
Pressure	30–50 Pa	~4 Pa	—
Processing time	90 min	—	—
Energy consumption	—	—	~1,150 kWh/t
Energy consumption per kg	—	—	~1.15 kWh/kg

Note: a dash (—) in Table 1 indicates that the corresponding parameter was not reported for that process in the source study, not that its value was zero or negligible. Because the three processes were reported in different studies under different conditions, the table juxtaposes rather than directly compares them.

3. Comparison with Hydrometallurgical Selenium Recovery Routes

To place the vacuum-based purification results in a broader technological context, they were compared with representative hydrometallurgical selenium recovery data reported independently in the literature. Table 2 summarizes selenium recovery, principal reagents, operating conditions, and byproduct handling for a reported alkaline hydrometallurgical leaching process [10], a multi-stage acid-based hydrometallurgical process [9], and the vacuum-based routes examined in Sections 3.3–3.4 [4].

Table 2. Comparison of vacuum-based and hydrometallurgical selenium recovery routes reported in the literature

Parameter	Alkaline hydrometallurgical leaching	Multi-stage acid hydrometallurgical process	Vacuum sludge treatment	Industrial vacuum process
Selenium recovery / yield	~86.8%	92.9% (Se); 95.8% Cu, 99.1% Au, 99.4% Ag, 99.8% Pb	90.76%	>96.5%
Principal reagents	NaOH solution, oxidant	H ₂ SO ₄ –H ₂ O ₂ ; NaClO ₃ –HCl–NaCl; Na ₂ SO ₃	None (physical separation)	None (physical separation)
Temperature	~90 °C	Not specified (ambient/near-ambient leaching)	693 K	—
Pressure	Atmospheric	Atmospheric	30–50 Pa	—
Process character	Multi-step leaching and precipitation	Multi-step leaching, reduction and precipitation	Single-step vacuum distillation	Single-step vacuum distillation
Reported byproduct handling	Aqueous alkaline leach effluent [6, 8]	Aqueous acid leach effluent [6, 8]	No liquid effluent; solid residue enriched in Ag, Au	No liquid effluent

Note: cell entries reproduce values and process descriptions as reported in the cited sources.

Alkaline leaching of copper anode slime in sodium hydroxide solution has been reported to achieve selenium recovery of approximately 86.8%, together with 94% copper recovery, under atmospheric-pressure conditions at approximately 90 °C [12]. This value is lower than the 90.76% selenium recovery reported for vacuum treatment of selenium sludge [4] and considerably lower than the >96.5% direct yield reported for the industrial vacuum process [4]. More recent multi-stage hydrometallurgical processes, which combine acid leaching with sequential chemical reduction and

precipitation to recover selenium, copper, gold, and silver from a single slime feed, have been developed specifically to improve the overall economics and cleanliness of the hydrometallurgical route, achieving a reported selenium recovery of approximately 92.9%, together with 95.8% copper, 99.1% gold, 99.4% silver, and 99.8% lead recovery under optimal conditions [10]. Beyond the numerical recovery values, an important distinction between the two technological families concerns process structure and byproduct handling. Hydrometallurgical routes generally require several sequential reagent-addition, leaching, and precipitation stages, together with the disposal or downstream treatment of the resulting aqueous leachate [6, 8, 11, 10]. In contrast, the vacuum-based routes examined in this study rely on a single physical separation step that does not consume chemical reagents and does not generate a liquid effluent [4, 6, 8]. This distinction is consistent with the broader technological comparison presented in Section 4 and supports the view, expressed in recent reviews, that vacuum distillation offers particular advantages in impurity removal and elimination of chemical effluents, even in cases where the reported selenium recovery of hydrometallurgical routes is of a comparable order of magnitude [8, 9].

Results and Discussion

The results indicate that the effectiveness of vacuum-based selenium purification should be evaluated using both product purity and impurity removal rather than selenium concentration alone. The increase from 99.4% to 99.992% Se represents an absolute increase of 0.592 percentage points and a relative increase of approximately 0.596% [5]. In a high-purity material, however, this apparently small increase corresponds to a substantial reduction in the concentration of non-selenium components [5]. The calculated impurity removal efficiency of at least 97.36% and purification factor of approximately 37.9 demonstrate that the principal purification effect is associated with the removal of accompanying impurities rather than a large increase in the selenium fraction itself [5]. This distinction is important when evaluating technologies intended for the production of high-purity selenium.

The vacuum process applied to selenium sludge demonstrated 90.76% selenium recovery at approximately 693 K and 30–50 Pa for 90 min, with a product purity of

98.68% [4]. The reported industrial process achieved a direct selenium yield exceeding 96.5% and a product purity exceeding 98.0%, while the reported energy consumption was approximately 1,150 kWh/t, equivalent to 1.15 kWh/kg of selenium ingot [4]. These values are consistent with the broader performance range described for vacuum distillation routes in the wider literature [7], and together indicate that vacuum processing can combine substantial selenium recovery with comparatively high product quality [4, 6]. The triple vacuum distillation results provide additional evidence of the purification potential of repeated treatment [5]. Under approximately 4 Pa and around 523 K, crude selenium containing 99.4% Se was purified to 99.992% Se, while total impurity concentration decreased from 2,997.38 ppmw to below 79.08 ppmw [5]. The calculated minimum impurity removal of 97.36% and purification factor of 37.9 quantitatively describe this improvement [5]. The different operating conditions reported for selenium sludge treatment and triple vacuum distillation also indicate that vacuum pressure and temperature are important components of the technological process [4, 5]. However, because the reported results originate from different studies and different starting materials, the available data do not allow the independent effect of temperature or pressure to be established quantitatively [4, 5]. Therefore, these parameters should not be interpreted as results of a controlled optimization experiment.

From a technological perspective, the ability to concentrate silver and gold in the non-volatile residue during selenium sludge treatment provides an additional feature of the vacuum process [4, 6]. The process therefore has relevance not only to selenium recovery but also to the subsequent treatment of the residual fraction [4, 6]. This feature is corroborated by an independent semi-industrial study, in which vacuum distillation of crude selenium concentrated gold and silver in the residue with direct recovery yields of 99.72% and 99.56%, respectively, representing enrichment of more than 20 times [9].

The comparison with hydrometallurgical selenium recovery presented in Section 3.7 further situates the vacuum-based results within the broader landscape of selenium-recovery technology. The 90.76–96.5% recovery reported for vacuum-based routes [4] compares favorably with the 86.8% selenium recovery reported for alkaline hydrometallurgical leaching [9], while requiring no leaching reagents and generating no

aqueous effluent. Even the more recent, reagent-optimized hydrometallurgical schemes designed to recover selenium together with copper, gold, and silver from a single slime feed still rely on multiple sequential chemical stages [10], underscoring a structural, rather than purely incremental, difference between the two technological families. This comparison should nonetheless be interpreted with the same caution applied throughout this study: the compared processes were reported for different feedstocks, scales, and operating conditions, and the observed differences in recovery and process complexity are indicative rather than the result of a controlled head-to-head trial.

Overall, the analyzed results demonstrate that vacuum-based purification can substantially reduce impurity concentrations while maintaining high selenium recovery that is competitive with, or exceeds, reported hydrometallurgical alternatives [4, 5, 10]. The calculated purification parameters provide a useful basis for evaluating the effectiveness of the process and demonstrate that impurity removal is a critical factor in achieving high-purity selenium [5].

Conclusion and Recommendations

The analysis of reported vacuum-based selenium purification data demonstrates that the technology can provide substantial improvement in product quality through effective removal of accompanying impurities [4, 5]. Triple consecutive vacuum distillation increased selenium content from 99.4% to 99.992%, corresponding to an absolute increase of 0.592 percentage points and a relative increase of approximately 0.596% [5]. At the same time, total impurity concentration decreased from 2,997.38 ppmw to below 79.08 ppmw [5]. Based on the reported upper-limit final impurity concentration, the calculated impurity removal efficiency was at least 97.36%, corresponding to a minimum purification factor of approximately 37.9 [5]. Vacuum treatment of selenium sludge achieved 90.76% selenium recovery at 693 K, 30–50 Pa, and 90 min [4], while the reported industrial process demonstrated a direct selenium yield exceeding 96.5% and an energy consumption of approximately 1.15 kWh/kg of selenium ingot [4].

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DEVELOPMENT OF A THICKENING PROCESS FOR GOLD-BEARING FLOTATION CONCENTRATES WITH CLARIFIED LIQUID RECOVERY

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Annotatsiya. Mazkur maqolada tarkibida oltin bo'lgan flotatsiya konsentratlarini quyultirish jarayonini takomillashtirish hamda yuqori darajada tiniqlangan quyilma (sliv) olish texnologiyasining ilmiy-amaliy asoslari ko'rib chiqiladi. Oltinli flotatsiya mahsulotlarini keyingi metallurgik qayta ishlashga tayyorlashda qattiq va suyuq fazalarni samarali ajratish, pulpaning qattiq faza konsentratsiyasini oshirish va texnologik suvni qayta foydalanish imkonini beradigan sifatli quyilma olish muhim ahamiyatga ega. Ayniqsa, mayda dispers zarrachalarning mavjudligi ularning cho'kish tezligini pasaytirib, quyultirish jarayonining samaradorligini kamaytirishi mumkin.

Tadqiqotning asosiy yo'nalishi sifatida flotatsiya konsentratining fizik-kimyoviy va granulometrik xususiyatlarini aniqlash, flokulyant turini va optimal sarfini tanlash, pulpa konsentratsiyasining cho'kish jarayoniga ta'sirini baholash, quyilmaning tiniqligi hamda quyultirilgan mahsulotning qattiq faza miqdorini aniqlash nazarda tutiladi. Zamonaviy tadqiqotlarda oltinli mayda dispers materiallarni flokulyatsion quyultirishda flokulyant sarfi va pulpa konsentratsiyasi cho'kish kinetikasiga sezilarli ta'sir ko'rsatishi qayd etilgan.

Kalit so'zlar: oltin, flotatsiya konsentrati, quyultirish, flokulyatsiya, quyilma, sliv, pulpa, cho'kish tezligi, flokulyant, qattiq faza konsentratsiyasi, quyultirgich.

Аннотация. В статье рассматриваются научно-практические основы совершенствования процесса сгущения золотосодержащих флотационных концентратов и технологии получения высокоосветлённого слива. При подготовке продуктов флотации золотосодержащего сырья к последующей

металлургической переработке важное значение имеют эффективное разделение твёрдой и жидкой фаз, повышение концентрации твёрдой фазы в пульпе и получение качественного слива, позволяющего повторно использовать технологическую воду. Наличие тонкодисперсных частиц может снижать скорость их осаждения и эффективность сгущения.

Основные направления исследования предусматривают определение физико-химических характеристик и гранулометрического состава флотационного концентрата, выбор типа флокулянта и его оптимального расхода, оценку влияния концентрации пульпы на процесс осаждения, а также определение прозрачности слива и содержания твёрдой фазы в сгущённом продукте. В современных исследованиях отмечается существенное влияние расхода флокулянта и концентрации пульпы на кинетику осаждения при флокуляционном сгущении тонкодисперсных золотосодержащих материалов.

Ключевые слова: золото, флотационный концентрат, сгущение, флокуляция, осветлённый слив, пульпа, скорость осаждения, флокулянт, концентрация твёрдой фазы, сгуститель.

Abstract. This article examines the scientific and practical foundations for improving the thickening of gold-bearing flotation concentrates and developing a process for producing a highly clarified overflow. Efficient solid–liquid separation, increased slurry solids concentration, and the production of a high-quality overflow suitable for process-water reuse are important in preparing gold-bearing flotation products for subsequent metallurgical processing. In particular, finely dispersed particles may settle slowly, thereby reducing thickening efficiency.

The principal research objectives include characterising the physicochemical properties and particle-size distribution of the flotation concentrate, selecting the flocculant type and optimal dosage, assessing the influence of slurry solids concentration on sedimentation, and determining overflow clarity and underflow solids content. Recent studies indicate that flocculant dosage and slurry solids

concentration significantly influence settling kinetics during the flocculation-assisted thickening of finely dispersed gold-bearing materials.

Key words: *gold, flotation concentrate, thickening, flocculation, clarified overflow, slurry, settling velocity, flocculant, solids concentration, thickener.*

Introduction

Flotation is an important method for concentrating gold associated with sulfide minerals and other mineral phases during the beneficiation of gold-bearing ores. In addition to valuable components, the resulting concentrate may contain finely dispersed mineral particles, water, and residual process reagents. Efficient solid–liquid separation is therefore an essential processing step before the concentrate proceeds to subsequent treatment. Thickening increases the solids concentration of a slurry and recovers a relatively clear liquid phase through gravitational settling, which may be enhanced by flocculation. Gravity thickening remains a widely used, high-throughput process for continuous solid–liquid separation in modern mineral processing. However, settling becomes more challenging when the material contains a substantial proportion of fine particles. Under these conditions, flocculants can enhance sedimentation by promoting particle aggregation. Studies on gold-bearing materials have shown that polyacrylamide-based flocculants can increase the settling velocity of fine particles. Accordingly, identifying optimal operating parameters for the efficient thickening of gold-bearing flotation concentrates and the production of a high-quality overflow suitable for reuse in the processing circuit constitutes an important scientific and practical challenge.

Research Aim. The primary aim of this study is to identify operating parameters that enable the efficient thickening of gold-bearing flotation concentrate, enhance the settling of solid particles, and produce a clarified overflow containing minimal suspended solids. To achieve this aim, the study will examine the physicochemical principles governing thickening, determine the optimal flocculant type and dosage, and evaluate the effects of slurry solids concentration and other operating factors on process performance.

Research Objectives

- The following objectives are proposed:

- Determine the mineralogical and chemical composition of the gold-bearing flotation concentrate.

- Characterise the particle-size distribution of the concentrate.
- Determine the initial solids concentration of the slurry.
- Investigate the effects of different flocculants on thickening performance.
- Determine the influence of flocculant dosage on settling velocity.
- Evaluate the effect of slurry solids concentration on thickening efficiency.
- Assess overflow clarity and suspended-solids content.
- Determine the solids concentration of the thickened underflow.
- Investigate the distribution of gold between the solid and liquid phases.
- Develop a suitable thickening flowsheet based on the results obtained.

Research Methodology

Gold-bearing flotation concentrate will be used as the study material. Its chemical and mineralogical composition will be determined during the initial characterisation stage. Particle-size analysis will be performed to quantify the fine fractions. This parameter is important for characterising thickening behaviour, as decreasing particle size can reduce settling velocity and complicate solid–liquid separation. Previous studies have identified a high proportion of fine particles as one of the factors limiting the throughput of gravity thickening.

The laboratory experiments will involve varying or monitoring the following principal parameters:

- Slurry solids concentration;
- Flocculant type;
- Flocculant dosage;
- Mixing conditions;
- Settling time;
- pH;
- Overflow volume;
- Underflow solids concentration.

Anionic, cationic, or nonionic polymer flocculants may be used in the flocculation experiments. However, a particular reagent should be identified as optimal only on the basis of experimental results obtained using the specific concentrate under investigation. In gold-ore processing, flocculant selection depends on the mineral composition, particle size, and surface properties of the material. For example, a published study on the Otjikoto gold plant employed flocculant screening, settling tests, and rheological measurements to establish thickener design parameters. The study reported that a high-molecular-weight anionic polyacrylamide provided favourable settling performance and overflow clarity. *Theoretical Fundamentals of Thickening*. Thickening involves the settling of solid particles in a liquid medium. Their settling behaviour depends on particle size, density, and shape, as well as slurry viscosity and solids concentration. During flocculation, polymer molecules adsorb onto mineral surfaces and may form bridges between particles, promoting the formation of larger aggregates. These flocs can settle more rapidly than individual particles, thereby enhancing solid–liquid separation. However, increasing the flocculant dosage excessively does not necessarily improve performance. A recent study on gold-mine tailings thickening indicated that exceeding the optimal dosage may produce loosely structured flocs and increase resistance to settling.

Results and Discussion

Accordingly, a central objective of the research should be to identify conditions that achieve the highest attainable settling velocity and a high-quality overflow at minimal reagent consumption, rather than assuming that a higher flocculant dosage invariably produces better results. *Assessment of Overflow Quality*. Overflow is the liquid stream discharged from the upper section of a thickener. Its quality directly influences its suitability for reuse as process water.

The following parameters may be used to assess overflow quality:

Suspended-solids concentration;

Turbidity;

pH;

Solids content;

Gold concentration;

Concentrations of other valuable components.

Thickening efficiency should be evaluated in terms of both the increase in underflow solids content and the clarity of the recovered overflow. Studies on thickener design for gold-processing plants have assessed overflow clarity and underflow density alongside flocculant screening. Gold losses through the overflow also require specific monitoring, as fine mineral particles carried into this stream may contain gold. Therefore, the assessment of process performance should account for both overflow clarity and gold distribution within the overall mass balance. *Optimisation of the Process.* Based on the research findings, the following process configuration may be recommended: Flotation concentrate → slurry preparation → flocculant addition and mixing → flocculation → thickening → clarified overflow and thickened underflow. The flocculant solution should be prepared separately at an appropriate concentration before being introduced into the thickener feed zone and effectively mixed with the slurry. Hydrodynamic conditions during flocculation influence the size and strength of the resulting flocs. Recent studies have identified feedwell hydrodynamics as an important factor governing flocculation kinetics and subsequent settling velocity. Thickener loading rate is another important operating parameter. Experiments involving gold-mine materials have shown that increasing the feed rate can reduce underflow solids concentration and increase the concentration of suspended particles in the overflow. Accordingly, the following interrelated parameters should be considered jointly when optimising operating conditions: Flocculant dosage, slurry solids concentration, feed rate, settling time, underflow solids concentration, and overflow quality.

Expected Scientific Outcomes. The study is expected to: Identify the principal physicochemical properties of the gold-bearing flotation concentrate that influence thickening;

Select an effective flocculant type;

Determine the optimal flocculant dosage;

Establish the optimal initial slurry solids concentration;

- Characterise settling kinetics;
- Evaluate overflow quality;
- Determine the optimal underflow solids concentration;
- Establish the distribution of gold between the solid and liquid phases;
- Develop an optimised operating regime for the thickening process.

Specific numerical results should be included in the article only after laboratory or pilot-scale experiments have been conducted. If no experiments have been performed, values obtained for materials from other deposits, such as an “optimal dosage of 20 g/t” or a “settling velocity of 8.8 cm/min,” must not be presented as findings of the current study. For example, the reported settling velocity of 8.80 cm/min was obtained for a different finely dispersed gold-bearing material at a flocculant dosage of 60 g/t.

Conclusion and Recommendations

Thickening gold-bearing flotation concentrates is an important process for achieving efficient solid–liquid separation, preparing concentrates for subsequent metallurgical treatment, and increasing opportunities for process-water reuse. The reviewed scientific literature indicates that thickening performance is significantly influenced by slurry solids concentration, particle-size distribution, flocculant type and dosage, feed rate, and hydrodynamic conditions within the thickener. Consequently, developing a thickening process for gold-bearing flotation concentrate should address not only the production of a high-solids underflow but also the recovery of a clarified overflow and the minimisation of gold losses through the overflow stream. Further research should include laboratory screening of different flocculants, optimisation of slurry solids concentration and reagent dosage, mathematical modelling of settling kinetics, and pilot-scale validation of the selected operating conditions. These investigations would provide a basis for improving the practical performance of the proposed technology.

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CHEMICAL ACTIVATION AND MODIFICATION OF WOOD WASTE-DERIVED CARBONIZATE WITH METAL SALTS

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Annotatsiya. Ushbu tadqiqot mahalliy yog‘och chiqindilarini karbonlash natijasida olingan ko‘mir (char) asosida yuqori samarali aktivlangan uglerodlarni ishlab chiqarish jarayonini optimallashtirish va soddalashtirishga bag‘ishlangan. Bunda kimyoviy aktivlash va metall komplekslash jarayonlarini bir bosqichli texnologik jarayonda birlashtirish taklif etilgan. Temir(III), mis(II) va rux(II) xlorid tuzlari bir vaqtning o‘zida aktivlovchi reagentlar hamda strukturaviy modifikatorlar sifatida muvaffaqiyatli qo‘llanildi. Olingan kompozit g‘ovakli materiallarning fizik-kimyoviy, strukturaviy, elementar va adsorbsion xususiyatlari batafsil tadqiq qilindi. Eksperimental natijalar shuni ko‘rsatdiki, metall xloridlar yordamida bir bosqichda amalga oshirilgan birgalikdagi aktivlash va modifikatsiyalash natijasida yaxshi rivojlangan mikro- va mezog‘ovaklar tarmog‘i, katta solishtirma sirt maydoni hamda oqova suv tarkibidagi organik ifloslantiruvchilarni samarali bog‘lash xususiyati yuqori bo‘lgan kompozit materiallar hosil bo‘ladi.

Kalit so‘zlar: *aktivlangan uglerod, yog‘och ko‘miri, bir bosqichli modifikatsiyalash, rux xlorid, temir(III) xlorid, mis(II) xlorid, g‘ovakli struktura, elementar tahlil.*

Аннотация. Данное исследование посвящено оптимизации и упрощению процесса получения высокоэффективных активированных углеродных материалов посредством объединения химической активации и комплексообразования с металлами в одностадийный процесс с использованием угольного остатка (char), полученного в результате карбонизации местных древесных отходов. Хлориды железа(III), меди(II) и цинка(II) были успешно применены одновременно в качестве активирующих реагентов и структурных модификаторов. Физико-химические, структурные, элементные и адсорбционные характеристики полученных композиционных пористых материалов были всесторонне исследованы. Экспериментальные результаты показали, что одностадийная совместная активация и модификация хлоридами металлов приводит к формированию хорошо развитой сети микро- и мезопор, высокой удельной поверхности и высокой способности к связыванию органических загрязнителей, содержащихся в сточных водах.

Ключевые слова: активированный углерод, древесный уголь, одностадийная модификация, хлорид цинка, хлорид железа(III), хлорид меди(II), пористая структура, элементный анализ.

Abstract. This study addresses the optimization and simplification of the production of high-performance activated carbons by integrating chemical activation and metal complexation into a single-step process utilizing char derived from the carbonization of local wood waste. Iron(III), copper(II), and zinc(II) chloride salts were successfully applied simultaneously as activating agents and structural modifiers. The physicochemical, structural, elemental, and adsorptive characteristics of the resulting composite porous materials were thoroughly evaluated. The experimental findings revealed that the single-step co-activation and modification with metal chlorides yielded a well-developed microporous and mesoporous network, large specific surface area, and exceptional binding affinity for organic pollutants in wastewater matrices.

Key words: *activated carbon, wood char, single-step modification, zinc chloride, ferric (III) chloride, cupric (II) chloride, porous structure, elemental analysis.*

Introduction

Activated carbons have gained immense global attention across environmental and industrial engineering fields due to their well-developed pore networks, thermal stabilities, and elevated surface energies. These frameworks are extensively implemented for wastewater remediation, selective gas captures, and as catalytic supports. However, raw or unmodified carbon structures face distinct limitations; their pristine surfaces lack consistent affinity for all chemical pollutants. While certain non-polar organic molecules bind tightly via hydrophobic interactions, other ionic, polar, and highly functionalized compounds are poorly retained due to adverse surface charge configurations or a lack of complementary surface groups. Consequently, target-oriented surface chemistry engineering and pore-size tailoring are mandatory to enhance active binding configurations [1].

The primary objective of structural modification is to generate newly accessible active centers, tune the surface charge, adjust hydrophilicity, and control surface acid-base dynamics. Traditional protocols employ an array of post-treatments involving mineral acids, strong bases, oxidizing formulations, heteroatom-containing (nitrogen/sulfur) compounds, and metal salts. Liquid-phase acid washing (utilizing agents such as HCl, H₂SO₄, HNO₃, and H₃PO₄) is widely utilized to demineralize carbon matrices, dissolve structural ash, open previously blocked pores, and increase oxygenated functional groups [2]. However, embedding metal oxides or complexes remains the most effective strategy for introducing targeted selectivity. For example, aluminum-based coordinates (such as Al-MOF configurations) improve binding capacities for anionic organic substances, whereas magnesium elements (MgO or Mg(OH)₂) impart strong basic functionalities that markedly boost the capture of cationic dyes like methylene blue [1, 2]. Concurrently, adding transitional metals like Fe, Cu, and Mn enables magnetic separation alongside excellent catalytic and photocatalytic (ZnO) efficiencies [1-3].

Conventional methodologies introduce metal components through distinct, multi-step routes—typically requiring the synthesis and purification of an activated carbon, followed by secondary liquid impregnation and high-temperature calcination. This approach increases energy consumption, labor, and chemical waste. To resolve these challenges, this study explores a unified, single-step chemical activation and modification strategy utilizing crude wood-derived char and metal chloride formulations, comprehensively evaluating the structural developments, elemental composition, and adsorption behaviors of the resulting composite materials.

Research Methodology

To streamline the fabrication process and achieve one-step embedding of metal functional species directly into the developing carbon framework, chemical activation and modification were executed concurrently. Analytical-grade iron(III) chloride hexahydrate ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$), copper(II) chloride dihydrate ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$), and anhydrous zinc(II) chloride (ZnCl_2) were selected to function as both pore-generating chemical activators and sources of metallic components. The precursor material consisted of raw wood char obtained via carbonization at 500 °C. The char was mechanically milled and sieved to collect uniform particle sizes. In a typical preparation, the dry char and the selected metal salt were blended at a strict 1:1 mass ratio. The designated metal salt was completely dissolved in a minimal volume of deionized water and thoroughly mixed with the char to form a homogeneous paste. To allow sufficient time for capillary diffusion and uniform transport of the metal ions deep into the inner pore capillaries, the mixtures were aged at room temperature for 12 hours [1, 2].

Following the impregnation phase, the wet samples were dried in a convection oven at 105 ± 2 °C until a constant weight was achieved. The dry composites were transferred into a quartz tubular reactor. To guarantee an entirely inert environment and eliminate residual oxygen, the system was thoroughly purged with high-purity argon gas. Pyrolysis was conducted under a continuous argon flow by heating the reactor at a well-controlled ramp rate of 10 °C/min up to a terminal activation temperature of 600 °C, where it was held for exactly 60 minutes.

After thermal processing, the samples were allowed to cool slowly to below 90 °C under an uninterrupted argon blanket. To eliminate free chlorides and unreacted precursor salts, the recovered composites were subjected to rigorous washing cycles using boiling deionized water. Washing was maintained until the filtrate tested entirely free of chloride ions (Cl^-), as verified via qualitative spot testing with a 0.1 M silver nitrate (AgNO_3) solution (monitored by the complete absence of any white AgCl precipitate). Finally, the purified materials were dried at 105 °C and preserved in hermetically sealed glass vials [1].

Results and Discussion

Executing chemical activation and metal embedding within a single thermal stage stimulated simultaneous pore propagation and the secure anchored fixation of active metal species on the forming carbon walls. At 600 °C, the metal chlorides act as powerful dehydrating and bond-cleaving agents that accelerate the degradation of organic cross-linkages, preventing excessive carbon gasification while promoting highly developed microporous regions [1, 2]. The thermal anchoring phase binds the metal complexes firmly as stable phases. If the processing temperature is too low, these metal phases remain highly water-soluble and leach out during purification; excessively high temperatures provoke severe particle aggregation (sintering), reducing surface area and destroying surface functional groups [2]. The key structural and porous textural parameters of the synthesised materials, along with their respective iodine and methylene blue (MB) uptake values, are compiled in Table 1.

Table 1. Porous structural and adsorptive properties of the single-step co-activated and modified carbons (T=600 °C, Ratio 1:1)

Sample Code	Specific Surface Area, S_{BET} (m^2/g)	Total Pore Volume, V_{total} (cm^3/g)	Iodine Adsorption (%)	MB Adsorption Capacity (mg/g)
Pristine Wood Char	180	0.09	35	45
Char + ZnCl_2	940	0.46	85	230
Char + FeCl_3	780	0.39	78	195
Char + CuCl_2	710	0.35	72	180

The elemental composition of the prepared samples was evaluated to confirm the successful incorporation of metal species into the carbon matrix and analyze the changes in the carbonaceous framework. The results of the elemental analysis are summarized in Table 2 [3-6].

Table 2. Elemental composition of the pristine and modified activated carbon samples

Sample	C, mass.%	O, mass.%	K, mass.%	Cl, mass.%	Fe, mass.%	Cu, mass.%	Zn, mass.%
C-500	90.842	7.913	—	—	—	—	—
Fe-1.0	86.028	9.733	—	0.084	3.215	—	—
Cu-1.0	85.556	10.077	—	0.093	—	3.386	—
Zn-1.0	84.823	10.304	—	0.078	—	—	3.932

The elemental analysis data clearly confirms that carbon forms the absolute structural backbone across all analyzed samples. In the pristine C-500 char, the carbon content reached 90.842 mass.%, with oxygen accounting for 7.913 mass.%. Following the single-step co-activation and modification with metal chlorides, a noticeable decrease in the carbon weight fraction (dropping to 84.823–86.028 mass.%) was observed alongside a corresponding increase in oxygen content (up to 9.733–10.304 mass.%). This trend is directly attributed to the fixing of metal oxide phases and the development of oxygen-containing functional groups on the carbon surface during chemical processing [2].

The successful embedding of target metals is validated by the clear presence of Fe (3.215 mass.%), Cu (3.386 mass.%), and Zn (3.932 mass.%) in their respective samples [3-7]. Crucially, the residual chloride (Cl⁻) concentration was kept extremely low across all modified matrices (0.078–0.093 mass.%), proving the high efficiency of the hot deionized water washing step monitored via AgNO₃ precipitation [1].

Conclusion and Recommendations

This work demonstrates a successful and highly efficient technology for manufacturing advanced composite adsorbents from cheap wood char via a single-step activation and modification process. Under optimized conditions (1:1 mass ratio, 600 °C treatment temperature, and an inert argon flow), the resulting modified carbons

exhibit exceptional surface areas and dense pore networks capable of rapid organic pollutant capture. The elemental analysis confirmed the high-efficiency immobilization of target metal frameworks (Fe, Cu, and Zn) with negligible residual impurities. This single-stage strategy reduces overall processing times and significantly cuts energy and reagent requirements, making it an economically viable and eco-friendly method for industrial water treatment applications.

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Section 4. ACTUAL PROBLEMS OF HISTORY, PHILOSOPHY AND SOCIOLOGY

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PHILOSOPHICAL-LOGICAL MODALITY AND EPISTEMOLOGICAL INTERPRETATION OF THE CONCEPTS OF “TRUTH” AND “BELIEF”

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Annotatsiya: Ushbu maqolada kontekstual argumentlashning ratsional va irratsional tasnifi falsafiy-nazariy jihatdan tahlil qilinadi. Tadqiqotda inson ongining voqeylikni aks ettirish darajalarini ifodalovchi bir qancha fundamental tushunchalar mavjud bo‘lib, ular orasida “ishonch” va “e’tiqod” alohida maqomi ochib berilgan. Bunda “ishonch” va “e’tiqod” farqlarni aniqlashtirish kontekstual argumentlarning inson ongiga ta’sir etish mexanizmini tushunishning asosiy omillari formol yoritilib berilgan. Ushbu maqola doirasida epistemik mantiqda bilim operatori K_ap , doksastik mantiqda esa ishonch yoki e’tiqod operatori B_ap qo‘llaniladi. Klassik bilim mantiq‘idan (epistemik mantiqdan) farqli o‘laroq, doksastik mantiq subyektlarning ishonch va e’tiqodlarini ifodalashga moslashtirilgan maxsus aksiomatik tizim haqida bafurcha yoritilgan. Mazkur maqolada KD45 tizimi va tizim agentning o‘z ishonch va ishonchsizlik holatlariga nisbatan refleksiv munosabat talqin qilinadi.

Kalit so‘zlar: “Ishonch” va “e’tiqod”, Klassik epistemologiya, Edmund Gettiyer, Epistemik mantiq, doksastik mantiq, KD45 tizimi.

Аннотация: В данной статье анализируется рациональная и иррациональная классификация контекстной аргументации с философской и теоретической точки зрения. Исследование включает ряд фундаментальных понятий, представляющих уровни отражения реальности человеческим разумом, среди которых раскрывается особый статус «убеждения» и «убеждения». При этом формально выделяются основные факторы понимания механизма влияния контекстных аргументов на человеческий разум путем уточнения различий между «убеждением» и «убеждением». В рамках данной статьи в эпистемической логике используется оператор знания

K_ap , а в доксистической логике — оператор убеждения или убеждения B_ap . В отличие от классической логики знания (эпистемической логики), доксистическая логика представляет собой особую аксиоматическую систему, адаптированную для выражения убеждений и взглядов субъектов. В данной статье интерпретируется система KD45 и рефлексивное отношение агента к собственным состояниям убеждений и недоверия.

Ключевые слова: «Вера» и «убеждение», классическая эпистемология, Эдмунд Геттиер, эпистемическая логика, доксистическая логика, система KD45.

Abstract: This article analyzes the rational and irrational classification of contextual argumentation from a philosophical and theoretical perspective. The study includes a number of fundamental concepts that represent the levels of reflection of reality by the human mind, among which the special status of “truth” and “belief” is revealed. In this, the main factors for understanding the mechanism of influence of contextual arguments on the human mind by clarifying the differences between “truth” and “belief” are formally highlighted. In the framework of this article, the knowledge operator K_ap is used in epistemic logic, and the belief or belief operator B_ap is used in doxastic logic. Unlike classical knowledge logic (epistemic logic), doxastic logic is a special axiomatic system adapted to express the beliefs and convictions of subjects. This article interprets the KD45 system and the reflexive attitude of the agent to his own states of belief and distrust.

Key words: “Truth” and “belief”, Classical epistemology, Edmund Gettier, Epistemic logic, doxastic logic, KD45 system.

Introduction

In the history of philosophy and the theory of knowledge, there are several fundamental concepts that represent the levels of reflection of reality by the human mind, among which “truth” and “belief” stand out with a special status. Although in many cases these two concepts are used synonymously in everyday speech or in psychological research, their logical-epistemological nature and modal properties differ

significantly. Clarifying these differences is a key factor in understanding the mechanism of influence of contextual arguments on the human mind [1]. In the framework of this study, “truth” means the cognitive attitude of the subject to the validity or probable truthfulness of a particular statement, and “belief” means the form of this belief that has acquired a relatively stable, valuable and practical content.

From an epistemological perspective, belief and truth are cognitive states associated with a subject’s acceptance of a particular proposition or idea as true, even if it has not been fully proven deductively or empirically. In classical epistemology, starting from the time of Socrates and Plato, the concept of knowledge has long been interpreted as a “founded true belief”. According to this approach, three main conditions must be met for a subject to know something: first, the proposition must be true; second, the subject must believe or be convinced of the truth of this proposition; third, the subject must have sufficient logical or empirical evidence, i.e. arguments, to justify this belief. Thus, in the classical approach, knowledge was viewed as a unity of truth, trust, and justification [2].

Literature Review

However, famous counterexamples put forward by the American philosopher Edmund Gettier in the 1960s showed that these three conditions—truth, certainty, and validity—are not always sufficient to describe knowledge [3]. According to this approach, which is called the Gettier problem, in some cases, even if the subject’s belief is true and sufficiently well-founded, it cannot be considered true knowledge, because its truth may have arisen by chance. For example, the subject may have reasonable evidence leading to a certain conclusion, but if some of this evidence is false, the final conclusion may accidentally turn out to be true. This situation raises the problem of “accidental true belief”. Therefore, Gettier’s counterexamples marked an important turning point in modern epistemology, in order to further clarify the boundary between knowledge and belief, and also to show that knowledge cannot be limited to true, well-founded belief alone. As a result, the need arose for a deeper study of the nature of knowledge, the justification of belief, and the relationship between them. The Gettier problem provides a clearer understanding of the difference between knowledge and

belief. From the point of view of logical modality, the most important difference between these two concepts is manifested in the relation to truth of the operators that represent them. In epistemic logic, the knowledge operator K_ap is used, while in doxastic logic, the belief or belief operator B_ap is used [4]. The main difference between these two operators is as follows:

$$K_ap \rightarrow p$$

This formula means “if an agent a knows a proposition p , then p is true.” That is, in epistemic logic, true knowledge must be consistent with objective truth. If an agent (a) knows a proposition but that proposition is actually false, this is not knowledge in the strict sense, but a false belief. For example, let p - be the proposition “Tashkent is the capital of Uzbekistan.” Then K_ap - means “agent a knows that Tashkent is the capital of Uzbekistan”. Logically, according to the relation $K_ap \rightarrow p$, if agent a really knows this fact, then the statement p must be true. That is, Tashkent is really the capital of Uzbekistan. If Tashkent were not the capital of Uzbekistan, the agent’s view of this would not be knowledge, but a misconception. Thus, one of the important properties of true knowledge is that it corresponds to objective reality.

Research Methodology

In doxastic logic, the belief or belief operator B_ap is used, and its main difference from knowledge is expressed as follows:

$$B_ap \rightarrow /p$$

This formula means that “if an agent a believes a proposition p , it does not logically follow that p is objectively true.” That is, a subject’s sincere belief in p does not guarantee that his belief is necessarily true. A person may believe a proposition, but that proposition may actually be false. The logical possibility of this situation can be expressed as follows:

$$\Diamond (B_ap \wedge \neg p)$$

Here, the modal operators are interpreted as follows: $\Diamond$ – probability, $\wedge$ – conjunction (and), $\neg$ – negation. Thus, this formula expresses the logical possibility that an agent a can believe p and at the same time p can be false. For example, let p - be the proposition “It will rain today”. Then B_ap means “agent a believes that it will rain

today.” If the agent believes that it will rain today based on weather data or other evidence, then his belief in p may be subjectively justified. However, it turns out later that it did not rain during the day. In this case, p is false and can be represented by $\neg p$. Therefore, the following is logically possible:

$$B_ap \wedge \neg p$$

That is, agent a believed that “it will rain today,” but this belief did not correspond to objective reality. Therefore, a person can sincerely and firmly believe in something, but his belief may not be true. Thus, the difference between epistemic and doxastic logic is clearly manifested in the relationship between the knowledge operator ($K_ap \rightarrow p$) and the belief operator ($B_ap \nrightarrow p$). A comparison of these two approaches shows that while the concept of knowledge requires correspondence to objective reality, there is no such firm guarantee in belief or belief. That is, the concept of knowledge has a truth condition, while the concept of belief or belief does not have such a guarantee. In other words, knowledge must correspond to reality, while belief may or may not correspond to reality [4]. Therefore, in modern epistemology, the difference between knowledge and belief and the degree of their justification are studied in more depth.

Results and Discussion

The results of the analysis show that if a person knows something, it must correspond to reality. That is, true knowledge cannot be a mistake. If the information that a person knows does not correspond to reality, then this is not knowledge, but a mistake (false belief). However, in doxastic (belief and trust) logic, such a condition does not exist. A person can sincerely believe in something, but his belief may not correspond to objective reality. Therefore, the presence of a belief or truth does not mean that its content is necessarily true. A person can also sincerely believe in something that is not true. Doxastic logic (from the Greek word “doxa” - thought, reasoning, belief) is one of the important areas of philosophical logic and epistemology that studies human beliefs and beliefs. It studies whether a person or subject believes or does not believe in something, understands his beliefs, and the logical relationships between these beliefs. In this sense, doxastic logic is a theoretical framework that describes the formation of a subject’s beliefs and their logical consistency [4].

In the 20th century, the scope of formal logic research has expanded significantly with the development of modal logic, epistemic logic, and agent-oriented logical systems. For centuries, it has worked mainly with considerations reflecting objective existence and the relationships between them. In the mid-20th century, under the influence of the work of scientists such as Georg von Wright and Jaakko Hintikka, it became possible to logically study the inner world of a person, his subjective assessments, thoughts, and beliefs. As a result, doxastic logic was formed, and it was fully substantiated that the beliefs of the subject can also be expressed on the basis of certain logical regularities and formal systems. B_ap . As we have seen above, the operator B_ap means “agent a believes the statement p ”. Belief is the fact that statement p is considered true in all possible worlds possible for the subject. In this sense, the operator B_ap represents the fact that the agent accepts statement p and considers it true in all possible worlds that correspond to the agent’s belief state. Unlike classical epistemic logic, doxastic logic has a special axiomatic system adapted to represent the beliefs and convictions of subjects. This system is called the KD45 system, also known as the doxastic system of Hintikka. The name KD45 comes from its main axioms – axioms K, D, 4 and 5, which express the agent’s reflexive attitude towards his own states of belief and disbelief [5]. The KD45 system consists of the following basic axioms. The first axiom is the K axiom, that is, the axiom of distributivity, which is expressed by the following formula:

$$K: B_a(p \rightarrow q) \rightarrow (B_ap \rightarrow B_aq)$$

This axiom implies that the agent’s beliefs obey the rules of logical inference. That is, if the agent believes that q follows from p and also believes in p , then he also believes in q . For example, if the agent believes that “if it rains, the street will be wet” and also believes in the proposition “it is raining,” then he logically also believes in the conclusion “the street will be wet.”

The second axiom is Axiom D, that is, the axiom of consistency of beliefs, which is expressed as follows:

$$D: B_ap \rightarrow \neg B_a\neg p$$

This axiom can also be expressed in equivalent form as follows:

$$\neg(B_a p \wedge B_a \neg p)$$

This axiom implies that an agent cannot simultaneously believe in both p and its negation $\neg p$. This means that the agent's beliefs must not be contradictory. For example, if an agent believes that "it is raining today," he cannot simultaneously believe that "it is not raining today". The third axiom is axiom 4, that is, the axiom of positive reflection or self-awareness, and is expressed by the following formula:

$$4: B_a p \rightarrow B_a(B_a p)$$

This axiom states that if an agent believes a p , then he also understands that he believes p . For example, if p – is the proposition "It is raining today," then $B_a p$ means that the agent believes this proposition. And $B_a(B_a p)$ means that the agent also understands his own belief, "I believe that it is raining today." Therefore, the agent not only believes a particular proposition, but also understands that he believes this proposition. The fourth axiom is Axiom 5, the axiom of negative reflection, which is expressed as follows:

$$5: \neg B_a p \rightarrow B_a(\neg B_a p)$$

This axiom states that if an agent a does not believe p , then he is also aware that he does not believe p . For example, if p – is the proposition "It is raining today", then $\neg B_a p$ means that the agent does not believe this proposition. If $B_a B_a(\neg B_a p)$ then the agent is also aware of his own state of disbelief, namely "I do not believe the proposition that it is raining today". This analysis shows that the KD45 system combines the following four basic axioms:

$$KD45 = K + D + 4 + 5$$

In this case, axiom K represents the correspondence of the agent's beliefs to logical conclusions, axiom D represents the consistency of beliefs, axiom 4 represents the agent's awareness of his own beliefs, and axiom 5 represents the agent's awareness of his own state of disbelief. In this regard, the KD45 system allows for the systematic representation of the subject's beliefs and convictions from a formal-logical perspective, their logical consistency, and the subject's awareness of his own belief state. However, a person's belief system is not always immutable and static. Under the influence of new information, evidence, and contextual arguments, the subject can maintain, reduce, or

revise his existing beliefs. This dynamic process of updating beliefs is modeled in doxastic logic through special theories.

Conclusion and Recommendations

At this point, it is necessary to determine the epistemological and cognitive hierarchy between the concepts of “truth” and “belief”. Trust is a relatively dynamic and flexible cognitive state associated with the subject’s perception of a particular statement as close to the truth or as credible. As the subject receives new information and evidence, he initially gains a certain degree of confidence in the truth of the statement, and this confidence can change or be refuted under the influence of new arguments. To analyze this process, we propose a conditional cognitive-probability model. Thus, the philosophical-logical and epistemological analysis of the phenomena of truth and belief shows that they are manifested as various forms of doxastic modality in the knowledge system of a cognitive agent. In this process, the possibility of an argument affecting the belief system depends on a number of conditions. These are the argument’s basis in reliable sources, logical consistency, relevance to the context, and reinforcement by significant evidence. As a result of repeated acceptance by the subject of new information and arguments, they logically align with the existing belief system. When these ideas are stably reflected in the subject’s values and practical activities, the initial truth gradually becomes an element of a solid belief and worldview.

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THE PHILOSOPHICAL REGULARITIES OF THE TRANSITION FROM CLASSICAL INTELLECTUALISM TO DIGITAL INTELLECTUALISM

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Annotatsiya. Maqolada klassik intellektualizmdan raqamli intellektualizmga o'tish jarayoni ijtimoiy-falsafiy jihatdan tahlil qilinadi. Muammo shundan kelib chiqadiki, raqamli sivilizatsiya sharoitida intellekt faqat individual aqlning qobiliyati sifatida emas, balki inson, axborot tizimlari, algoritmlar va sun'iy intellektning o'zaro aloqador faoliyati sifatida namoyon bo'lmoqda. Tadqiqot Arastu, Dekart, Kant, Gegel, A. Tyuring, L. Floridi, E. Klark va D. Chalmers, J. Syorl asarlari hamda intellektual madaniyat va sun'iy intellekt falsafasiga oid o'zbek tadqiqotlariga tayanadi; dialektik metod, tarixiy-falsafiy rekonstruksiya, qiyosiy tahlil va tizimli yondashuvdan foydalaniladi. Tadqiqotda aniqlandiki, mazkur o'tish oddiy texnologik yangilanish emas, balki bilish subyekti, bilimning shakllanishi va tafakkurning tashkiliy mexanizmlari o'zgarishi bilan bog'liq falsafiy jarayondir. O'tishning beshta qonuniyati ajratib ko'rsatiladi: vorisiylik va sifatii yangilanish birligi; miqdoriy o'zgarishlarning sifatii o'zgarishlarga o'tishi; differensiatsiya va integratsiya dialektikasi; subyekt–obyekt munosabatlarining transformatsiyasi; hisoblashdan kontekstual hamkorlikka o'tish. Raqamli intellektual mas'uliyat tushunchasi asoslab beriladi.

Kalit so‘zlar: intellektualizm, klassik intellektualizm, raqamli intellektualizm, tafakkur, aql, sun’iy intellekt, algoritm, raqamli jamiyat, bilish subyekti, intellektual madaniyat, axborot, transformatsiya, raqamli intellektual mas’uliyat.

Аннотация. В статье с социально-философских позиций анализируется переход от классического интеллектуализма к цифровому. Проблема обусловлена тем, что в условиях цифровой цивилизации интеллект проявляется уже не только как способность индивидуального разума, но и как взаимосвязанная деятельность человека, информационных систем, алгоритмов и искусственного интеллекта. Исследование опирается на труды Аристотеля, Декарта, Канта, Гегеля, А. Тьюринга, Л. Флориди, Э. Кларка и Д. Чалмерса, Дж. Сёрла, а также на работы узбекских исследователей по интеллектуальной культуре и философии искусственного интеллекта; используются диалектический метод, историко-философская реконструкция, сравнительный анализ и системный подход. Установлено, что данный переход представляет собой не простое технологическое обновление, а философский процесс, связанный с изменением субъекта познания, способов формирования знания и организационных механизмов мышления. Выделены пять закономерностей перехода: единство преемственности и качественного обновления; переход количественных изменений в качественные; диалектика дифференциации и интеграции; трансформация субъект-объектных отношений; переход от вычисления к контекстуальному сотрудничеству. Обосновано понятие цифровой интеллектуальной ответственности.

Ключевые слова: интеллектуализм, классический интеллектуализм, цифровой интеллектуализм, мышление, разум, искусственный интеллект, алгоритм, цифровое общество, субъект познания, интеллектуальная культура, информация, трансформация, цифровая интеллектуальная ответственность.

Abstract. The article examines, from a socio-philosophical standpoint, the transition from classical intellectualism to digital intellectualism. The problem arises because, under the conditions of digital civilisation, intellect is no longer

manifested solely as a capacity of the individual mind but increasingly as the interconnected activity of the human being, information systems, algorithms and artificial intelligence. The study draws on the works of Aristotle, Descartes, Kant, Hegel, A. Turing, L. Floridi, A. Clark and D. Chalmers and J. Searle, as well as on Uzbek research into intellectual culture and the philosophy of artificial intelligence; it employs the dialectical method, historical-philosophical reconstruction, comparative analysis and the systemic approach. It is established that the transition is not a mere technological update but a philosophical process involving changes in the knowing subject, in the formation of knowledge and in the organisational mechanisms of thinking. Five regularities of the transition are identified: the unity of continuity and qualitative renewal; the passage of quantitative changes into qualitative ones; the dialectic of differentiation and integration; the transformation of subject–object relations; and the shift from computation to contextual collaboration. The concept of digital intellectual responsibility is substantiated.

Key words: *intellectualism, classical intellectualism, digital intellectualism, thinking, reason, artificial intelligence, algorithm, digital society, knowing subject, intellectual culture, information, transformation, digital intellectual responsibility.*

Introduction

Throughout the history of human development, intellect has been one of the principal forces determining humanity's capacity to comprehend nature and society, to transform the reality it encounters and to design its own future. In philosophy the concept of intellect is considerably wider than a simple ability to acquire knowledge: it unites reason, thinking, logical reflection, understanding, generalisation and the capacity to organise purposeful activity. It was in this sense that intellectualism took shape as a philosophical principle affirming the primacy of reason and rational cognition in human existence. The defining feature of classical intellectualism is that the human being is regarded as the central bearer of intellect. Knowledge is acquired, analysed, systematised and applied by a person, and for a long time even the technical means that people created were understood as auxiliary devices that eased intellectual labour without taking part in it. Contemporary digital transformation has significantly changed

the content of this relation. Technology no longer merely executes a task that a person has formulated in advance: it analyses data, generates alternatives, forecasts probable outcomes and produces texts, images and other informational products. It is therefore no longer sufficient to explain intellect solely in terms of the natural capacities of the human brain, since a considerable part of intellectual activity is moving into the sphere of relations between the human being, technology and information systems.

The Uzbek philosopher G. G. Gaffarova, analysing intellectual culture in digital society, shows that digitalisation and informatisation are bringing about new changes in human thinking, in decision-making and in the structural organisation of society.¹ The problem also has a practical dimension for Uzbekistan, which has adopted the Strategy for the Development of Artificial Intelligence Technologies until 2030, providing for the broad introduction of these technologies into social and economic life.² When algorithms become part of the everyday environment in which students learn, specialists take decisions and citizens form opinions, the question of what it means to think and to know ceases to be purely academic.

This situation calls for the theoretical substantiation of a new form of intellectualism – digital intellectualism. The aim of this article is to reveal the philosophical regularities of the transition from classical to digital intellectualism. Four tasks follow from this aim: to characterise classical intellectualism and its model of the knowing subject; to clarify the content of digital intellectualism and distinguish it from the mere use of digital technologies; to identify and substantiate the regularities of the transition; and to determine the status and responsibility of the human being within the new paradigm. The novelty of the study lies in interpreting the transition not as the replacement of human reason by technology but as a dialectical transformation governed by identifiable regularities, and in proposing the concept of digital intellectual responsibility as its normative counterpart.

¹ G'affarova G. G'. Raqamli jamiyatning intellektual madaniyati: falsafiy tahlil [Intellectual culture of digital society: a philosophical analysis] // FarDU ilmiy xabarlar. 2023. Vol. 29, No. 4. DOI: 10.56292/SJFSU/vol29_iss4/a2.

² Resolution of the President of the Republic of Uzbekistan No. PP-358 of 14 October 2024 "On Approval of the Strategy for the Development of Artificial Intelligence Technologies until 2030". URL: <https://lex.uz/docs/7159258>.

Research Methodology

The study rests on three groups of sources. The first comprises the classical texts in which the intellectualist ideal of the autonomous rational subject was formulated: Aristotle's *Metaphysics*, Descartes's *Meditations on First Philosophy* and Kant's essay on enlightenment; Hegel's *Science of Logic* is drawn upon for the doctrine of measure, that is, for the passage of quantitative changes into qualitative ones. The second group consists of works that call the boundaries of intellect into question in the age of computation: A. Turing's paper on computing machinery and intelligence, J. Searle's critique of "strong" artificial intelligence, the extended-mind thesis of A. Clark and D. Chalmers, E. Hutchins's theory of distributed cognition, L. Floridi's philosophy of information, and empirical studies of cognitive offloading. The third group includes the research of Uzbek scholars – G. G. Gaffarova on intellectual culture in digital society and N. Rakhimbabaeva on the continuity of the philosophy of artificial intelligence – together with the national strategy for the development of artificial intelligence.

The dialectical method serves as the general methodological basis, since it allows the transition to be grasped as a unity of continuity and negation, of quantitative and qualitative change. Historical-philosophical reconstruction traces how the understanding of intellect shifted from antiquity to the digital era. Comparative analysis sets classical and digital intellectualism side by side across a common set of parameters. The systemic approach treats intellect as a property of the system "human – technology – information" rather than of any isolated element, while conceptual analysis distinguishes digital intellectualism from adjacent notions such as digital literacy or the simple use of artificial intelligence tools. The argument proceeds from a characterisation of the two models to the regularities of the transition, and from these regularities to the status and responsibility of the human being.

Results and Discussion

1. Classical intellectualism: the autonomous knowing subject

Historically, classical intellectualism was formed by confidence in human reason and its rational capacities. From ancient philosophy onward, reason was regarded as the feature that distinguishes the human being from all other living beings; Aristotle opened

his *Metaphysics* with the claim that “all men by nature desire to know”.³ Later philosophical systems likewise affirmed the decisive role of thinking in comprehending truth, establishing cause-and-effect relations and disclosing regularities. In Descartes the thinking subject became the foundation of all reliable knowledge: certainty was to be attained by an individual mind that subjects every conviction to methodical doubt and accepts only what it apprehends clearly and distinctly.⁴

In the classical model the boundary between the “knower” and the “known” was relatively clear: the human being was the subject, while nature and social reality were objects of cognition. Books, writing, calculating devices and technical instruments served as means of cognition, but none of them was regarded as the source of an independent intellectual act. Another important feature of classical intellectualism is the inseparable bond between knowledge, on the one hand, and human memory and individual thinking, on the other. A knowledgeable person was understood to be one who had mastered a large body of knowledge, could systematise it logically and was able to apply it in a variety of situations.

In the digital environment, however, the very concept of “knowing” is changing. A person is no longer obliged to keep all information in memory. Experimental research shows that when people expect information to remain accessible, they tend to remember less of the information itself and more of where it can be found.⁵ The core intellectual competence is thus increasingly bound up with locating the necessary information, verifying and comparing it, critically evaluating algorithmic recommendations and turning them into meaningful conclusions. Consequently, whereas in classical intellectualism intellect appeared as individual, anthropocentric and predominantly internal cognitive activity, in digital intellectualism it is gradually acquiring a networked, technologically mediated and distributed character.

³ Aristotle. *Metaphysics*. Trans. W. D. Ross. In: *The Complete Works of Aristotle: The Revised Oxford Translation* / Ed. J. Barnes. Vol. 2. Princeton: Princeton University Press, 1984. Book I, 980a21.

⁴ Descartes R. *Meditations on First Philosophy*. Trans. J. Cottingham. Cambridge: Cambridge University Press, 1996. P. 12–24.

⁵ Sparrow B., Liu J., Wegner D. M. Google Effects on Memory: Cognitive Consequences of Having Information at Our Fingertips // *Science*. 2011. Vol. 333, No. 6043. P. 776–778.

2. Digital intellectualism: concept and genesis

It would be methodologically incorrect to equate digital intellectualism with the mere use of computers or artificial intelligence. Its content is considerably broader: it denotes a new form of cognition that emerges from the systemic integration of human intellectual activity with digital technologies. Of particular significance for understanding this process is the question “Can machines think?”, posed by Alan Turing as early as the middle of the twentieth century. Turing took the problem beyond a merely terminological dispute and proposed that the intellectual activity of a machine be discussed on the basis of its observable behaviour.⁶ This approach marked an important turn from interpreting intellect exclusively as an attribute of biological human consciousness towards a functional and technological interpretation. Today’s generative artificial intelligence systems have made the issue still more complex. A contemporary algorithm not only performs numerical calculations but also operates with language, groups data, answers questions, proposes alternative lines of reasoning and generates information with new content. Technology has thus begun to turn from an external instrument of intellectual activity into an active component that performs some of its functions. The Uzbek researcher N. Rakhimbabaeva, examining the historical continuity of the philosophy of artificial intelligence, interprets its contemporary forms as a process interconnected with classical rationalism, cybernetic thinking and the development of digital civilisation. Her analysis makes it possible to understand artificial intelligence not as a phenomenon absolutely opposed to human thinking, but within the historical and logical continuity of intellectual progress.⁷ From this standpoint, the relation between classical and digital intellectualism is not one of negation but one of successive transformation. Digital intellect does not abolish the historical role of human reason; on the contrary, it develops as the form in which the logical, mathematical, linguistic and algorithmic knowledge created by humanity has been materialised in technological

⁶ Turing A. M. Computing Machinery and Intelligence // Mind. 1950. Vol. LIX, No. 236. P. 433.

⁷ Raximbabayeva N. Sun’iy intellekt falsafasining davomiyligi va istiqbollari [Continuity and prospects of the philosophy of artificial intelligence] // O’zMU xabarlar. Ijtimoiy-gumanitar fanlar. Toshkent, 2026. No. 1/1.2. B. 166–168.

systems. The differences between the two models identified in the course of the analysis are summarised in Table 1.

Table 1. Comparative characteristics of classical and digital intellectualism

Parameter	Classical intellectualism	Digital intellectualism
<i>Bearer of intellect</i>	The individual human mind	The system “human – technology – information”
<i>Locus of knowledge</i>	Memory and individual thinking	Distributed among people, databases and algorithms
<i>Role of technology</i>	Passive auxiliary instrument	Active component performing some intellectual functions
<i>Subject–object relation</i>	Clear boundary between the knower and the known	Mediated relation: algorithms influence the course of cognition, while goals and responsibility remain with the human being
<i>Criterion of an intellectual person</i>	Volume of mastered knowledge and the ability to systematise and apply it	Ability to find, verify, compare and critically interpret information, including algorithmic output
<i>Dominant mode of intellect</i>	Individual, anthropocentric, internal	Networked, technologically mediated, distributed
<i>Characteristic risk</i>	Dogmatism; the limits of individual memory	Uncritical reliance on algorithms; weakening of independent reasoning

3. The philosophical regularities of the transition

A comparison of the two models makes it possible to identify five regularities governing the transition from classical to digital intellectualism. They are regularities in the philosophical sense: stable, recurrent and necessary relations that express the direction of the process rather than isolated observations.

The first regularity is the unity of continuity and qualitative renewal. No new intellectual paradigm completely negates the forms of thinking that preceded it. Formal logic, mathematics, language, classification, causal analysis and other traditional forms of cognition lie at the foundation of digital intellectualism as well. What is new is that certain intellectual operations once performed by the human being are being transferred to algorithmic systems. The new form thus preserves the content of the old one while changing the manner in which it is carried out; the relation is one of dialectical sublation rather than abolition. *The second regularity is the passage of quantitative changes into qualitative ones.* At earlier stages of history the growth of information was expressed mainly in the appearance of new libraries, archives and scientific centres – that is, in the

extensive enlargement of one and the same mode of intellectual work. In the digital era the volume of data has exceeded the limits within which it can be processed directly by a human being. Quantitative growth has here crossed what Hegel called a measure, beyond which a change in quantity becomes a change in quality.⁸ A need has arisen for the automatic sorting, linking and analysis of vast amounts of information, and it is this need that has made artificial intelligence and algorithmic analysis a structural component of intellectual activity rather than an optional aid to it. *The third regularity is the dialectic of differentiation and integration, through which intellect passes from an individual to a networked form.* In the classical period a scientific discovery was usually associated with the name of an individual scholar. Present-day research, by contrast, is becoming a complex networked process involving databases, international scientific platforms, digital models, supercomputers and artificial intelligence systems. Intellectual functions are differentiated – memory, search, calculation, pattern recognition, evaluation and decision-making are distributed among different agents and devices – and are at the same time integrated into a single cognitive system. Philosophy of mind has articulated this shift in the thesis of the “extended mind”, according to which external resources reliably coupled with a person’s cognitive processes become part of those processes,⁹ and in the theory of distributed cognition, which shows that cognitive work is frequently accomplished by systems of people and artefacts rather than by an individual alone.¹⁰ Contemporary intellect is therefore not only the “inner property” of an individual but also a potential realised in the connections between people, data and technological systems.

The fourth regularity is the transformation of subject–object relations. In the classical model the human being was the active subject and technology the passive instrument. Contemporary algorithms, however, propose options for human decisions,

⁸ Hegel G. W. F. The Science of Logic. Trans. and ed. G. di Giovanni. Cambridge: Cambridge University Press, 2010. Book One, Section Three “Measure”.

⁹ Clark A., Chalmers D. The Extended Mind // Analysis. 1998. Vol. 58, No. 1. P. 7–19.

¹⁰ Hutchins E. Cognition in the Wild. Cambridge, MA: MIT Press, 1995.

give priority to some of them, formulate recommendations and thereby actively influence the process of cognition. It does not follow from this that the algorithm has become an ontological subject equal to the human being in the full sense. Determining the social significance of a goal, choosing values, bearing moral responsibility and assessing the human consequences of a result remain the province of the human being. The relation that emerges is thus neither the former subject–instrument scheme nor a symmetrical relation between two subjects; it is a mediated relation in which the human being remains the bearer of goals and responsibility while sharing the operational side of cognition with technology. *The fifth regularity is the shift of intellect from computation to contextual collaboration.* Whereas rapid calculation was the principal task of the first computers, today’s digital systems work with language, images, sound and context. As a result, interaction between human and machine is moving from the level of issuing technical commands towards a form of dialogue, which indicates that the concept of intellect itself is undergoing change. L. Floridi, analysing how digital technologies are transforming the structure of the informational environment in which people live, argues that the contemporary human being must be understood within an ever-expanding “infosphere”. His treatment of intelligence likewise shows that machine intelligence should not be understood as a simple copy of human intelligence, and that the specific functional capacities of digital systems must be taken into account.¹¹ Proceeding from this idea, digital intellectualism moves the relation between human and algorithm away from the naive comparison “which of them is smarter?” towards the philosophical question “in what proportion are their intellectual functions being combined?”

Results and Discussion

1. The human being in the paradigm of digital intellectualism

Digital intellectualism need not diminish the intellectual status of the human being. On the contrary, it compels a fresh understanding of the essence of human

¹¹ Floridi L. The Fourth Revolution: How the Infosphere Is Reshaping Human Reality. Oxford: Oxford University Press, 2014. Chapter “Intelligence: Inscribing the World”. P. 129–143.

intellect. If an algorithm processes vast volumes of data faster than a person can, it becomes evident that human superiority cannot be measured by computational speed or memory capacity alone. The distinctiveness of human intellect appears more clearly in the capacity to create meaning, to establish values, to understand lived experience, to make moral choices and to assess the social and spiritual consequences of one's goals.

This conclusion is supported by a long-standing line of philosophical criticism. J. Searle's "Chinese room" argument was intended to show that manipulating symbols according to formal rules, however successful its outward results, does not by itself amount to understanding.¹² Contemporary critics of large language models make a similar point: such systems produce fluent text on the basis of statistical patterns in their training data without access to meaning in the sense in which a human speaker possesses it, and they can reproduce the biases contained in that data.¹³ One need not accept every conclusion of these critics to recognise the methodological lesson they offer: the functional success of an algorithm does not settle the questions of understanding, purpose and responsibility. For this reason digital intellectualism is not a paradigm of replacing the human being with technology. It is a paradigm of determining which human intellectual functions are reproduced, which are technologically amplified, and which are preserved as distinctive features of human existence.

2. The central contradiction and digital intellectual responsibility

At this point a new contradiction emerges. Artificial intelligence extends human cognitive capacities, yet excessive reliance on it may weaken a person's ability to reason independently. Psychological research on cognitive offloading shows that people readily delegate cognitive demands to external tools; this generally improves performance, but it can also reduce what is retained internally, and the decision to offload depends on how people judge their own abilities.¹⁴ The contradiction has a philosophical precedent. Kant

¹² Searle J. R. Minds, Brains, and Programs // Behavioral and Brain Sciences. 1980. Vol. 3, No. 3. P. 417–424.

¹³ Bender E. M., Gebru T., McMillan-Major A., Shmitchell S. On the Dangers of Stochastic Parrots: Can Language Models Be Too Big? // Proceedings of the 2021 ACM Conference on Fairness, Accountability, and Transparency. New York: ACM, 2021. P. 610–623.

¹⁴ Risko E. F., Gilbert S. J. Cognitive Offloading // Trends in Cognitive Sciences. 2016. Vol. 20, No. 9. P. 676–688.

defined enlightenment as humanity's emergence from its self-incurred immaturity – the inability to use one's own understanding without the guidance of another – and observed how comfortable it is to remain immature when a book, a spiritual adviser or a physician can do one's thinking for one.¹⁵ In the digital era the algorithm can easily assume the role of such a guardian, and the Kantian demand to use one's own reason acquires new urgency. The development of digital intellectualism must therefore be accompanied by the formation of digital intellectual responsibility. Digital intellectual responsibility means not the passive acceptance of a ready-made algorithmic answer, but the critical analysis of its source, logic, reliability and consequences. It includes at least four components: verification of the source and factual basis of an algorithmic output; examination of its internal logic and of possible alternative answers; awareness of the limits of both human and machine competence; and accountability for the use of the result, including openness about the part technology played in obtaining it. The intellectual person of the future will be not merely someone who has memorised a vast amount of information, but someone who understands the limits of human and artificial intellect and is able to organise a conscious collaboration between them. In this respect the mature form of digital intellectualism rests not on the opposition "human or machine" but on the unity of the human being, technology, critical thinking and ethical responsibility.

Conclusion and Recommendations

The transition from classical to digital intellectualism is an important philosophical stage of civilisational development. It signifies neither the disappearance of human intellect nor its simple replacement by technical intellect. Rather, it expresses the growing complexity of the form of intellectual activity, of its organisational mechanisms, of its sources of information and of its intersubjective connections.

Whereas classical intellectualism relied on the autonomy and rational capacities of human reason, digital intellectualism presents human reason in a state of interaction

¹⁵ Kant I. An Answer to the Question: What Is Enlightenment? In: Kant: Political Writings / Ed. H. S. Reiss. Cambridge: Cambridge University Press, 1991. P. 54–60.

with algorithms, information systems and artificial intelligence. The study has identified five philosophical regularities of this transition: the unity of continuity and qualitative renewal; the passage of quantitative changes into a qualitative transformation; the dialectic of differentiation and integration, through which individual intellect becomes networked; the transformation of subject–object relations into a mediated relation in which the human being remains the bearer of goals and responsibility; and the shift from computation to contextual collaboration, which entails a differentiation of human and artificial intellectual functions. On this basis, digital intellectualism may be defined as a new philosophical and intellectual paradigm that arises from the integration of human thinking with the technological environment and that interconnects biological and artificial intellectual capacities in the processes of creating and processing knowledge and of making decisions. Within such a paradigm the principal task of the human being is not to compete with technology but to determine the purpose, criteria and ethical limits of its use. The true content of the intellectualism of the future will therefore be determined not only by how “intelligent” technology becomes, but by how consciously, critically and responsibly human beings are able to use these intellectual capacities. Several recommendations follow from the study. First, in higher education the emphasis should shift from the reproduction of knowledge to its verification, comparison and interpretation, including assignments in which students assess outputs generated by artificial intelligence against primary sources. Second, digital intellectual responsibility should be treated as a component of intellectual culture and reflected in teaching practice and in academic integrity policies, including the transparent disclosure of the use of artificial intelligence tools in academic work. Third, further research is needed on the empirical side of the problem – how regular use of artificial intelligence tools changes the reasoning of students and specialists – and on the ethical criteria for implementing the national artificial intelligence strategy in education and the humanities.



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Section 5. ACTUAL PROBLEMS OF NATURAL SCIENCES

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SYNTHESIS AND STUDY OF THE COORDINATION COMPOUND OF LANTHANUM(III) NITRATE SALT WITH 4-AMINOBENZOIC ACID

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Annotatsiya. Mazkur maqolada lantan(III) nitrat tuzining 4-aminobenzoy kislotasi (PABA) bilan hosil qilgan koordinatsion birikmasining sintezi va fizik-kimyoviy tadqiqot natijalari keltirilgan. Tadqiqot davomida 4-aminobenzoy kislotasining lantan(III) ioni bilan o'zaro ta'sirlashuvi hamda koordinatsion birikma hosil bo'lish sharoitlari o'rganildi. Sintez qilingan birikmaning tarkibi va tuzilishini aniqlash maqsadida zamonaviy fizik-kimyoviy tahlil usullaridan foydalanildi. Jumladan, IQ-spektroskopiya yordamida ligand tarkibidagi karboksil va amin guruhlarining koordinatsiyalanish jarayonidagi o'zgarishlari tahlil qilindi. Shuningdek, birikmaning termik barqarorligi va parchalanish bosqichlarini aniqlash uchun termik tahlil usullaridan foydalanish imkoniyatlari ko'rib chiqildi. Olingan natijalar 4-aminobenzoy kislotasining lantanoid ionlari bilan koordinatsion birikmalar hosil qilishdagi xususiyatlarini baholash hamda ularning tarkibiy-tuzilish xususiyatlarini aniqlash uchun muhim ahamiyatga ega.

Kalit so'zlar: lantan(III) nitrat, 4-aminobenzoy kislota (PABA), koordinatsion birikma, lantanoidlar, kompleks birikma, IQ-spektroskopiya, termik tahlil, koordinatsiyalanish, karboksil guruhi, amin guruhi.

Аннотация. В данной статье представлены результаты синтеза и физико-химического исследования координационного соединения, образованного нитратом лантана(III) и 4-аминобензойной кислотой (PABA). В ходе исследования изучены взаимодействие 4-аминобензойной кислоты с ионами лантана(III), а также условия образования координационного соединения. Для определения состава и строения синтезированного

соединения использованы современные физико-химические методы анализа. В частности, с помощью ИК-спектроскопии проанализированы изменения карбоксильной и аминогрупп в процессе координации лиганда. Кроме того, рассмотрены возможности применения методов термического анализа для определения термической устойчивости соединения и стадий его термического разложения. Полученные результаты имеют важное значение для оценки координационных свойств 4-аминобензойной кислоты при образовании координационных соединений с ионами лантаноидов, а также для установления их структурно-составных характеристик.

Ключевые слова: нитрат лантана(III), 4-аминобензойная кислота (PABA), координационное соединение, лантаноиды, комплексное соединение, ИК-спектроскопия, термический анализ, координация, карбоксильная группа, аминогруппа.

Abstract. This article presents the results of the synthesis and physicochemical investigation of a coordination compound formed by lanthanum(III) nitrate and 4-aminobenzoic acid (PABA). The interaction of 4-aminobenzoic acid with lanthanum(III) ions, as well as the conditions for the formation of the coordination compound, were investigated. Modern physicochemical analytical methods were used to determine the composition and structure of the synthesized compound. In particular, changes in the carboxyl and amino groups of the ligand during the coordination process were analyzed using infrared (IR) spectroscopy. In addition, thermal analysis methods were considered for determining the thermal stability of the compound and the stages of its thermal decomposition. The obtained results are important for evaluating the coordination properties of 4-aminobenzoic acid in the formation of coordination compounds with lanthanide ions and for determining their compositional and structural characteristics.

Key words: lanthanum(III) nitrate, 4-aminobenzoic acid (PABA), coordination compound, lanthanides, complex compound, IR spectroscopy, thermal analysis, coordination, carboxyl group, amino group.



Introduction

Currently, one of the most important directions of coordination chemistry is the synthesis of new types of biologically active, catalytic and practically important complex compounds based on rare earth elements (REEs) and the study of their structure. Lanthanides have a unique electronic structure, a tendency to high coordination numbers and the ability to form stable complexes with various organic ligands, so their compounds are widely used in pharmacology, medicine, new materials technology and agriculture. It is known that aromatic amino acids and their derivatives, including 4-aminobenzoic acid (PABA), are biologically active substances that play an important role in biochemical processes in the body. The amine ($-\text{NH}_2$) and carboxyl ($-\text{COO}^-$) groups in PABA allow the formation of various bidentate or monodentate coordination bonds with metal ions. Therefore, the synthesis of new coordination compounds based on lanthanum(III) salt and 4-aminobenzoic acid, the study of their spatial structure and physicochemical properties are one of the most relevant issues from a theoretical and practical point of view. An analysis of the literature data shows that the synthesis conditions of complex compounds formed by lanthanum(III) nitrate with 4-aminobenzoic acid, their thermal stability, structural features and other physicochemical properties require a systematic and comprehensive study.

The aim of this work is to synthesize a new coordination compound based on the interaction of lanthanum(III) nitrate hexahydrate with 4-aminobenzoic acid, determine its optimal conditions for its preparation, and comprehensively study its structure and properties using modern physicochemical analysis methods (IR spectroscopy, X-ray phase and thermal analysis).

Literature review

Lanthanides and coordination compounds formed on their basis are one of the promising research directions of modern inorganic and coordination chemistry. The tendency of lanthanum(III) ion to high coordination numbers, the formation of stable complexes with organic ligands containing oxygen and nitrogen donor atoms, and the structural, thermal, optical, and biological properties of the resulting compounds increase interest in this class of compounds. In recent studies, La(III) complexes are

considered promising objects in materials science, luminescent systems, biologically active compounds, and the creation of various functional materials [1]. Kadam and co-authors, studying complexes of La(III) with organic ligands, noted that aromatic carboxylic acids can have several coordination centers and can bind to lanthanum ions in various coordination modes. The authors characterized the synthesized La(III) complexes using elemental analysis, FTIR, TG–DTA, SEM, XRD, and luminescence methods [1]. Of particular importance is the complexation of lanthanum(III) ion with carboxyl-containing ligands. Complexes of La(III) with nicotinic acid and other nitrogen-containing organic ligands have been studied by Shubina and Orlova (Figure 1) [2].

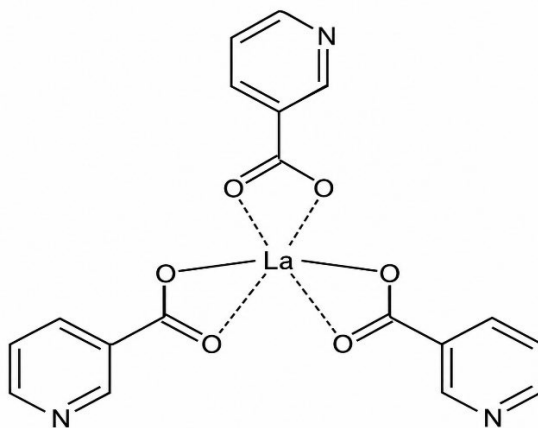


Figure 1. Structure of the complex compound molecule $[La(C_4H_5NCOO)_3]$

The authors showed the influence of the pH value of the medium and the ratio of reagents on the complexation reaction between metal ions and ligand in the preparation of La(III) complexes with nicotinic acid. In particular, a poorly soluble complex was formed by reacting La^{3+} ions with a threefold excess of ligand at $pH \approx 4$. It was also shown that nicotinic acid can be obtained by first converting it to its sodium salt and then reacting it with $La(NO_3)_3 \cdot 6H_2O$ to obtain a lanthanum carboxylate complex [2]. These results indicate that the degree of deprotonation of the ligand and the solution medium are important factors in the synthesis of La(III) complexes with aromatic carboxylic acids. Not only structural, but also biological properties of lanthanide complexes are an important object of research. Philip and Mohanan synthesized Sm(III) and Dy(III) complexes based on pyrazolone derivatives and studied their antimicrobial and

antibiofilm properties [3]. According to the results obtained, the metal complexes exhibited higher antibacterial and antifungal activity compared to the free ligand. The authors explained this phenomenon by the decrease in the polarity of the metal ion as a result of chelation, the delocalization of electron density along the ligand, and the increase in the lipophilicity of the complex [3]. These data indicate that the complexation of lanthanide ions with bioactive organic ligands can lead to the formation of compounds with new functional properties.

In the coordination chemistry of La(III) nitrate, the location of the nitrate anions in the inner or outer coordination sphere, as well as the coordination number of the metal center, are important structural parameters. Natreba and Fedorenko synthesized a complex of $\text{La}(\text{NO}_3)_3$ with 4,4,10,10-tetramethyl-1,3,7,9-tetraazapyro[5.5]undecane-2,8-dione and analyzed its single-crystal X-ray structure [4]. According to the results of the study, the La(III) atom is coordinated by the oxygen donor atoms of the ligands, three bidentate nitrate anions and two water molecules, and the coordination number of the metal is determined to be 10 [4]. This clearly demonstrates the high coordination capacity of the La(III) ion and its tendency to oxygen-donating ligands. The thermal properties of lanthanum(III) complexes are also important in determining their composition, coordination environment and practical applications. Gandhi et al. synthesized a nanodispersed La(III) coordination compound and demonstrated the possibility of obtaining La_2O_3 nanoparticles by thermal decomposition [5]. The starting La(III) compound was characterized by FESEM, X-ray powder diffraction, and elemental analysis, and then its thermal decomposition was used to obtain crystalline La_2O_3 nanoparticles [5]. These results indicate that studying the thermal decomposition products of La(III) coordination compounds not only provides a characterization of their structure and stability, but also allows the preparation of functional oxide materials.

The complexation of lanthanide ions with organic ligands also plays an important role in their separation and concentration processes. Quintriqueo and co-authors studied the extraction of La(III) and Ce(III) complexes in the presence of β -diketones and trioctylphosphine oxide in ionic liquids and kerosene [6]. The authors found that the combined use of two different extractants showed a synergistic effect, significantly

affecting the extraction efficiency and separation coefficient of La(III) and Ce(III) complexes [6]. These results indicate that the ability of La(III) to form complexes with organic donor molecules is important not only in synthetic chemistry, but also in the separation and selective binding of lanthanides. The complexation of La(III) nitrate with amide-type oxygen donor ligands was also studied in detail. Namazova and co-authors studied the interaction of $\text{La}(\text{NO}_3)_3$ with methylenediacetamide in aqueous solution and found that a new complex compound with the composition $\text{La}(\text{NO}_3)_3 \cdot 2\text{C}_5\text{H}_{10}\text{O}_2\text{N}_2 \cdot 2\text{H}_2\text{O}$ was formed (Figure 2) [7].

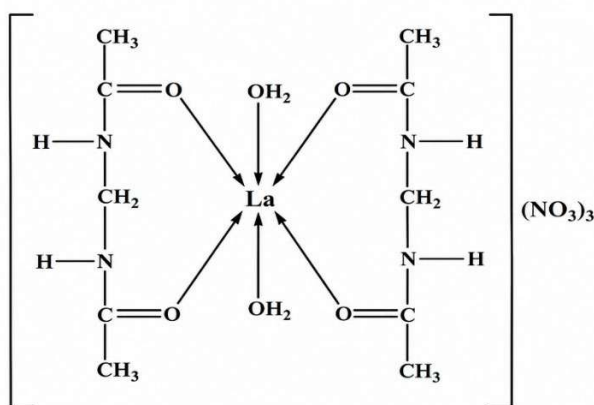


Figure 2. Structure of the coordination compound of lanthanum(III) nitrate with methylenediacetamide

The individuality of the complex was confirmed by derivatographic and X-ray phase analysis, and IR spectroscopic studies showed that the ligand is coordinated to the metal ion through the carbonyl oxygen [7]. It was also found that the crystal lattice of the obtained complex belongs to the monoclinic syngony. This information once again confirms that La(III) has a high affinity for O-donor groups. In lanthanum complexes with mixed ligands, the coordination sphere can have a more complex structure. Ruzieva and co-authors synthesized mixed ligand complexes of La(III) and Ce(III) with 2-amino-1-methylbenzimidazole and diisopropyldithiophosphate (Fig. 3) [8]. The complexes were studied by elemental analysis, X-ray diffraction, differential thermal analysis, and IR spectroscopy. According to the IR spectroscopy results, it was proposed that the diisopropyldithiophosphate and NO_3^- groups coordinate to the metal center in a bidentate-cyclic manner, and the 2-amino-1-methylbenzimidazole molecules in a

monodentate manner, resulting in the formation of a distorted dodecahedral coordination environment [8].

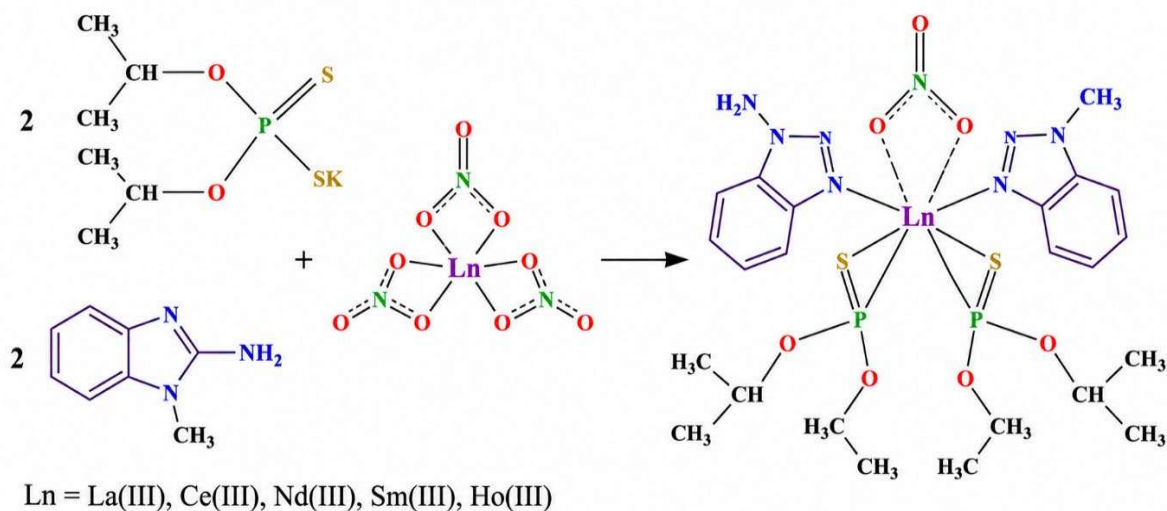


Figure 3. Scheme for the synthesis of mixed ligand complexes of Ln(III) ions with 2-amino-1-methylbenzimidazole and diisopropyldithiophosphate.

These results indicate that the combined presence of donor atoms of different nature and nitrate groups in the La(III) coordination sphere leads to complex structural formations.

The above studies show that La(III) ions form stable coordination complexes with various organic ligands containing oxygen, nitrogen, and sulfur donor atoms [1,2,4,7,8]. In particular, aromatic ligands with carboxyl groups are able to bind La(III) ions through oxygen atoms, resulting in the formation of complexes with various coordination structures [1,2]. At the same time, complexes of lanthanides with aminobenzoic acid derivatives have also been reported to be promising in terms of biological activity [1].

However, within the framework of these eight analyzed literature sources, there was no study that comprehensively studied the synthesis, coordination method and physicochemical properties of an individual coordination compound formed by La(III) nitrate with 4-aminobenzoic acid. In this regard, the presence of carboxyl and amino functional groups in the composition of 4-aminobenzoic acid determines that it is an interesting ligand for coordination interactions with La(III) ions. Therefore, the synthesis of a new coordination compound based on $\text{La}(\text{NO}_3)_3$ and 4-aminobenzoic acid, and the study of its composition and structure using modern physicochemical methods

such as IR spectroscopy, X-ray phase and thermal analysis are of great scientific importance.

Research Methodology

To obtain the coordination compound of lanthanum(III) nitrate with 4-aminobenzoic acid, 0.325 g (0.75 mmol) $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ was initially dissolved in 10 ml of distilled water. In a separate vessel, 0.309 g (2.25 mmol) 4-aminobenzoic acid (4-ABA) was dissolved in 20 ml of ethanol–water mixture. In order to increase the solubility of the ligand and partially deprotonate the carboxyl group, a solution of 0.126 g (2.25 mmol) KOH in a small amount of water was added dropwise to the solution [9,10]. The resulting clear ligand solution was slowly added to the lanthanum(III) nitrate solution under constant stirring. The pH of the reaction mixture was maintained between 5.0–6.0, as a strong alkaline medium may precipitate $\text{La}(\text{OH})_3$. The mixture was stirred at room temperature for 40–60 min on a magnetic stirrer.

The solution was then slowly evaporated and left at room temperature for 24–48 h for crystallization. The resulting white or light-colored crystalline precipitate was filtered off, washed successively with distilled water and ethanol, and dried at room temperature [11,12]. The structure of the synthesized coordination compound is shown in Figure 4.

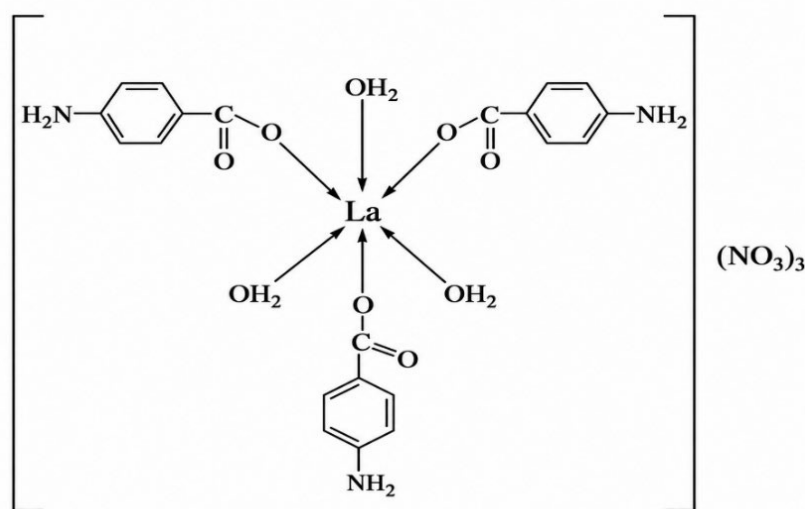


Figure 4. Structure of the molecule of the coordination compound of lanthanum(III) nitrate with 4-aminobenzoic acid (PABA)

Results and Discussion

IR spectroscopic studies were carried out to determine the composition of the synthesized $[\text{La}(\text{4-ABA})_3(\text{H}_2\text{O})_3]$ complex and the coordination properties of the La(III) ion with 4-aminobenzoate ligands. The IR spectrum of the complex was analyzed in comparison with the spectrum of free 4-aminobenzoic acid (4-ABA), and changes in the vibrational frequencies associated with the characteristic functional groups of the ligand were evaluated [13]. In particular, special attention was paid to the position of the $\nu_{\text{as}}(\text{COO}^-)$ and $\nu_{\text{s}}(\text{COO}^-)$ vibrations associated with the carboxyl group, as well as the appearance of new absorption lines characteristic of the La–O bond in the low-frequency region (Fig. 5). A broad absorption band is observed in the range of $3500\text{--}3000\text{ cm}^{-1}$ of the spectrum, with one of its maxima at 3062.96 cm^{-1} . This band can be explained by the superposition of the $\nu(\text{O--H})$ stretching vibrations of the water molecules in the complex, the $\nu(\text{N--H})$ stretching vibrations of the amino group, and the aromatic $\nu(\text{C--H})$ stretching vibrations. The broadening of the absorption band indicates the formation of hydrogen bonds with the participation of coordination water molecules and functional groups in the complex.

A very intense absorption line was observed in the spectrum of the complex at 1678.07 cm^{-1} . This line was mainly interpreted as belonging to the asymmetric stretching vibration $\nu_{\text{as}}(\text{COO}^-)$ of the carboxylate group; deformational vibrations of the --NH_2 group may also contribute to this region. The absorption line at 1537.27 cm^{-1} can be attributed to the combined contribution of the skeletal vibrations of the aromatic ring $\nu(\text{C=C})$ and the vibrations belonging to the carboxylate group. Also, the line at 1485.19 cm^{-1} belongs to the skeletal vibrations of the C=C bonds of the aromatic ring. An intense line corresponding to the symmetrical stretching vibration of the carboxylate group was observed at 1305.81 cm^{-1} . The stretching vibrations of the aromatic C--N bond may also be present in this region. If the value 1678.07 cm^{-1} is taken as $\nu_{\text{as}}(\text{COO}^-)$ and 1305.81 cm^{-1} as $\nu_{\text{s}}(\text{COO}^-)$, the difference between them is: $\Delta\nu = 1678.07 - 1305.81 = 372.26\text{ cm}^{-1}$ constitutes. The observed large $\Delta\nu$ value is consistent with the proposed structural model that the carboxylate group is coordinated to the La(III) ion in a monodentate manner, i.e. through a single oxygen atom. In this case, the

second carboxylate oxygen of the 4-aminobenzoate ligand is directly attached to the metal center. does not participate in coordination.

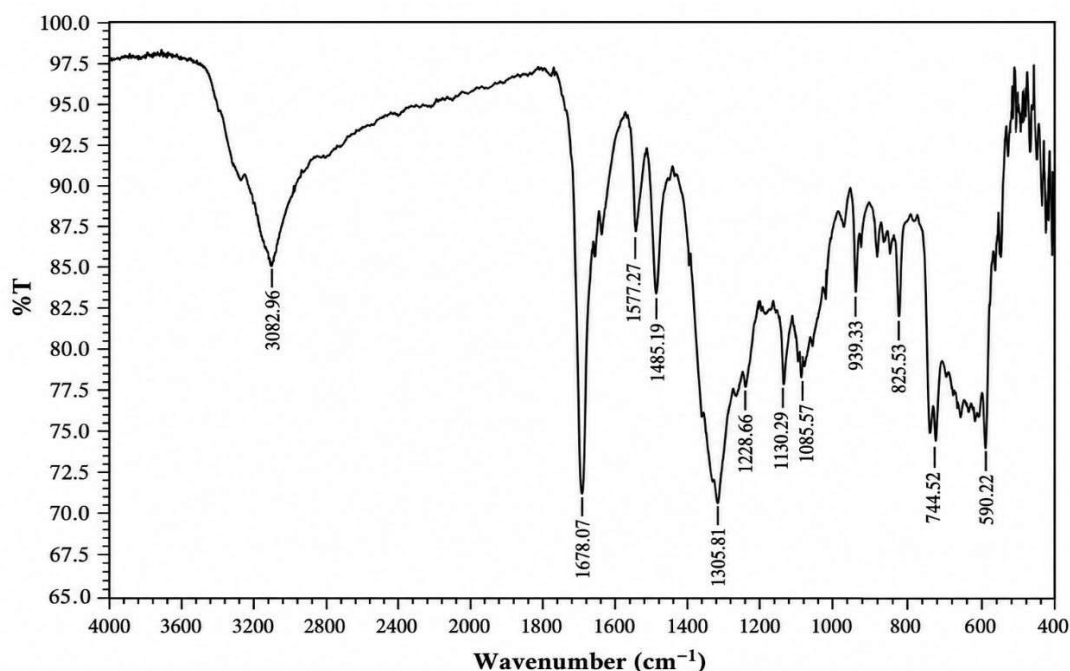


Figure 5. IR spectroscopy image of the complex compound $[\text{La}(4\text{-ABA})_3(\text{H}_2\text{O})_3]$

A number of absorption lines were also observed in the “fingerprint” region of the spectrum, characterizing the structure of the complex. In particular, the absorption at 1228.66 cm^{-1} can be attributed to the C–N valence and in-plane deformation vibrations, while the lines at 1130.29 and 1095.57 cm^{-1} can be attributed to the in-plane C–H deformation vibrations of the aromatic ring. The absorptions in the 939.33 , 825.53 and 744.52 cm^{-1} regions are associated with the out-of-plane deformation vibrations of the aromatic C–H bonds. In particular, the characteristic absorption around 825.53 cm^{-1} corresponds to the presence of a 1,4-substituted, i.e. para-substituted, benzene ring.

The low-frequency region is of particular importance in characterizing the complex formation. The absorption line observed at 590.22 cm^{-1} can be interpreted as belonging to the $\nu(\text{La-O})$ stretching vibration. This line supports the existence of a coordination bond between the La(III) center and the oxygen donor atoms. In the proposed $[\text{La}(4\text{-ABA})_3(\text{H}_2\text{O})_3]$ structure, such La–O bonds are formed by the carboxylate oxygens of the 4-aminobenzoate ligands and the oxygen atoms of the coordinating water molecules [14].

Thus, the IR spectroscopic data indicate the formation of the complex $[\text{La}(\text{4-ABA})_3(\text{H}_2\text{O})_3]$ and the monodentate coordination of the 4-aminobenzoate ligands to the La(III) center, mainly through the oxygen atom of the carboxylate group, is consistent with the proposed structure. According to this model, the three O-donor atoms of the three monodentate 4-ABA⁻ ligands and the three O-donor atoms of the three coordinating H₂O molecules form a total of six donor centers around La(III), and the coordination number of the metal ion is proposed to be 6. The broad absorption band around 3062.96 cm⁻¹ is consistent with the presence of water molecules and hydrogen bonds, and the low-frequency line at 590.22 cm⁻¹ is consistent with the formation of La–O coordination bonds. In order to determine the thermal stability and decomposition properties of the synthesized complex $[\text{La}(\text{4-ABA})_3(\text{H}_2\text{O})_3]$ (4-ABA⁻ — 4-aminobenzoate anion), thermal analysis was performed by TG, DTG and DTA methods [15]. The study was carried out in air atmosphere in the temperature range of 22–1000 °C. Comparative analysis of thermal analysis curves showed that the complex decomposed in several successive stages during heating. The initial stage of thermal decomposition was observed in the temperature range of 22–183 °C. The endothermic effect observed at around 96.68 °C in the DTA curve is associated with the decomposition of water molecules in the complex. The TG curve shows a gradual decrease in the mass of the sample in this temperature range, and by about 183 °C the residual mass was 95.35%. This process is explained by the dehydration of the complex, i.e., the separation of water molecules bound by hydrogen bonds in the coordination sphere. This result is also consistent with the IR spectroscopic data on the presence of water molecules in the complex. Further increase in temperature leads to intensive thermal destruction of the organic part of the complex. In the range of 183–325 °C, a significant mass loss is observed in the TG curve, and the residual mass decreases to about 57.55%. At this stage, the manifestation of obvious thermal effects around 155.38 and 183.45 °C in the DTA/DTG curves indicates that the decomposition process is proceeding with high intensity. This mass loss is associated with the thermo-oxidative destruction of 4-aminobenzoate ligands, including the decomposition of carboxylate fragments and decarboxylation processes.

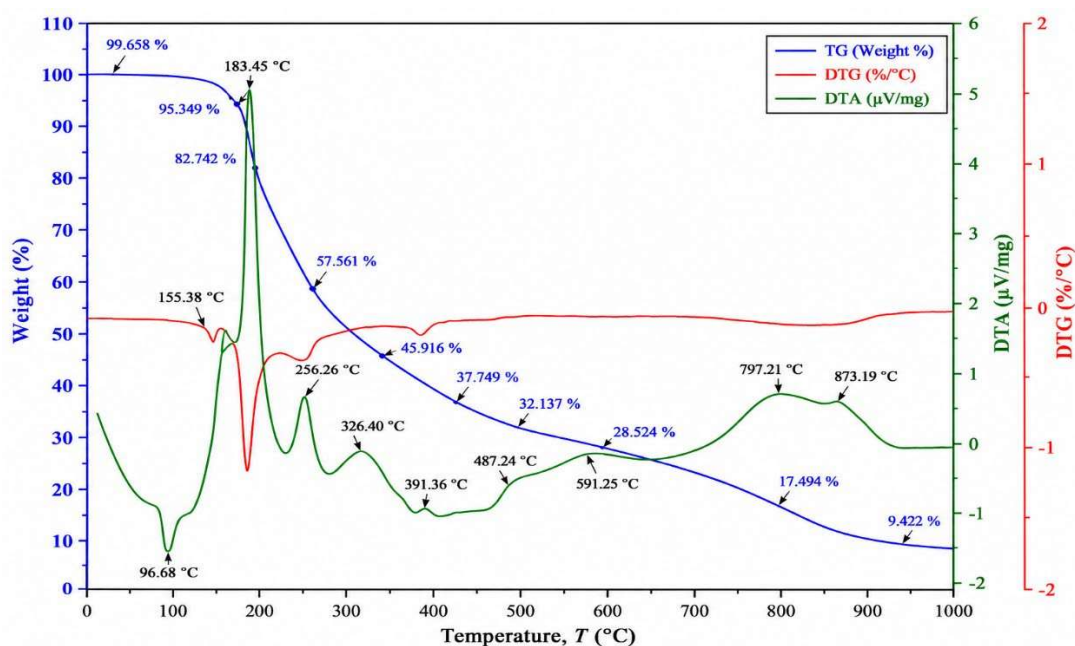


Figure 6. Results of TG–DTA–DTG thermal analysis of the complex compound $[\text{La}(4\text{-ABA})_3(\text{H}_2\text{O})_3]$

The next complex stage of thermal decomposition occurs in the range of approximately 325–609 °C. In this temperature range, a number of thermal effects are observed at around 326.40, 391.36, 487.24 and 591.25 °C. The mass fraction in the TG curve gradually decreases and reaches approximately 28.52% at around 608.8 °C. These processes are explained by the deep thermooxidative destruction of organic ligand residues, the decomposition of amino groups and aromatic ring fragments [16]. Since the process is carried out in an air atmosphere, oxidation of organic components and the release of volatile products containing CO_2 , H_2O and nitrogen are observed at these stages. The final stage of complex decomposition is observed in the high-temperature range of 609–1000 °C. The broad thermal effects observed in the DTA curve around 797.21 and 873.19 °C are interpreted as being related to the subsequent oxidation of carbonaceous and other intermediate decomposition products formed in the previous steps. In the TG curve, the residual mass decreases from 28.52% to 17.49%, and at the end of the process to approximately 9.42% at 1000 °C. The inorganic residue retained at high temperatures is associated with the formation of a lanthanum-containing oxide phase. In general, the TG–DTA–DTG analysis of the $[\text{La}(4\text{-ABA})_3(\text{H}_2\text{O})_3]$ complex shows that its thermal decomposition proceeds in the following sequence: dehydration → thermooxidative destruction of organic ligands → deep decomposition of aromatic

and amino-containing residues → formation of an inorganic lanthanum-containing residue at high temperatures.

Conclusion and Recommendations

A coordination compound $[\text{La}(\text{4-ABA})_3(\text{H}_2\text{O})_3]$ was synthesized based on lanthanum(III) nitrate and 4-aminobenzoic acid. In IR spectroscopic analysis, the $\Delta\nu = 372.26 \text{ cm}^{-1}$ value corresponds to the monodentate coordination of 4-aminobenzoate anions to the La(III) ion through the carboxylate oxygen, and the $\nu (\text{La-O})$ absorption line at 590.22 cm^{-1} indicates the formation of a metal-oxygen coordination bond. According to the proposed structural model, the coordination number of the La(III) ion is 6. TG–DTA–DTG analyses showed a multi-stage thermal decomposition of the complex, initially with the release of water molecules, followed by the thermo-oxidative destruction of organic ligands and the formation of an inorganic phase containing lanthanum at high temperature.

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UDC: 581.145.1:582.542.1

FLOWERING DYNAMICS OF AEGILOPS L. SPECIES

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Annotatsiya. Maqolada *Aegilops* L. turkumiga mansub turlarning gullash dinamikasi yoritilgan. *Aegilops* turkumiga mansub turlarning gullash biologiyasini ilmiy jihatdan o'rganish ushbu turkum turlarini xalq xo'jaligida intensiv foydalanish uchun tavsiya etishda katta ahamiyatga ega. Tadqiqot davomida ayrim ekologik omillarning, xususan, havo harorati va nisbiy namlikning, mazkur turlarning gullash jarayoniga ta'siri qayd etildi.

Kalit so'zlar: *Aegilops triuncialis* L., *Aegilops cylindrica* Host., *Aegilops tauschii* Coss., *Aegilops crassa* Boiss., gullash dinamikasi, ekologik omillar.

Аннотация. В статье рассматривается динамика цветения видов рода *Aegilops* L. Научное изучение биологии цветения видов рода *Aegilops* имеет большое значение при рекомендации видов данного рода для интенсивного использования в народном хозяйстве. В ходе исследования было зарегистрировано влияние отдельных экологических факторов, в частности температуры воздуха и относительной влажности, на процесс цветения изучаемых видов.

Ключевые слова: *Aegilops triuncialis* L., *Aegilops cylindrica* Host., *Aegilops tauschii* Coss., *Aegilops crassa* Boiss., динамика цветения, экологические факторы.

Annatation. The article describes the flowering dynamics of species of the genus *Aegilops* L. The scientific study of the flowering biology of *Aegilops* species is of great importance when recommending species of this genus for intensive use in the national economy. During the experiment, the influence of certain environmental factors (air temperature and relative humidity) on the flowering process of the species was recorded.

Key words: *Aegilops triuncialis* L., *Aegilops cylindrica* Host., *Aegilops tauschii* Coss., *Aegilops crassa* Boiss., flowering dynamics, environmental factors.

Introduction.

Flowering and pollination are among the most important processes in the reproductive biology of plants and provide valuable information for assessing the ecological and biological characteristics of plant species. Flowering is a critical stage in the life cycle of higher plants, during which the transition to reproductive development is completed and the processes associated with sexual reproduction take place. The onset, duration, and intensity of flowering are determined by the genetic and biological characteristics of a species and are strongly influenced by environmental conditions. A number of abiotic and agronomic factors, including temperature, moisture availability, photoperiod, soil conditions, and cultivation practices, can significantly affect the timing, duration, and dynamics of flowering. Consequently, the study of flowering phenology and its variability is essential for understanding the developmental patterns and reproductive strategies of plant species. This is particularly relevant for representatives of the family Poaceae, in which flowering characteristics may vary considerably depending on both species-specific traits and environmental conditions.

R.Ye. Levina [4; 1–95] established that the flowering process in plants is associated with the maturation of the male and female reproductive structures and is completed with fertilization. According to M.A. Pavlova [6; 1–12], the duration of flowering in different plant species is related to the number of lateral generative buds, while the development and distribution of these buds may, in turn, be influenced by plant density. These findings indicate that flowering dynamics are determined by a complex interaction between endogenous developmental processes and external environmental factors. The genus *Aegilops* L. is of particular interest because its species represent an important genetic resource for wheat improvement and possess valuable biological and adaptive traits. A comprehensive understanding of their reproductive biology, including flowering phenology and pollination characteristics, is therefore essential for assessing their potential for utilization in breeding programs, genetic resource conservation, and agricultural applications. In particular, the evaluation of flowering characteristics under introduced environmental conditions can provide important information on the adaptability and reproductive potential of *Aegilops* species outside

Research Methodology

The seasonal rhythm of development of the studied *Aegilops* species was investigated using the methods described by I.V. Borisova [2; 619–626] and I.N. Beydeman [1; 1–154]. The duration of the principal developmental phases was recorded, including the vegetative phases-emergence, formation of the third leaf, tillering, and booting-as well as heading, flowering, and grain maturation. Grain maturation was assessed according to the milk, dough, and full maturity stages.

The flowering biology and seasonal dynamics of the studied plants were investigated using the methods proposed by A.N. Ponomaryov [7; 115–179; 61; 1440] and the methodological recommendations of X.K. Karshiboyev [5; 1–84]. The timing, duration, and seasonal dynamics of flowering were recorded throughout the growing season. Seed productivity of the plants was evaluated according to the methodological recommendations of I.V. Vaynagiy [3; 826–831].

Results and Discussion

After the formation of spikes, flowering began in the studied species. This phenological phase occurred during the first ten days of May.

In *A. triuncialis*, the flowering phase was observed on May 1, 2022, when the air temperature was +28 °C and the relative humidity was 31%. In 2023, the onset of flowering in this species was observed on April 28, when the air temperature was +28 °C and the relative humidity was 24%.

In *A. cylindrica*, this stage was observed on April 30, 2022, when the air temperature was +29 °C and the relative humidity was 34%. In 2023, this phase occurred on April 28, when the air temperature was +28 °C and the relative humidity was 24%.

In *A. tauschii*, the flowering phase was observed on May 1, 2022, when the air temperature was +28 °C and the relative humidity was 31%. In 2023, flowering began on April 28, when the air temperature was +28 °C and the relative humidity was 24%.

In *A. crassa*, the flowering stage was observed on May 2, 2022, when the air temperature was +33 °C and the relative humidity was 29%. In 2023, this stage was observed on April 30, when the air temperature was +30 °C and the relative humidity was 22%.

In all the species studied, flowering also began in the middle part of the spike. Subsequently, the lower and upper spikelets flowered. During flowering, the floral glumes of each spikelet opened, exposing the anthers, and pollination took place within a short period of time. A correlation analysis was also performed for this phenological phase. The results showed that temperature had a negative effect on flowering, with a correlation coefficient of $r = -0.4$. This indicates that an increase in temperature slows down the flowering process in the studied species. In addition, the relationship between the flowering process and humidity was analyzed. The correlation coefficient for humidity was $r = 0.4$, indicating that higher humidity promotes phenological development and the flowering process in these species.

These results provide scientific evidence that environmental factors have an important influence on the dynamics of flowering. Additionally, the diurnal and seasonal flowering patterns of these species were studied.

Table 1. Seasonal flowering period of *Aegilops* L. species under introduction conditions (2022–2023; $n = 100$).

Species name	Flowering period, days			Flowering duration, days
	Onset of flowering	Peak flowering	End of flowering	
<i>A. triuncialis</i>	01.05	04.05	07.05	7
	28.04	03.05	08.05	10
<i>A. cylindrica</i>	30.04	04.05	08.05	9
	28.04	03.05	11.05	13
<i>A. tauschii</i>	25.04	01.05	06.05	11
	23.04	26.04	04.05	11
<i>A. crassa</i>	26.04	01.05	07.05	11
	24.04	29.04	05.05	11

The flowering process of species belonging to the genus *Aegilops* L. was monitored under introduction conditions during 2022–2023. Depending on the meteorological conditions of each year, the studied species exhibited differences in the timing of flowering (Table 1). In 2022–2023, flowering in the studied species occurred from the third decade of April to the first decade of May (see Table 1). Depending on the meteorological conditions of the respective year, the flowering period of the species varied by several days. In 2022, the duration of flowering among the studied species ranged from 7 days in *A. triuncialis* to 11 days in *A. tauschii* and *A. crassa*. In 2023,

flowering lasted from 10 days in *A. triuncialis* to 13 days in *A. cylindrica*. During the study period, flowering in some species began in the lower part of the spike, as observed in *A. triuncialis*. In other species, such as *A. cylindrica*, *A. tauschii*, and *A. crassa*, flowering initially occurred in the second and third spikelets, followed by flowering of the spikelets in the upper part of the spike. Prior to anthesis, the glumes of the spikelets opened, after which the filaments of the stamens protruded outward and hung from the spikelets (Fig. 3).

The results of the study showed that flowering in the studied species occurred under conditions of relatively high air humidity and low air temperature (Fig. 1).

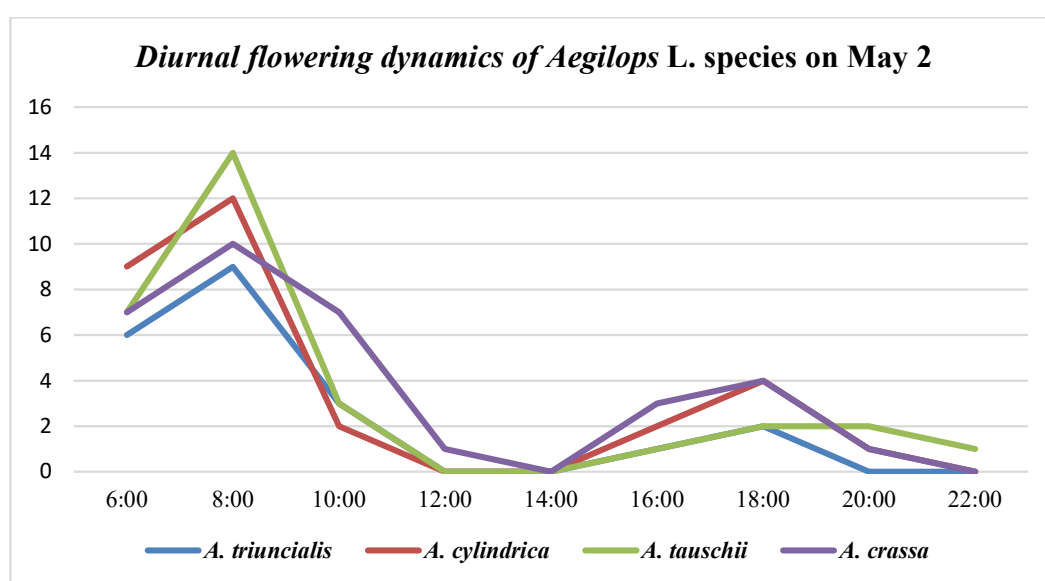


Figure 1. Diurnal flowering dynamics of *Aegilops* L. species.

The highest number of flowers opened during the period from 06:00 to 10:00 (May 2, 2022). During the middle part of the day, flowering was almost completely absent in the studied species. From 16:00 to 18:00, the number of newly opened flowers decreased, while no newly opened flowers were recorded after 20:00.

During the study period, the influence of certain environmental factors, particularly air temperature and relative humidity, on the flowering process of the studied species was observed (Fig. 2). The flowering process of plants is closely associated with a number of environmental factors, including temperature, light availability, air humidity, and mineral nutrition [9; pp. 7–204]. The species examined in

our study exhibited several common patterns in their flowering dynamics, with the timing of flowering being closely associated with the number of spikelets per spike.

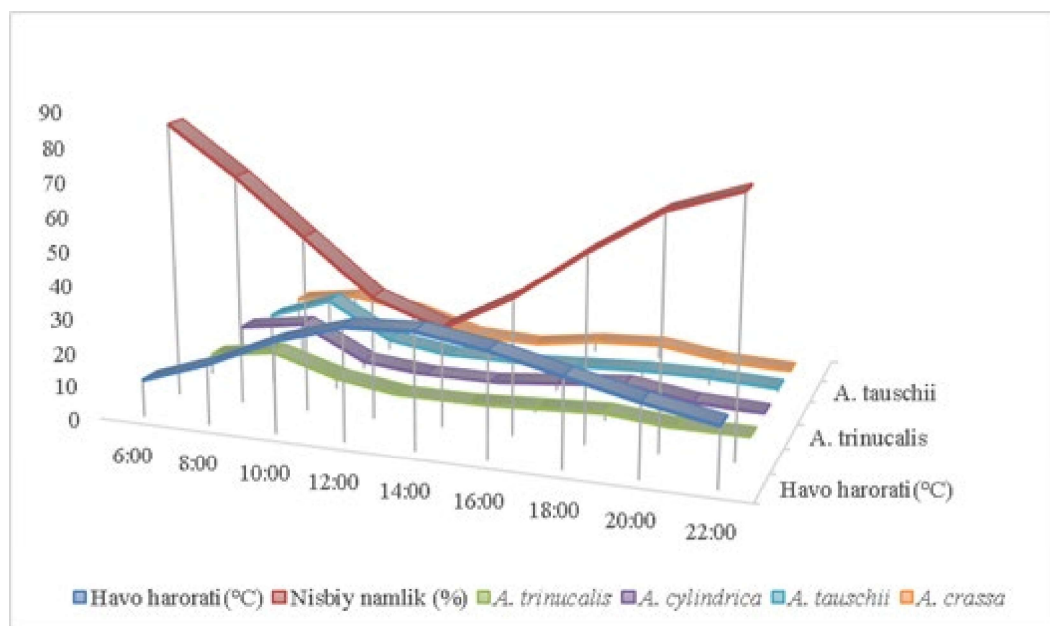


Figure 2. Effects of air temperature and relative humidity on flowering in *Aegilops* L. species.



Figure 3. Flowering process of *Aegilops* L. species.

Seed productivity in plants is largely determined by the quantity and quality of pollen grains. Flowering and pollination are important biological processes with

considerable practical significance and play an important role in addressing a number of issues related to plant evolution [8; pp. 1–43].

Although anemophilous plants generally produce large quantities of pollen, information on the fertility of pollen grains in representatives of the genus *Aegilops* L. remains limited. The pollen grains examined in the present study are shown in Fig. 4. Pollen fertility is of considerable importance for taxonomic studies and plant breeding programs, as it provides valuable information on reproductive potential and can contribute to the assessment of genetic relationships among taxa.

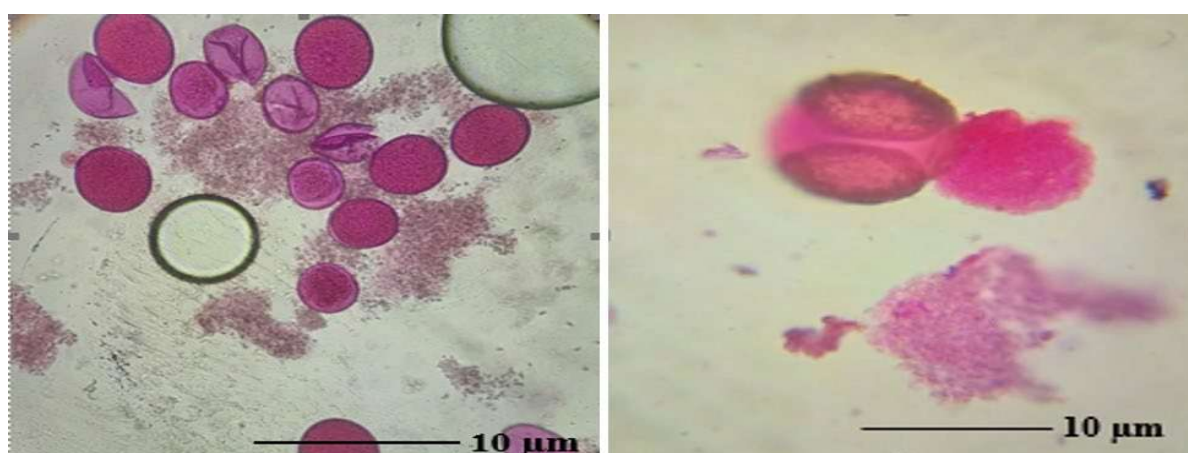


Figure 4. Pollen grains of *Aegilops* L. species. ×400. Scale bar = 10 μm.

Furthermore, pollen fertility is a key factor determining whether sexual reproduction provides sufficient reproductive regeneration to ensure the persistence and survival of a particular species within a plant population [10; pp. 30–33].

Table 2. Pollen fertility of flowers in *Aegilops* L. species (n = 100).

№	Species	Pollen collection time	Pollen fertility (%)
1	<i>Aegilops tauschii</i>	2022	94,0
		2023	92,5
2	<i>Aegilops cylindrica</i>	2022	96,6
		2023	93,4
3	<i>Aegilops crassa</i>	2022	96,4
		2023	92,1
4	<i>Aegilops triuncialis</i>	2022	99,1
		2023	95,2

During the study, pollen fertility in representatives of the genus *Aegilops* L. was determined and expressed as a percentage. The results obtained during 2022–2023

showed that pollen fertility in *Aegilops crassa* exceeded 92.1%, indicating a high level of reproductive stability in this species (Table 2).

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Section 6. ACTUAL PROBLEMS OF MATHEMATICS, PHYSICS AND MECHANICS

UDK 546.824-31

HYDROTHERMAL SYNTHESIS OF TiO_2 NANOTUBES: EFFECTS OF HCL TREATMENT TIME AND ANNEALING TEMPERATURE ON CRYSTAL STRUCTURE, MORPHOLOGY, AND OPTICAL PROPERTIES

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Annotatsiya. TiO_2 nanonayli tuzilmalar sferik TiO_2 nanozarrachalaridan iborat boshlang'ich kukunga ishqoriy gidrotermal ishlov berish, keyinchalik HCl kislota bilan va termik ishlov berish orqali sintez qilindi. Kislota bilan ishlov berish davomiyligi hamda termik ishlov berish haroratining hosil bo'lgan nanostrukturalarning fazaviy tarkibi, morfologiyasi va optik xossalariga ta'siri XRD, SEM, o'lchamlar taqsimoti tahlili va UV-Vis spektroskopiyasi yordamida baholandi. XRD tahlili HCl bilan 1 soatlik ishlov berish anataz fazasining to'liq shakllanishi uchun yetarli emasligini, 3 soatlik ishlov esa anataz fazasining aniq hosil bo'lishini ta'minlashini ko'rsatdi. Termik ishlov berish natijasida kristallik darajasi yaxshilanib, harorat 450 dan 650 °C gacha oshirilganda kristallit o'lchami 13,44 nm dan 15,12 nm gacha ortdi. SEM tasvirlari boshlang'ich sferik TiO_2 nanozarrachalarining o'rtacha diametri 18,4 nm bo'lgan nanonayli morfologiyaga aylanganini tasdiqladi. HCl bilan 3 soat ishlov berilgan namunalarda optik taqiqlangan zona kengligi termik ishlov berishdan oldingi 3,45 eV dan termik ishlovdan so'ng taxminan 3,32 eV gacha kamaydi. Olingan natijalar kislota bilan ishlov berish davomiyligi TiO_2 nanonaylarining fazaviy shakllanishida, termik ishlov berish esa ularning kristallik darajasi va optik xossalarini boshqarishda muhim rol o'ynashini ko'rsatdi.



Kalit soʻzlar: *TiO₂ nanonaylari; gidrotermal sintez; ishqoriy ishlov berish; HCl bilan ishlov berish; termik ishlov berish; anataz; rentgen difraktsiyasi; diffuz qaytish; optik taqiqlangan zona kengligi*

Аннотация. Нанотрубчатые структуры TiO₂ были синтезированы путем щелочной гидротермальной обработки коммерческого порошка TiO₂ с последующей обработкой HCl и термическим отжигом. Влияние продолжительности кислотной обработки и температуры отжига на структурные, морфологические и оптические свойства исследовали методами рентгеновской дифракции (XRD), сканирующей электронной микроскопии (SEM), анализа распределения по размерам и УФ–видимой спектроскопии диффузного отражения. Результаты XRD показали, что обработка HCl в течение 1 ч была недостаточной для получения характерной анатазной фазы TiO₂, тогда как увеличение продолжительности обработки до 3 ч привело к отчетливому формированию фазы анатаза. Последующий термический отжиг улучшил кристалличность, при этом размер кристаллитов увеличился с 13,44 до 15,12 нм в диапазоне температур от 450 до 650 °С. SEM-анализ подтвердил превращение частиц исходного коммерческого материала в нанотрубчатые структуры со средним диаметром 18,4 нм. Ширина оптической запрещенной зоны образцов, обработанных HCl в течение 3 ч, уменьшилась с 3,45 эВ до отжига приблизительно до 3,32 эВ после термической обработки. Эти результаты показывают, что продолжительность кислотной обработки является критически важным параметром фазообразования, тогда как термический отжиг позволяет эффективно регулировать кристалличность и оптические свойства гидротермально синтезированных нанотрубок TiO₂.

Ключевые слова: *нанотрубки TiO₂; гидротермальный синтез; щелочная обработка; обработка HCl; термический отжиг; анатаз; рентгеновская дифракция; диффузное отражение; ширина оптической запрещенной зоны*

Abstract. TiO₂ nanotubes structures were synthesized by alkaline hydrothermal treatment of commercial TiO₂ powder, followed by HCl treatment

and thermal annealing. The effects of acid-treatment time and annealing temperature on the structural, morphological, and optical properties were investigated by XRD, SEM, size-distribution analysis, and UV–Vis diffuse-reflectance spectroscopy. XRD showed that 1 h HCl treatment was insufficient to obtain the characteristic anatase TiO_2 structure phase, whereas extending the treatment to 3 h resulted in clear anatase phase formation. Subsequent annealing improved crystallinity, with the crystallite size increasing from 13.44 to 15.12 nm between 450 and 650 °C. SEM confirmed the transformation of the commercial precursor particles into nanotubes structures with an average diameter of 18.4 nm. The optical band gap of the 3 h HCl-treated samples decreased from 3.45 eV before annealing to approximately 3.32 eV after thermal treatment. These results demonstrate that acid-treatment duration is a critical parameter for phase formation, while annealing effectively controls the crystallinity and optical properties of hydrothermally synthesized TiO_2 nanotubes.

Key words: *TiO_2 nanotubes; hydrothermal synthesis; alkaline treatment; HCl treatment; annealing; anatase; X-ray diffraction; diffuse reflectance; optical band gap.*

Introduction

Titanium dioxide (TiO_2) is one of the most extensively investigated oxide semiconductors because of its chemical stability, low toxicity, corrosion resistance, and useful electronic and optical properties. These characteristics have led to its widespread investigation in photocatalysis, environmental remediation, photoelectrochemical systems, sensors, and energy-conversion technologies [1,2]. For photocatalytic applications in particular, material performance is strongly influenced by crystalline phase, crystallinity, particle dimensions, surface structure, defect chemistry, and optical response. Consequently, controlling these properties during synthesis and post-treatment is as important as selecting TiO_2 itself.

One-dimensional TiO_2 - and titanate-based nanostructures, including nanotubes, nanorods, and nanowires, have received considerable attention because their anisotropic geometry can provide large accessible surfaces and short radial transport distances while

retaining extended pathways along the one-dimensional structure [3,4]. TiO_2 nanotubes have therefore been studied for photocatalysis, photoelectrochemistry, sensing, solar-energy conversion, and electrochemical energy storage [3,11]. Their properties, however, depend strongly on the route by which the nanotubes structure is produced and on the subsequent chemical and thermal treatments.

Among the available synthesis approaches, alkaline hydrothermal processing is attractive because it is comparatively simple, does not require a sacrificial template, and can directly convert commercial TiO_2 powders into one-dimensional titanate-derived structures. The pioneering work of Kasuga et al. demonstrated the formation of tubular titanium oxide structures through treatment of TiO_2 in concentrated NaOH [5]. Later studies established that the products formed under strongly alkaline hydrothermal conditions are commonly better described as layered sodium titanates or protonated titanates rather than phase-pure anatase TiO_2 [4,6,7]. The conversion process is generally associated with partial dissolution and rearrangement of Ti–O frameworks, formation of layered titanate species, and subsequent scrolling or restructuring into tubular morphologies.

Acid treatment is therefore a critical step after alkaline hydrothermal synthesis. Exposure to dilute HCl promotes Na^+/H^+ ion exchange and removal of sodium-containing species from the interlayer region, producing protonated titanate structures whose subsequent thermal behavior differs markedly from that of sodium-rich titanates [6,7]. Morgado et al. showed that residual sodium content has a pronounced influence on the structure and thermal transformation of hydrothermally synthesized titanate nanotubes [7]. Similarly, Tsai and Teng demonstrated that the HCl-washing conditions influence the physical characteristics and formation of titania nanotube aggregates [6]. More recent work has also shown that acid washing and annealing are coupled parameters governing the stability and phase evolution of hydrothermally prepared nanotubes [9].

Thermal treatment is commonly used to increase crystallinity and convert protonated titanate structures toward TiO_2 phases. At the same time, annealing can induce dehydration, grain growth, sintering, and partial loss of the nanotubes morphology when

the temperature becomes sufficiently high [7–9]. Thus, an appropriate annealing window is required to obtain a crystalline TiO_2 structure without unnecessarily compromising nanoscale morphology. Previous studies have reported significant changes in crystallite size, pore structure, and phase composition with increasing calcination temperature [8,9].

In the present work, commercial TiO_2 powder was transformed into nanotubes structures by hydrothermal treatment in 10 M NaOH at 130 °C. The study focuses on two processing variables that are often treated only as secondary steps: HCl treatment time and post-annealing temperature. HCl treatment durations of 1 and 3 h were compared, followed by annealing at 450, 550, and 650 °C for 2 h. XRD, SEM, SEM-derived size distributions, and UV–Vis diffuse-reflectance spectroscopy were used to establish correlations between processing conditions, phase evolution, morphology, crystallite size, and optical response. Although the materials were prepared with photocatalytic applications in mind, the present paper is limited to synthesis and physicochemical characterization and does not report photocatalytic activity measurements.

Research Methodology

1. Materials. A commercial TiO_2 powder was used as the titanium-containing precursor. Sodium hydroxide (NaOH, $\geq 99\%$), hydrochloric acid (HCl, 37%), ethanol, and distilled water were used as received.

2. Hydrothermal synthesis and post-treatment. TiO_2 nanotubes products were prepared by an alkaline hydrothermal route adapted from the method originally introduced by Kasuga et al. [5]. The synthesis process of the TiO_2 nanotubes is schematically shown in the Fig. 1. Briefly, a 10 M NaOH solution was prepared by dissolving 20 g of NaOH in distilled water to a final volume of 50 mL. Certain amount of commercial TiO_2 powder was added to the alkaline solution. The suspension was magnetically stirred at 80 °C for 30 min and was subjected twice to ultrasonic treatment for 2 min during mixing. The resulting suspension was transferred to a Teflon-lined autoclave and hydrothermally treated at 130 °C for 24 h.

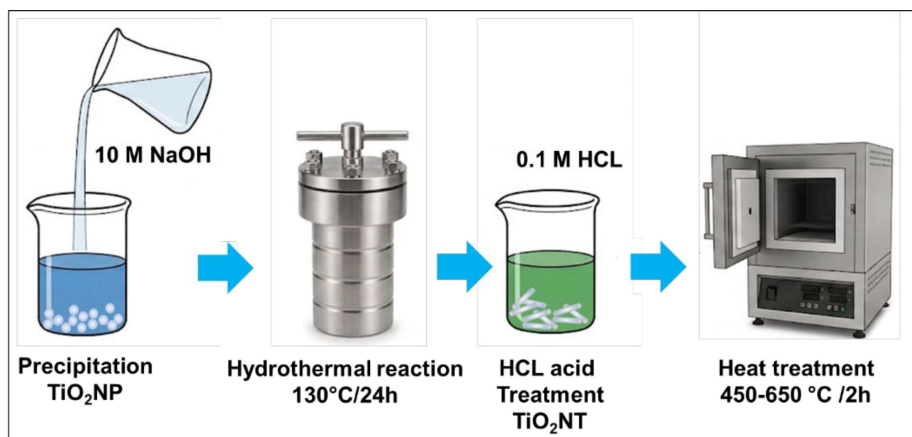


Figure 1. Schematic illustration of the TiO₂ nanotube fabrication process using alkaline hydrothermal method.

After hydrothermal treatment, the solid product was separated by filtration and washed repeatedly with distilled water until approximately neutral pH was reached. The material was dried at 65 °C for 24 h. The dried hydrothermal product was then divided into two groups and treated in 125 mL of 0.1 M HCl for either 1 h or 3 h. After acid treatment, the samples were washed with distilled water and finally with ethanol until the washing solution reached approximately pH 6, followed by drying at 65 °C for 24 h.

For each acid-treatment series, portions of the dried material were retained without thermal treatment, while the remaining portions were annealed in air at 450, 550, or 650 °C for 2 h using a heating rate of 20 °C min⁻¹. For clarity, the samples are referred to as NT-1h (HCL) and NT-3h (HCL) for the unannealed products after 1 and 3 h HCl treatment, respectively, and as NT-1h (HCL) -T or NT-3h (HCL) -T, where T denotes the annealing temperature in °C.

3. Characterization. The phase composition and crystal structure of the samples were examined by X-ray diffraction using a Rigaku MiniFlex 600 diffractometer with Cu K α radiation ($\lambda = 1.5406$ Å). The average coherent crystallite size was estimated from the width of the principal anatase reflection using the Scherrer equation:

$$D = K\lambda / (\beta \cos \theta)$$

where D is the coherent crystallite size, K is the Scherrer constant (0.89 in this work), λ is the X-ray wavelength, β is the full width at half maximum (FWHM) of the diffraction peak in radians, and θ is the Bragg angle. The calculated Scherrer size represents a coherent diffraction-domain size and should not be interpreted as the physical particle

diameter or nanotube diameter. Surface morphology was investigated using an Thermo Scientific Apreo ChemiSEM scanning electron microscope. Size-distribution histograms were obtained from the SEM images by measuring the apparent lateral size of the commercial TiO_2 precursor particles and the external diameter of the nanotubes structures. Because these quantities describe different geometrical features, they are reported separately and are not used as directly equivalent particle-size metrics. Optical properties were investigated by UV–Vis diffuse-reflectance spectroscopy using a SPECORD 210 PLUS spectrophotometer. Apparent optical band-gap values were estimated from Tauc plots constructed from the diffuse-reflectance data [10].

Results and Discussion

1. Effect of HCl treatment time and annealing temperature on crystal structure.

Figure 2 compares the XRD patterns of the commercial TiO_2 precursor with the hydrothermally synthesized products subjected to 1 h and 3 h HCl treatment. The commercial precursor exhibits the characteristic diffraction pattern of crystalline TiO_2 with prominent anatase reflections. In comparison, the 1 h HCl treated series demonstrated a different behavior (Figure 2a). The as-treated NT-1h sample and the corresponding samples annealed at 450, 550, and 650 °C do not reproduce the characteristic anatase pattern of the commercial reference. Instead, the diffraction profiles remain dominated by reflections and broad features associated with the hydrothermally generated titanate-derived structure. This result indicates that, under the present synthesis conditions, 1 h in 0.1 M HCl was insufficient to produce the structural state required for recovery of an anatase-type TiO_2 diffraction pattern, even after subsequent thermal treatment. This observation is consistent with the established chemistry of alkaline-hydrothermal titanate synthesis. Concentrated NaOH converts TiO_2 into sodium-containing layered titanate species, and acid washing promotes Na^+/H^+ ion exchange and structural reorganization [4,6,7]. Importantly, the present XRD data provide evidence for a difference in phase evolution but do not directly measure residual sodium concentration. Therefore, the 1 h result is most appropriately interpreted as being consistent with incomplete acid-induced ion exchange and persistence of titanate-derived phases rather than as direct quantitative proof of sodium retention. A

substantially different XRD response was obtained when the HCl treatment was extended to 3 h (Figure 2b). The NT-3h series displays the characteristic anatase TiO_2 reflections, including the intense peak near $2\theta \approx 25.3^\circ$ assigned to the (101) plane, together with reflections around 37.8° , 48.0° , 53.9° , 55.1° , 62.7° , and 68.8° corresponding to the (004), (200), (105), (211), (204), and (116) planes, respectively. The persistence of the anatase pattern after annealing at $450\text{--}650^\circ\text{C}$ indicates that the longer acid treatment produced a precursor more readily converted to anatase TiO_2 during subsequent thermal processing. Comparable effects of acid washing on titanate composition and thermally induced TiO_2 formation have been reported previously [7,9].

The diffraction peaks of the annealed NT-3h samples become sharper with increasing temperature, indicating increased crystallinity and growth of coherent diffraction domains. Scherrer analysis of the annealed 3 h series gave crystallite sizes of 13.44, 14.51, and 15.12 nm for 450, 550, and 650°C , respectively (Table 1). The gradual increase is consistent with thermally activated atomic diffusion and grain growth. The commercial TiO_2 reference showed a larger Scherrer size of 36.92 nm; however, this value should not be compared directly with the SEM-derived apparent particle size because XRD and SEM quantify fundamentally different structural length scales.

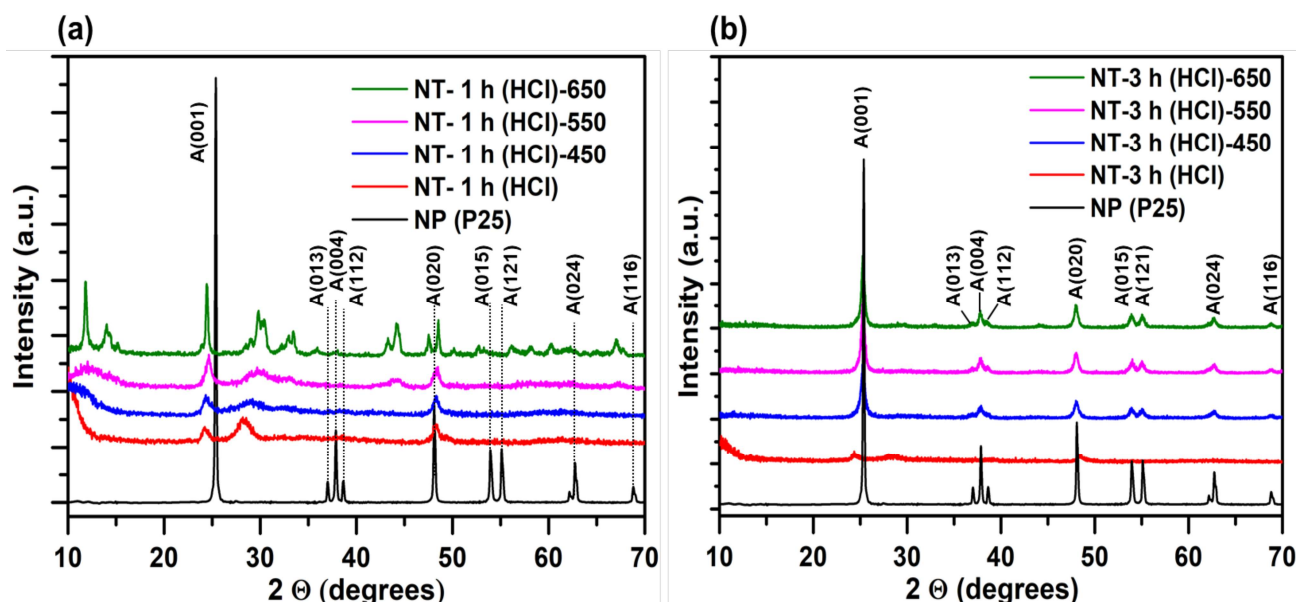


Figure 2. (a) XRD patterns of the commercial TiO_2 precursor and hydrothermally derived samples treated with 0.1 M HCl for 1 h, before and after annealing at 450, 550, and 650°C for 2 h; (b) corresponding XRD patterns for the 3 h HCl-treated series.

Table 1. Scherrer crystallite sizes obtained from XRD.

Sample	Crystallite size (nm)
Commercial TiO ₂	36.92
NT-3h-450	13.44
NT-3h-550	14.51
NT-3h-650	15.12

2. Morphology and SEM-derived size distribution. Figure 3a shows the morphology of the commercial TiO₂ precursor. The powder consists of irregularly shaped particles and agglomerates without a preferred one-dimensional morphology. After alkaline hydrothermal treatment and post-washing, the morphology changes dramatically (Figure 3b), and the product is dominated by elongated, high-aspect-ratio structures arranged in an entangled network. The observed morphology is consistent with the formation of nanotubes TiO₂ structures through alkaline hydrothermal conversion of the starting powder, as widely reported for related systems [4–6]. The corresponding SEM-derived size distributions are presented in Figure 4. The commercial precursor has a mean apparent particle size of 125.4 nm based on the dimensions measured in the SEM micrograph, whereas the nanotubes product exhibits a mean external diameter of 18.4 nm. It should be noted that the mean value of 125.4 nm corresponds to the apparent lateral size of the commercial TiO₂ particles or particle agglomerates observed by SEM, whereas the value of 18.4 nm represents the average outer diameter of the synthesized nanotubes. Therefore, the ratio between these values does not reflect the efficiency of the hydrothermal conversion.

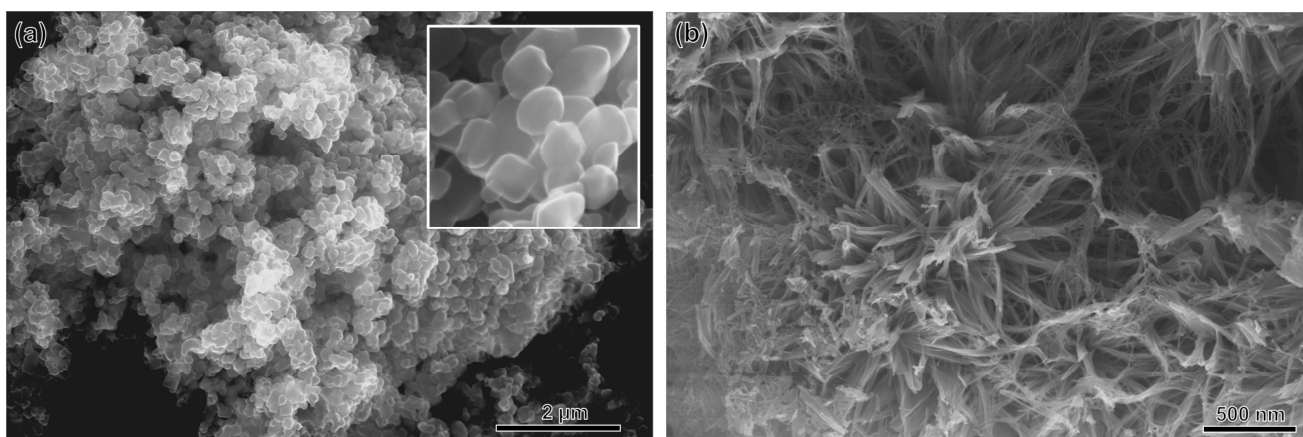


Figure 3. SEM images of (a) the commercial TiO₂ precursor and (b) the as-formed nanotubes product obtained after hydrothermal treatment at 130°C for 24 h and post-washing with 0.1M HCL for 3h.

Instead, the corresponding size distributions provide evidence of a pronounced morphological transformation from relatively coarse and irregular particulate structures to much finer one-dimensional nanotubes features.

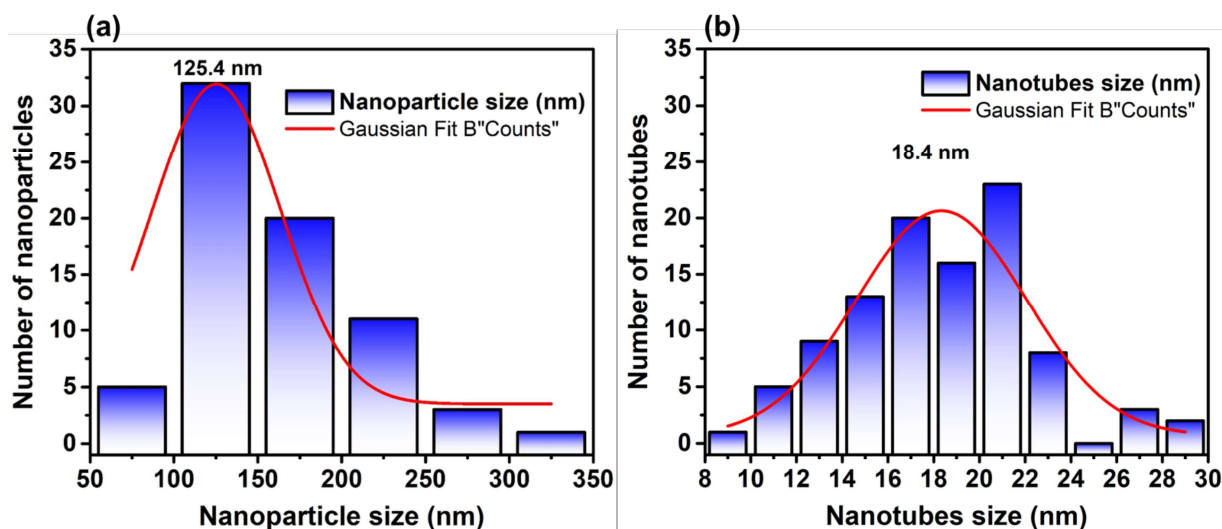


Figure 4. SEM-derived size distributions of (a) the commercial TiO_2 precursor, with a mean apparent particle size of 125.4 nm, and (b) the as-formed nanotubes product, with a mean external diameter of 18.4 nm.

3. UV–Vis diffuse-reflectance and optical band-gap analysis. The UV–Vis diffuse-reflectance spectra and corresponding Tauc plots are shown together in Figure 5, with the 1 h HCl-treated series in (a,b) and the 3 h HCl-treated series in (c,d). This presentation makes it possible to distinguish the optical consequences of acid-treatment time from those of the subsequent annealing step.

Table 2. Apparent optical band-gap values derived from Tauc analysis.

Sample	1 h HCl series, Eg (eV)	3 h HCl series, Eg (eV)
Commercial TiO_2	3.27	3.27
Unannealed NT	3.72	3.45
NT-450 °C	3.43	3.32
NT-550 °C	3.43	3.32
NT-650 °C	3.48	3.32

For the 1 h HCl-treated series (Figure 5a,b), the unannealed NT-1h sample exhibited an apparent optical band gap of 3.72 eV, considerably higher than the 3.27 eV value obtained for the commercial TiO_2 reference. After annealing, the estimated values decreased to 3.43 eV at 450 °C, 3.43 eV at 550 °C, and 3.48 eV at 650 °C (Table 2). The relatively high values of the 1 h series are consistent with the XRD evidence showing

that these samples do not possess the same anatase structure as the commercial TiO_2 reference. Accordingly, their optical response should not be interpreted simply as a temperature-dependent shift of anatase TiO_2 , it is more likely reflects the different electronic structure of titanate-derived phases together with changes in crystallinity and structural disorder during heating. The 3 h HCl-treated series shows a different trend (Figure 5c,d). The unannealed NT-3h sample had an apparent band gap of 3.45 eV, while all three annealed samples gave values close to 3.32 eV. This value is close to that of the commercial TiO_2 reference and is consistent with the anatase-type XRD pattern observed for the 3 h series.

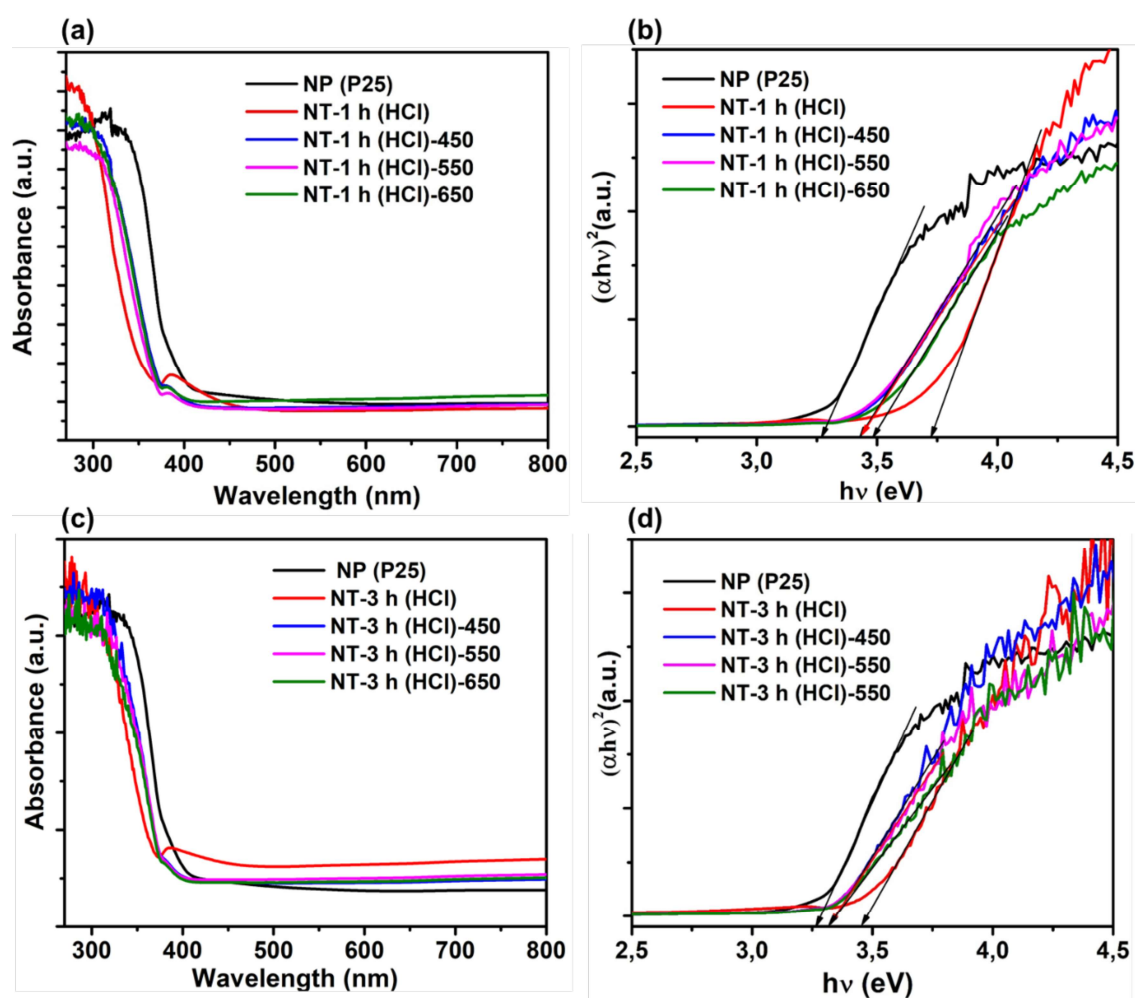


Figure 5. UV-Vis diffuse-reflectance spectra and corresponding Tauc plots of the commercial TiO_2 precursor and the HCl-treated series before and after annealing at 450, 550, and 650 °C for 2 h: (a) diffuse-reflectance spectra and (b) Tauc plot for the 1 h HCl-treated series; (c) diffuse-reflectance spectra and (d) Tauc plot for the 3 h HCl-treated series.

The near-constant band-gap values from 450 to 650 °C indicate that, once the longer acid treatment has enabled formation of an anatase-type phase, increasing the annealing temperature within this range has a smaller effect on the optical edge than the initial acid-treatment duration. The main temperature-dependent structural change in this interval is therefore better reflected by the increase in crystallite size than by a large shift in the apparent band gap. Taken together, the XRD and optical results show that HCl treatment time is a key parameter governing the structural state of the hydrothermally formed material. The difference between the 1 h and 3 h series is larger than the variation produced by changing the annealing temperature within either series. This finding supports the use of acid-treatment duration as an independent synthesis variable rather than treating the HCl wash merely as a routine cleaning step.

Conclusion and Recommendations

Commercial TiO₂ powder was successfully transformed into anatase TiO₂ nanotubes by alkaline hydrothermal treatment. HCl treatment time was found to be the key parameter controlling phase formation, with 3 h treatment required to obtain clear anatase reflections. Subsequent annealing increased the crystallite size from 13.44 to 15.12 nm. SEM confirmed nanotube formation with an average diameter of 18.4 nm, while UV–Vis analysis showed band-gap stabilization near 3.32 eV for the 3 h HCl-treated samples. These results highlight the dominant role of acid treatment in determining the structural and optical properties of the synthesized TiO₂ nanotubes.

Acknowledgement

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NUMERICAL ALGORITHMS AND SOFTWARE FOR FINITE ELEMENT ANALYSIS OF TWO-DIMENSIONAL ELASTICITY PROBLEMS

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Annotatsiya. Ushbu maqolada ikki o'lbhovi elastiklik masalalarini yechishda chiziqli va kvadratik to'rtburchak chekli elementlarning yaqinlashuvi va aniqligi sonli tadqiq etilgan. Hisoblash jarayonida to'rtburchak qurish, global bikrlilik matritsasini shakllantirish, algebraik tenglamalar sistemasini yechish, xatolikni baholash va to'rtburchak bosqichma-bosqich maydalash jarayonlari ko'rib chiqilgan. Chiziqli elementlar belgilangan aniqlikka erishish uchun ko'proq elementlar va erkinlik darajalarini talab qilishi, kvadratik elementlar esa yuqori tartibli approksimatsiya hisobiga tezroq yaqinlashishi ko'rsatilgan. Natijalar chekli element tartibi, to'rtburchak zichligi va hisoblash samaradorligi o'rtasidagi bog'liqlikni ko'rsatadi.

Kalit so'zlar: chekli elementlar usuli, sonli algoritmlar, to'rtburchak chekli elementlar, yaqinlashuv, aniqlik, hisoblash to'rtburchak, to'rtburchak maydalash, hisoblash samaradorligi.

Аннотация: В статье проведено численное исследование сходимости и точности линейных и квадратичных четырехугольных конечных элементов при решении двумерных задач теории упругости. Рассмотрена вычислительная процедура, включающая построение сетки, формирование глобальной матрицы жесткости, решение системы алгебраических уравнений, оценку погрешности и последовательное сгущение сетки. Показано, что линейные элементы требуют значительного увеличения числа элементов и степеней свободы для достижения заданной точности, тогда как квадратичные элементы обеспечивают более быструю сходимость благодаря более высоким аппроксимационным возможностям. Полученные результаты

характеризуют взаимосвязь между порядком конечного элемента, плотностью сетки и вычислительной эффективностью.

Ключевые слова: метод конечных элементов, численные алгоритмы, четырехугольные конечные элементы, сходимость, точность, расчетная сетка, сгущение сетки, вычислительная эффективность.

Abstract: The paper presents a numerical comparison of linear and quadratic quadrilateral finite elements for two-dimensional elasticity problems. The analysis considers the accuracy of displacement and stress calculations as the finite element mesh is refined. For each mesh, the boundary-value problem is solved independently, and the numerical results are compared with the analytical solution.

The calculations show a clear difference in the convergence behavior of the two element types. Linear quadrilateral elements approach the reference solution relatively slowly and require a finer mesh to obtain the required accuracy. Quadratic elements give considerably better results on coarse meshes and approach the analytical solution more rapidly as the mesh is refined. This behavior is related to the higher-order interpolation used in the quadratic formulation.

The results also show that the element order has a direct effect on the number of elements required for a given accuracy. The comparison can therefore be useful when selecting a finite element formulation for numerical calculations in two-dimensional elasticity and in the development of corresponding computational procedures.

Key words: finite element method, numerical algorithms, quadrilateral finite elements, convergence, accuracy, computational mesh, mesh refinement, computational efficiency.

Introduction

The finite element method (FEM) is widely used for numerical analysis of problems in continuum mechanics and engineering. The method allows a computational domain to be divided into a finite number of elements and is therefore suitable for problems with different geometries and boundary conditions. Various interpolation functions can be used depending on the required accuracy and the type of problem. The

basic principles of FEM, including domain discretization, construction of finite element approximations, formation of stiffness matrices, and applications to solid mechanics, are described in [1]. These concepts form the basis for the construction and implementation of finite element algorithms. Mathematical aspects of the method, including variational formulations, convergence, and error estimation, are considered in [2]. Practical aspects of finite element calculations are discussed in [3], with particular attention to structural mechanics and numerical implementation. Reference [4] also considers engineering applications of FEM, including computational model construction, selection of element types, and interpretation of numerical results. The accuracy of a finite element solution depends on several factors. Among them are the interpolation order, mesh size, element geometry, and the characteristics of the problem being solved [5]. The basic principles of finite element approximation, interpolation functions, and the derivation of finite element equations are discussed in [6]. These theoretical results provide a basis for studying the convergence of finite element approximations. In practical calculations, however, the choice of element type also depends on how many elements are needed to achieve the required accuracy. For this reason, a direct numerical comparison of linear and quadratic quadrilateral elements under successive mesh refinement is useful. In the present study, the two formulations are considered for a two-dimensional linear elasticity problem. Displacement and stress results are analyzed, and their convergence toward the analytical solution is examined.

Literature Review

The theoretical foundations of the finite element method, including variational formulations, finite element approximation, element matrices, assembly procedures, and applications to two-dimensional elasticity, are systematically presented by Zienkiewicz, Taylor, and Zhu [1]. Their work also considers mesh generation, error estimation, and computational procedures used in finite element analysis. Bathe [2] presents finite element procedures for static and dynamic analysis, with emphasis on the formulation of element equations, assembly of global systems, numerical solution, and computational implementation. Hughes [3] considers FEM from both mathematical and computational viewpoints, including weak formulations, stiffness matrices, assembly

procedures, and computer implementation. The mathematical analysis of finite element approximation and convergence is developed in the works of Strang and Fix [4] and Brenner and Scott [5]. These studies establish the relationship between approximation spaces, mesh size, and the convergence of finite element solutions. Szabó and Babuška [6] discuss the construction and verification of finite element models, including issues related to approximation and error estimation. Their later work [7] further considers the relationship between mathematical formulation, verification, validation, and the practical structure of finite element procedures. A posteriori error estimation and adaptive mesh refinement have been studied in a number of works. Babuška and Rheinboldt [8] developed a mathematical approach to computable error estimates. Kelly et al. [9] considered a posteriori error analysis, while Gago et al. [10] investigated adaptive mesh refinement. These studies show that mesh refinement and error estimation are important parts of reliable finite element calculations. Babuška and Szabó [11] analyzed convergence rates in relation to the number of degrees of freedom and the refinement strategy. This issue is directly related to the present comparison, since linear and quadratic elements are examined under systematic mesh refinement. A broader treatment of the mathematical and practical aspects of finite element analysis is given by Ern and Guermond [12]. Their work provides additional theoretical background for the approximation and numerical treatment of finite element problems. The literature therefore provides a well-established basis for analyzing finite element convergence. The present study focuses on a direct numerical comparison of linear and quadratic quadrilateral elements for the same two-dimensional elasticity problem and under the same mesh-refinement procedure.

Research Methodology

The numerical experiment is formulated for a two-dimensional linear elasticity problem. The equilibrium equations are written in the standard form

$$\nabla \cdot \sigma + b = 0$$

where σ is the stress tensor and b is the body-force vector. The strain-displacement relationship is expressed as

$$\varepsilon = 1/2 (\nabla u + \nabla u^T)$$

where u is the displacement vector. Assuming linear elastic isotropic material behavior, the constitutive relation is written as

$$\sigma = D \varepsilon$$

where D is the elasticity matrix. In the finite element approximation, the displacement field is represented through shape functions and nodal degrees of freedom:

$$u = N d$$

where N is the matrix of shape functions and d is the vector of nodal unknowns. Application of the Galerkin finite element procedure gives the algebraic system

$$K d = F$$

where K is the global stiffness matrix and F is the external force vector.

The computational procedure uses successive mesh refinement. At each refinement level, the boundary-value problem is solved independently. The calculated displacement and stress fields are then compared with the analytical reference solution.

The relative error is used as the main measure of numerical accuracy. For a numerical quantity q_h and an analytical reference value q , the relative error is calculated as

$$e = |q_h - q| / |q| \times 100\%$$

The characteristic mesh size h is progressively reduced during the calculation. According to finite element approximation theory, first-order quadrilateral elements are associated with a convergence behavior of $O(h)$, whereas second-order elements are associated with $O(h^2)$. The numerical experiment is therefore used to compare these two convergence characteristics under the same computational conditions.

1. Computational sequence

Table 1. The numerical procedure consists of the following stages:

Stage	Computational operation
1	Define the computational domain, material properties, loads, and boundary conditions.
2	Generate the initial structured finite element mesh.
3	Construct the element approximation and calculate local element contributions.
4	Assemble the local contributions into the global stiffness matrix and load vector.
5	Apply the prescribed boundary conditions.
6	Solve the resulting algebraic system for the nodal displacements.
7	Calculate displacement and stress fields and evaluate the relative error.
8	Refine the mesh and repeat the calculation for the next refinement level.
9	Compare the convergence behavior of the linear and quadratic formulations.

Results and Discussion

The numerical investigation was carried out using a structured finite element mesh with successive uniform refinement. The initial coarse mesh was subdivided into smaller elements while preserving the geometry and connectivity of the computational domain. The resulting mesh levels and numerical values are given in Table 2. The results in Table 2 show a clear effect of both mesh density and element order on the numerical solution. For the linear quadrilateral elements, the displacement and stress values gradually approach the analytical reference values as the mesh is refined. On the coarse meshes, the difference from the exact solution is relatively large, and a considerable increase in the number of elements is required to obtain higher accuracy.

The quadratic quadrilateral elements give a closer approximation on the same coarse meshes. For the 2×1 mesh, for example, the calculated displacement is 214.994 compared with the exact value of 225, while the corresponding result for the linear element is 152.533. For the 4×3 mesh, the quadratic displacement reaches 224.813, which is already close to the reference value.

Table 2. Comparison of numerical solutions obtained using linear and quadratic quadrilateral finite elements under successive mesh refinement.

Mesh	Number of elements	Linear displacement	Linear stress	Quadratic displacement / stress
2×1	2	152.533	6.667	214.994 / 11.833
2×2	4	156.155	6.834	221.119 / 12.449
3×2	6	184.360	8.938	223.092 / 12.678
4×3	12	200.797	10.340	224.813 / 13.396
6×4	24	213.086	11.699	224.974 / 14.176
8×5	40	218.304	12.476	— / 14.613
24×12	288	224.956	15.094	— / —
Exact solution	—	225	15.1	225 / 15.1

The stress results show the same general tendency. The quadratic formulation approaches the analytical stress value of 15.1 more rapidly, whereas the linear

formulation requires a substantially finer discretization. This difference is consistent with the higher-order interpolation used in the quadratic elements.

The results also show that mesh refinement has a different practical effect for the two formulations. For linear elements, increasing the number of elements is necessary to reduce the error to a small value. With quadratic elements, a comparable level of accuracy can be reached with fewer refinement steps.

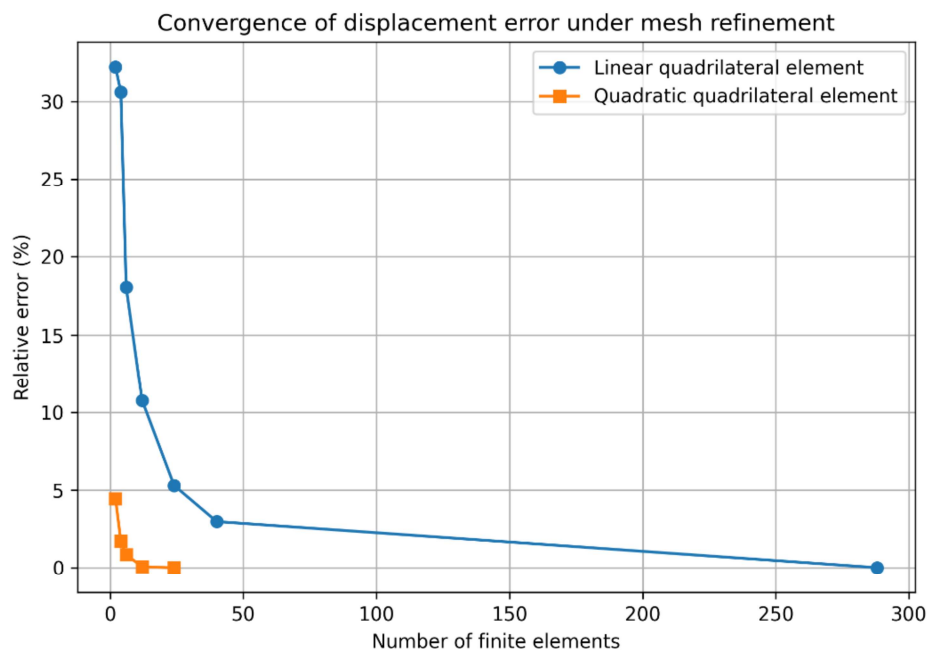


Figure 1. Relative displacement error under mesh refinement for linear and quadratic quadrilateral finite elements.

Figure 1 shows the convergence behavior obtained during the mesh-refinement procedure. The relative displacement error decreases much faster for the quadratic formulation than for the linear formulation. The curve corresponding to the linear element has a more gradual decline, whereas the quadratic element reaches a small error after only a limited number of refinement steps.

The observed behavior agrees with the theoretical difference between first-order and second-order approximations. Higher-order interpolation allows displacement gradients and local curvature to be represented more accurately within an element. This leads to a faster reduction of the discretization error as the mesh is refined.

The results obtained for stress show the same general trend. The linear formulation approaches the analytical value gradually, while the quadratic formulation reaches values close to the reference solution at an earlier stage of mesh refinement.

From the viewpoint of numerical software, the element order should therefore be treated as an important computational parameter. A software implementation that includes both linear and quadratic elements can use the same mesh-refinement and error-evaluation procedures to compare the accuracy and computational requirements of the two formulations.

Conclusion and Recommendations

The study considered the convergence and accuracy of linear and quadratic quadrilateral finite elements for a two-dimensional elasticity problem using systematic mesh refinement. The numerical results show that the interpolation order has a direct effect on the accuracy of the solution and on the number of elements required to reach a prescribed accuracy. The quadratic formulation approaches the analytical reference solution more rapidly than the linear formulation under comparable mesh-refinement conditions. The difference is especially clear on coarse meshes, where the quadratic elements provide substantially closer displacement and stress values.

The numerical results are consistent with the theoretical convergence behavior of first- and second-order finite element approximations. The higher-order interpolation used in quadratic elements gives a more accurate representation of the displacement field and reduces the amount of mesh refinement required in the considered problem.

Based on the numerical results, the following recommendations can be made:

- 1) For computational models where relatively high numerical accuracy is required with a limited number of elements, quadratic quadrilateral finite elements can be considered because of their faster convergence.
- 2) Finite element software should include systematic mesh refinement and error evaluation as integral parts of the computational procedure. This makes it possible to check the reliability of numerical results at successive discretization levels.
- 3) The choice between linear and quadratic elements should be made together with an assessment of mesh density, number of degrees of freedom, numerical accuracy, and

computational cost. The element order should therefore not be considered separately from the mesh-refinement strategy.

The obtained results can be used in the development and testing of numerical algorithms and software modules for finite element modeling of two-dimensional elasticity problems. They also provide a computational basis for further studies involving more complex geometries, material models, and adaptive mesh refinement.

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ANALYSIS OF STRUCTURAL CHANGES IN NEODYMIUM -DOPED SILICON BY RAMAN SPECTROSCOPY

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Annotatsiya. Ushbu ishda neodim (Nd) atomlarining p-tipli kremniy (KDB-48, $\rho=48 \Omega \cdot \text{cm}$) monokristaliga termik diffuziya usulida legirlash natijasida yuzaga keladigan strukturaviy o'zgarishlar Raman spektroskopiyasi yordamida tadqiq qilindi. Namunalar 1300°C haroratda 10 soat davomida vakuumli kvarts ampulalarda diffuziya qilindi va tez sovutish rejimida tayyorlandi. Raman spektrlari 785 nm to'liq uzunlikdagi lazer bilan jihozlangan spektrometrda xona haroratida o'lchandi. Dastlabki va nazorat namunalarida TA ($127, 183 \text{ cm}^{-1}$), LA ($311/315 \text{ cm}^{-1}$), TO/LO ($523,9 \text{ cm}^{-1}$) va ikkinchi tartibli optik (952 cm^{-1}) fonon rejimlari aniqlandi. Termik ishlov berish natijasida fazaviy tarkib o'zgarmagan, biroq barcha rejimlar intensivligi strukturaviy tartiblanish hisobiga oshgan (LA rejimida $+71,1\%$). Neodim diffuziyasi qilingan namuna spektrida tubdan farqli o'zgarishlar kuzatildi: $288, 398, 478, 672 \text{ cm}^{-1}$ da yangi piklarning paydo bo'lishi Nd_2O_3 va Nd-Si (silitsid) fazalarining hosil bo'lishini tasdiqlaydi. 520 cm^{-1} dagi TO fonon cho'qqisining yuqori intensivligi (7882 a.u) va uning past chastotaga siljishi ($\Delta\nu = -3,9 \text{ cm}^{-1}$) diffuziya qatlamida yuqori kristallanish darajasi va mexanik kuchlanishning kamayganligini ko'rsatadi. Natijalar neodimiyning kremniyda yangi fazalar hosil qilish orqali uning strukturaviy va vibratsion xossalarini sezilarli o'zgartirishini tasdiqlaydi.

Kalit soʻzlar: *Kremniy, neodim, termik diffuziya, Raman spektroskopiyasi, fonon rejimlari, silitsid, strukturaviy tartiblanish.*

Аннотация. В данной работе с помощью рамановской спектроскопии исследованы структурные изменения, возникающие при легировании монокристаллов кремния р-типа (КДБ-48, $\rho=48 \text{ Ом}\cdot\text{см}$) атомами неодима (Nd) методом термической диффузии. Образцы диффундировали в вакуумных кварцевых ампулах при 1300°C в течение 10 часов и готовились методом быстрого охлаждения. Спектры комбинационного рассеяния измерялись при комнатной температуре на спектрометре, оснащённом лазером с длиной волны 785 нм. В исходном и контрольном образцах были идентифицированы ТА ($127, 183 \text{ см}^{-1}$), LA ($311/315 \text{ см}^{-1}$), TO/LO ($523,9 \text{ см}^{-1}$) и оптические фононные моды второго порядка (952 см^{-1}). После термической обработки фазовый состав не изменился, но интенсивности всех мод увеличились за счёт структурного упорядочения (LA-мода на $+71,1\%$). В образце, легированном неодимом, наблюдались принципиально иные изменения: появление новых пиков при $288, 398, 478$ и 672 см^{-1} подтверждает образование фаз Nd_2O_3 и Nd-Si (силицида). Высокая интенсивность фононного пика TO при 520 см^{-1} (7882 у.е.) и его сдвиг в сторону низких частот ($\Delta\nu = -3,9 \text{ см}^{-1}$) указывают на высокую степень кристалличности и снижение механических напряжений в диффузионном слое. Результаты подтверждают, что неодим значительно изменяет структурные и колебательные свойства кремния путём образования новых фаз.

Ключевые слова: *Кремний, неодим, термическая диффузия, рамановская спектроскопия, фононные моды, силицид, структурное упорядочение.*

Abstract. In this work, structural changes arising from the doping of p-type silicon (KDB-48, $\rho=48 \text{ }\Omega\cdot\text{cm}$) single crystals with neodymium (Nd) atoms by thermal diffusion were studied using Raman spectroscopy. Samples were diffused in vacuum quartz ampoules at 1300°C for 10 hours and prepared by rapid cooling. Raman spectra were measured at room temperature using a spectrometer equipped

with a 785 nm laser. In the initial and control samples, TA ($127, 183 \text{ cm}^{-1}$), LA ($311/315 \text{ cm}^{-1}$), TO/LO (523.9 cm^{-1}), and second-order optical (952 cm^{-1}) phonon modes were identified. After thermal treatment, the phase composition did not change, but the intensities of all modes increased due to structural ordering (LA mode by +71.1%). In the neodymium-diffused sample, fundamentally different changes were observed: the appearance of new peaks at 288, 398, 478, and 672 cm^{-1} confirms the formation of Nd_2O_3 and Nd-Si (silicide) phases. The high intensity of the TO phonon peak at 520 cm^{-1} (7882 a.u.) and its shift to lower frequency ($\Delta\nu = -3.9 \text{ cm}^{-1}$) indicate a high degree of crystallinity and reduced mechanical stress in the diffused layer. The results confirm that neodymium significantly alters the structural and vibrational properties of silicon by forming new phases.

Key words: *Silicon, neodymium, thermal diffusion, Raman spectroscopy, phonon modes, silicide, structural ordering.*

Introduction

Silicon (Si) is the main material of modern microelectronics and occupies a leading position in industry due to its low cost, mature technology, and compatibility with MOS (metal-oxide-semiconductor) [1-2]. However, due to the indirect bandgap structure of silicon, electrons do not emit light during their motion. Therefore, silicon itself is not an efficient light-emitting material. To use it in light-emitting devices, additional methods such as doping with rare earth elements are employed [3]. This drawback is a serious obstacle to the development of silicon-based optoelectronics, in particular optical communication and on-chip light sources. Doping with rare earth elements is a promising way to solve this problem. Since the 4f electrons in rare earth elements are surrounded by filled 5s and 5p shells, their energy levels are little affected by the external crystal field, and the emission wavelength is almost independent of the matrix material [4]. Neodymium (Nd) has emission in the near-infrared region ($1.06 \mu\text{m}$ and $1.34 \mu\text{m}$), and these wavelengths are important in optical communication and laser technology [5]. By introducing neodymium into silicon, it becomes possible to integrate silicon-based light sources with existing microelectronics technology. The solid solubility of neodymium in silicon is very low (not exceeding 10^{16} cm^{-3}), which limits

high-concentration doping by conventional thermal diffusion. However, under non-equilibrium conditions, neodymium can form a supersaturated solid solution or nanoscale precipitate phases [6]. These structures significantly affect the microscopic structure and macroscopic properties of silicon. The infrared emission of neodymium ions can be used to create optical amplifiers, lasers, and light-emitting diodes. The achievements obtained in erbium-doped silicon (20.6% quantum efficiency at 1540 nm, 272 cm⁻¹ optical gain) are also promising for neodymium [7]. In this experiment, Raman spectrometry was used to determine structural changes when neodymium atoms are doped into a silicon single crystal. As a result, new molecular bonds were identified, namely peaks at 288 cm⁻¹, 398 cm⁻¹, 478 cm⁻¹, and 672 cm⁻¹ were analyzed.

Research Methodology

For the experiment, single-crystal silicon samples with resistivities of KDB-48 Ω·cm (p-Si) and KEF-150 Ω·cm (n-Si) were selected. The initial thickness of the samples was $d_0=2000\text{ }\mu\text{m}$. To remove contaminants and oxide layers from the surface, 20 μ was removed from both sides of the sample using M=20, M=14, M=8 grade carborundum powders. Then, a complete chemical cleaning step was carried out [8].

After cleaning, a high-purity (99.999%) neodymium layer was evaporated onto the silicon surface. To form the neodymium layer, evaporation was performed using a VUP-4 apparatus under high vacuum conditions (10⁻⁶ Torr), which ensured uniform distribution of neodymium atoms on the silicon surface. The alloying process was carried out by thermal diffusion. The prepared p-Si samples were placed in clean quartz ampoules. First, a vacuum (10⁻⁴ Torr) was created inside the ampoule, and diffusion was carried out at 1573 K (1300°C) for 10 hours. Subsequently, to study the formation of defects and the formation of tungsten atoms in the silicon crystal lattice, the samples were rapidly cooled. Rapid cooling helps to prevent the increase of internal defects in the samples, which could affect the formation of nanocrystallites and other structural changes [9]. Raman spectra of the samples were measured using a Raman spectrometer manufactured by Ocean Insight, equipped with a 785 nm laser. The 785 nm wavelength belongs to the near-infrared range and has several advantages for studying silicon materials. It is optimal for assessing the degree of crystallinity of silicon, significantly

reduces background luminescence, and allows deeper penetration into the sample. The spectral measurement range covers wavenumbers from 0 to 3000 cm^{-1} , which is sufficient to detect the main optical phonon of silicon (523.9 cm^{-1}), peaks characteristic of tungsten silicide, and other possible vibrational modes. All measurements were performed at room temperature [10].

Results and Discussion

Raman spectra of the silicon samples were measured using a Raman spectrometer equipped with a 785 nm laser. In Figure 1, part a shows the initial (p-Si) sample, part b shows the control sample, i.e., thermally treated at $T=1300\text{ }^{\circ}\text{C}$ for $t=10$ hours, and part c shows the p-Si<Nd> doped samples.

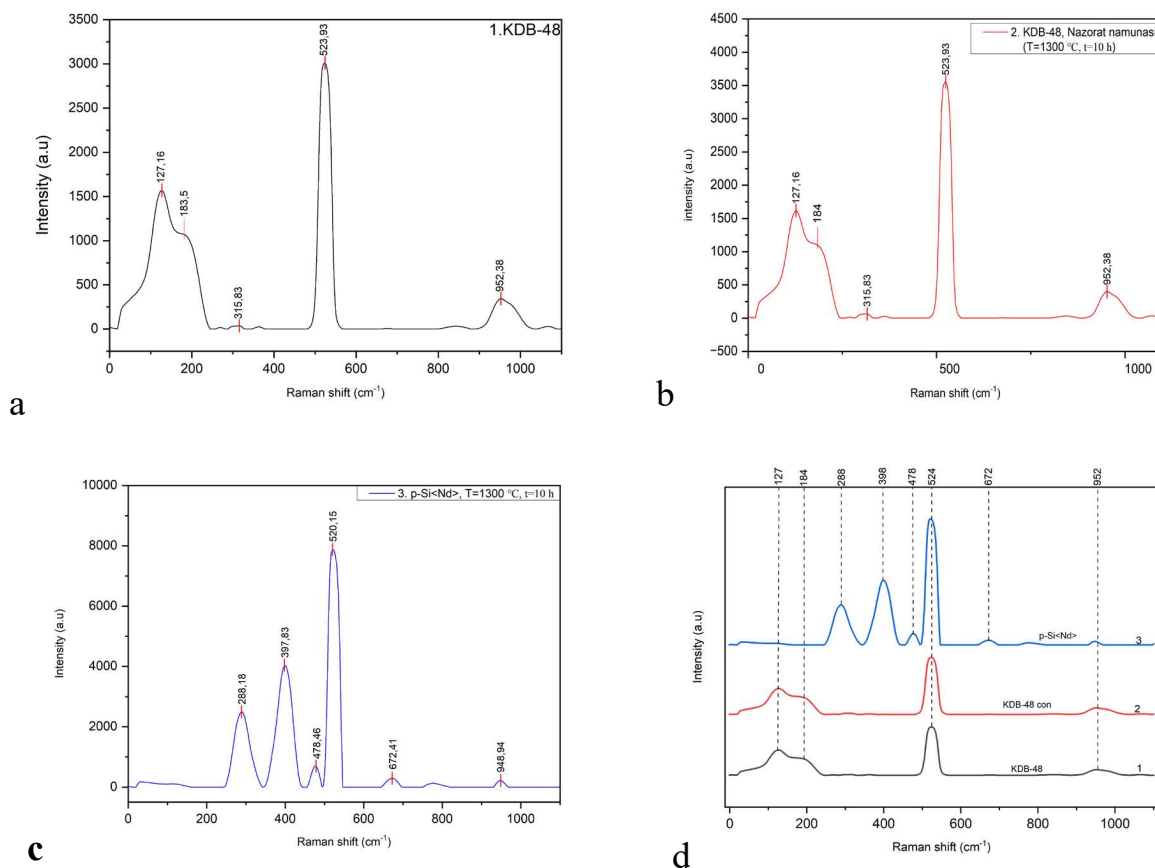


Figure 1. a) Initial sample (KDB-48), b) Control sample, $T=1300\text{ }^{\circ}\text{C}$, $t=10\text{ h}$, rapidly cooled, c) p-Si<Nd>, $T=1300\text{ }^{\circ}\text{C}$, $t=10\text{ h}$, rapidly cooled, d) general results

In the Raman spectrum of the initial KDB-48 sample, five main peaks were recorded at 127, 183, 311, 523.9, and 952 cm^{-1} . 127 cm^{-1} (TA mode). In the literature,

for amorphous silicon (a-Si), the broad band in the range $80\text{--}200\text{ cm}^{-1}$ is considered as the transverse acoustic (TA) phonon mode. This mode is mainly of the nature of changes in the bond angle between atoms and indicates structural disorder [11]. The 183 cm^{-1} peak also falls in the TA mode region. Studies have shown that the peaks at 127.16 cm^{-1} and 196.24 cm^{-1} are related to amorphous structures, and a decrease in their intensity confirms a reduction in defects [12]. 311 cm^{-1} (LA mode). For amorphous silicon, the longitudinal acoustic (LA) mode is observed around $\sim 300\text{--}330\text{ cm}^{-1}$ [13]. The LA mode is associated with the tetrahedral bending mode and also includes overtones of acoustic and combination (TO + TA) modes. This mode is less sensitive to intermediate-range order [14]. 523.9 cm^{-1} (TO/LO mode). This peak is the classical transverse optical (TO) phonon mode of crystalline silicon (c-Si). In the literature, the TO mode of crystalline silicon is recorded as a sharp line at $520\text{--}522\text{ cm}^{-1}$, and accordingly, this peak contains Si-Si bonds. The sharp peak at 523.9 cm^{-1} indicates the presence of a crystalline phase in the sample [13-14]. 952 cm^{-1} peak corresponds to the second-order optical phonon mode of crystalline silicon. The literature indicates that peaks around $\sim 940\text{--}952\text{ cm}^{-1}$ belong to the first and second-order optical phonons of crystalline silicon [14]. In the control sample, the peak centers hardly changed ($127, 184, 315, 523.9, 952\text{ cm}^{-1}$), which indicates that the phase composition of the material was preserved after thermal treatment. At the same time, the intensities of all peaks increased. The largest relative change is observed in the $311/315\text{ cm}^{-1}$ (LA mode) peak (+71.1%). Although the intensity of the LA mode is less sensitive to intermediate-range order, its significant increase indicates that a structural ordering process occurred in the material as a result of thermal treatment. The increase in the intensity of the 523.9 cm^{-1} (TO) peak (+18%) indicates an improvement in the degree of crystallinity [15-16]. Thermal treatment at $T=1300^{\circ}\text{C}$ for 10 hours does not change the phase composition of the KDB-48 sample, but increases the intensity of all phonon modes due to structural ordering. The spectrum of the neodymium-diffused sample differs fundamentally from that of the initial KDB-48 sample. In the spectrum, six peaks were recorded at $288, 398, 478, 520, 672, \text{ and } 949\text{ cm}^{-1}$. 288 cm^{-1} . This peak was not present in the initial samples. In the literature, a peak at 307.94 cm^{-1} has been recorded as a 2TA phonon mode in dysprosium

(Dy)-doped silicon [17]. Similarly, the 288 cm^{-1} peak may be related to a new phase formed as a result of Nd diffusion, possibly Nd_2O_3 or an Nd-Si compound. Nd_2O_3 has an A-type hexagonal structure, and 288 cm^{-1} may correspond to the frequency of one of these modes (probably the A_{1g} bending mode) [18]. 398 cm^{-1} . This peak also belongs to a new phase. The literature contains information on the observation of peaks around $\sim 398\text{ cm}^{-1}$ in the Nd-Si system. Characteristic Raman peaks for NdSi_2 compounds have been recorded around 256 and 690 cm^{-1} [19]. Also, in the A-type hexagonal structure of Nd_2O_3 , the A_{1g} stretching mode for La_2O_3 is known to be located at $\sim 404\text{ cm}^{-1}$ [20]. For Nd, the frequency of this mode is expected to be slightly lower, around 398 cm^{-1} , due to the atomic mass difference. Therefore, the 398 cm^{-1} peak can be taken as the A_{1g} mode of Nd_2O_3 or an intermediate phase formed at the Nd-Si interface. 478 cm^{-1} . This peak is located near the LO (longitudinal optical) mode of amorphous silicon. For amorphous silicon, the LO mode is observed around $\sim 380\text{--}410\text{ cm}^{-1}$. The 478 cm^{-1} falls in the region of the TO mode ($\sim 475\text{--}480\text{ cm}^{-1}$) of amorphous silicon. This peak indicates the presence of an amorphous or microcrystalline silicon phase formed as a result of recrystallization during diffusion [13]. 520 cm^{-1} . This peak has a very high intensity (7882 a.u.) and is the classical TO phonon mode of crystalline silicon (c-Si). A shift from 523.9 cm^{-1} in the initial sample to 520 cm^{-1} ($\Delta\nu = -3.9\text{ cm}^{-1}$) is observed [21]. This shift indicates a decrease in mechanical stress in the material or an increase in crystallite size. The increase in intensity from 3012 a.u. to 7882 a.u. (by a factor of 2.6) confirms the formation of a highly crystalline silicon layer as a result of diffusion [22]. This result is fully consistent with observations in the literature related to silicon crystallization. 672 cm^{-1} . This new peak may belong to a Raman-active mode of Nd_2O_3 . The literature records a band characteristic of the A-form around $\sim 660\text{--}672\text{ cm}^{-1}$ for Nd_2O_3 . This frequency may also correspond to phonon modes of Nd-Si compounds. The 672 cm^{-1} peak indicates the presence of a neodymium oxide or neodymium silicide phase formed as a result of Nd diffusion [19-20].

949 cm^{-1} . This peak was also present in the initial samples (952 cm^{-1}), but after diffusion its intensity decreased significantly ($345\rightarrow 222\text{ a.u.}$). This peak is assigned to

the second-order optical phonon mode of crystalline silicon. The decrease in intensity indicates that the crystalline phase partially changed during the diffusion process [20].

Table 1. General results of Raman measurements

Peak center (cm ⁻¹)	KDB-48 initial (a.u.)	KDB-48 control (a.u.)	p-Si<Nd> KDB-48 (a.u.)
127	1570	1618	—
183	1052	—	—
184	—	1100	—
288	—	—	2493
311	38	—	—
315	—	65	—
398	—	—	4040
478	—	—	695
520	—	—	7882
523,9	3012	3555	—
672	—	—	292
949	—	—	222
952	345	402	—

Thermal treatment (1300°C, 10 hours) does not cause phase changes in the KDB-48 sample. All phonon modes (TA, LA, TO, 2nd-order optical) are preserved, only their intensities increase due to structural ordering. The largest relative change is observed in the LA mode (+71.1%), which indicates an improvement in intermediate-range order. The high intensity of the 520 cm⁻¹ peak indicates a high degree of crystallinity in the diffused layer. This may have a positive effect on the electronic properties of the material. The shift of peak centers (523.9→520 cm⁻¹) indicates a decrease in stress and a change in crystallite size as a result of diffusion.

Conclusion and Recommendations

In this study, structural changes arising from the thermal diffusion of neodymium into p-type silicon single crystals were systematically studied by Raman spectroscopy. Based on the obtained results, the following main conclusions were drawn. Thermal treatment at T=1300°C for 10 hours does not change the phase composition of the KDB-48 sample. All phonon modes (TA, LA, TO, 2nd-order optical) are preserved, only their intensities increase due to structural ordering. The largest relative change is observed in the LA mode (+71.1%), which indicates an improvement in intermediate-range order.

The increase in the intensity of the 523.9 cm^{-1} (TO) peak (+18%) indicates an improvement in the degree of crystallinity. The spectrum of the neodymium-diffused sample differs fundamentally from that of the initial KDB-48 sample. In the spectrum, six peaks were recorded at 288, 398, 478, 520, 672, and 949 cm^{-1} . The disappearance of the TA and LA modes indicates a change in the initial structural state during diffusion. Analysis of the new peaks appearing at 288, 398, and 672 cm^{-1} confirms the formation of Nd_2O_3 and Nd-Si (silicide) phases as a result of Nd diffusion. The 288 cm^{-1} peak was assigned to the A_{1g} bending mode in the A-type hexagonal structure of Nd_2O_3 , the 398 cm^{-1} peak to the A_{1g} stretching mode, and the 672 cm^{-1} peak to a band characteristic of the A-form. The 478 cm^{-1} peak indicates the presence of an amorphous or microcrystalline silicon phase formed as a result of recrystallization during diffusion. The very high intensity of the 520 cm^{-1} peak (7882 a.u.) indicates a high degree of crystallinity in the diffused layer. The shift from 523.9 cm^{-1} in the initial sample to 520 cm^{-1} ($\Delta\nu = -3.9\text{ cm}^{-1}$) indicates a decrease in mechanical stress or an increase in crystallite size. The increase in intensity from 3012 a.u. to 7882 a.u. (by a factor of 2.6) confirms the formation of a highly crystalline silicon layer as a result of diffusion. The obtained results show that neodymium significantly alters the structural and vibrational properties of silicon by forming new phases. These results are important for creating a material basis for the use of neodymium-doped silicon in optoelectronic and photovoltaic devices. The simplicity of the thermal diffusion method and its compatibility with silicon technology increase its practical applicability.

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PHASE TRANSFORMATIONS AND X-RAY DIFFRACTION PATTERNS IN THE SI-MN SYSTEM

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Annotatsiya: Ushbu tadqiqot ishida monokristall kremniy asosida yuqori haroratli vakuumli diffuziya usuli orqali sintez qilingan Si-Mn geterotizimining fazaviy tarkibi va kristallanish qonuniyatlarining termik ishlov berish haroratiga (600-1200°C) bog'liqligi rentgen-difraksion tahlil (XRD) yordamida chuqur o'rganildi. Haroratning ko'tarilishi jarayonida kremniy kristall panjarasining dastlabki qisman amorflanishidan boshlab, kubik B20 tuzilishga ega bo'lgan MnSi monofazasi, tetragonal simmetriyadagi Mn₄Si₇ yuqori silitsidi hamda 950°C dan yuqori haroratlarda marganetsning qayta taqsimlanishi oqibatida Mn₅Si₃ va qayta barqarorlashgan MnSi fazalarining ketma-ket hosil bo'lishi aniqlandi. Sherrer formulasi asosida kristallitlar o'lchamining 30 nm dan 45 nm gacha o'sishi hamda ichki panjara zo'riqlarining fazaviy chegaralardagi evolyutsiyasi miqdoriy baholandi.

Kalit soʻzlar: *Si-Mn tizimi, marganets silitsidlari, $MnSi$, Mn_4Si_7 , rentgen nurlari difraktsiyasi (XRD), diffuziya, kristallit oʻlchami, fazaviy oʻtishlar kinetikasi.*

Аннотация: В настоящей работе методом рентгенофазового анализа (РФА) подробно исследованы фазовый состав и кинетика кристаллизации гетеросистемы Si-Mn, синтезированной на подложках монокристаллического кремния путем высокотемпературной термической вакуумной диффузии в диапазоне температур отжига 600-1200°C. Установлено, что с повышением температуры отжига система последовательно эволюционирует от начальной частичной аморфизации кристаллической решетки кремния к зарождению кубической монофазы $MnSi$ со структурой B20, с последующим формированием высшего силицида марганца Mn_4Si_7 тетрагональной симметрии. При температурах выше 950°C термическое перераспределение марганца приводит к появлению фазы Mn_5Si_3 наряду с рестабилизированной фазой $MnSi$. На основе формулы Шеррера количественно определен рост размеров кристаллитов от 30 до 45 нм, а также охарактеризована структурная эволюция микродеформаций кристаллической решетки на межфазных границах.

Ключевые слова: *система Si-Mn, силициды марганца, $MnSi$, Mn_4Si_7 , рентгеновская дифракция (РФА), термическая диффузия, размер кристаллитов, кинетика фазовых превращений.*

Abstract: In this study, the phase composition and crystallization kinetics of a Si-Mn heterosystem synthesized on single-crystal silicon substrates via high-temperature thermal vacuum diffusion were comprehensively investigated as a function of annealing temperature (600-1200°C) using X-ray diffraction (XRD) analysis. As the annealing temperature increased, the system progressed from initial partial amorphization of the host silicon lattice to the sequential nucleation of a cubic B20-type $MnSi$ monophase, followed by the formation of the higher manganese silicide Mn_4Si_7 exhibiting tetragonal symmetry. At temperatures exceeding 950°C, thermal redistribution of manganese triggered the appearance of

the Mn_5Si_3 phase along with restabilized MnSi. Using the Scherrer formulation, crystallite size growth from 30 nm up to 45 nm and the structural evolution of lattice-induced microstrains across interphase boundaries were quantitatively determined.

Key words: *Si-Mn system, manganese silicides, MnSi, Mn_4Si_7 , X-ray diffraction (XRD), thermal diffusion, crystallite size, phase transformation kinetics.*

Introduction

Doping silicon matrices with 3d transition metals represents a strategic technological pathway in the development of multifunctional semiconductor architectures. Incorporating transition metal species, particularly manganese, into the silicon crystal framework substantially broadens its electronic, magnetic, and optoelectronic capabilities [1-10]. Manganese is particularly notable for promoting spin-dependent transport phenomena within the Si host lattice, establishing room-temperature weak ferromagnetism, and yielding thermodynamically stable silicide phases characterized by superior thermoelectric metrics. The binary silicon-manganese (Si-Mn) system features a complex phase diagram populated by an array of intermetallic stoichiometric variants. Among these compounds, cubic B20-structured MnSi and tetragonal Mn_4Si_7 are recognized as the most technologically promising phases. Nonetheless, comprehensive systemic insight into the nucleation kinetics, interphase boundary transitions, and lattice strain dynamics of these silicides during high-temperature thermal diffusion remains incomplete. Accordingly, this study aims to systematically investigate and elucidate the structural-phase evolution mechanisms across the Si-Mn framework over a broad thermal regime (600-1200°C) via detailed X-ray diffraction (XRD) characterization [11-20].

Research Methodology

Single-crystal p-type and n-type silicon wafers with electrical resistivities ranging between 5 and 35 $\Omega\cdot\text{cm}$ were utilized as the precursor substrates. High-purity manganese ($\geq 99.999\%$) served as the diffusion dopant. Specimen processing proceeded via the following technological protocol:

Thermal Vacuum Deposition: Metallic Mn thin films were deposited onto clean silicon surfaces within a high-vacuum chamber evacuated by an oil-free turbomolecular pumping unit down to a base pressure of $P \leq 10^{-7}$ - 10^{-8} Torr.

High-Temperature Diffusion: Isothermal diffusion treatments were conducted within sealed, evacuated quartz ampoules across a temperature spectrum of 600°C to 1200°C for durations spanning from 0.5 to 10 hours.

Cooling Protocols: Following thermal annealing, specimens were subjected either to rapid quenching or slow in-furnace cooling to ambient temperature, thereby allowing the selective preservation of both metastable and near-equilibrium structural phases.

Structural Diagnostics: Phase identification was carried out using a Rigaku MiniFlex II X-ray diffractometer operating with $\text{CuK}\alpha$ radiation ($\lambda = 1.5406 \text{ \AA}$). Angular scanning spanned 2θ values from 3° to 60° at a scan increment of 0.02° with a dwelling time of 2 seconds per step. Experimental diffraction profiles were indexed against the standard ICDD PDF-4+ crystallographic database.

Results and Discussion

X-ray phase identification confirmed a distinct step-by-step structural evolution within the Si-Mn system as the annealing temperature rose. The structural changes observed across different thermal regimes are detailed below:

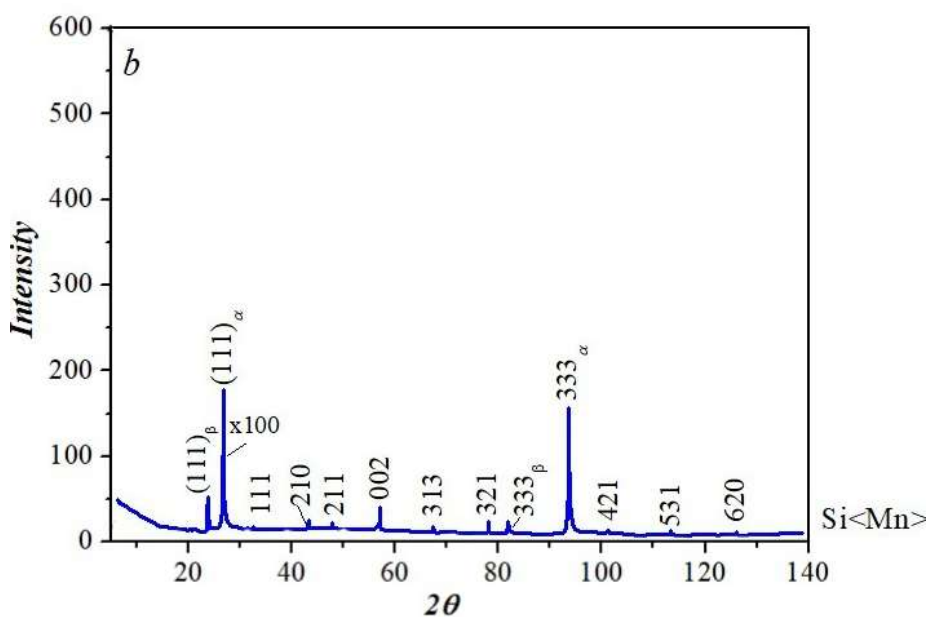


Fig. 1. X-ray diffraction pattern of the Si<Mn> heterostructure following thermal annealing at $T = 900$ - 1000°C .

Initial State and Surface Amorphization ($T \leq 600^\circ\text{C}$). At preliminary thermal stages, the diffractograms show an absence of sharp Bragg reflections, dominated instead by a broad, low-intensity diffuse background. In particular, the emergence of a broad feature in the $2\theta \approx 28^\circ$ - 29° interval indicates interstitial insertion of Mn adatoms into the outer silicon sublattices, causing localized near-surface amorphization. This defect-driven state induces host lattice dilatation and significantly degrades crystalline coherence. **Nucleation of Intermetallic MnSi Monosilicide (600 - 700°C).** As the processing temperature reaches 600 - 700°C , the onset of the cubic MnSi compound (space group $P2_13$) occurs. Diffractograms exhibit distinct diffraction maxima located at $2\theta \approx 31.6^\circ$, 36.1° , 47.3° , and 55.5° , consistent with standard ICDD PDF card #01-072-0566. Although the silicon substrate reflections-namely $(111)_\alpha$ and $(220)_\alpha$ -remain clearly visible, their pronounced peak broadening suggests the build-up of residual mechanical microstrains along the propagating diffusion front.

Transition to the Higher Silicide Mn_4Si_7 (800 - 900°C). Within this higher thermal window, accelerated interdiffusion kinetics of silicon atoms promote chemical interaction with the existing MnSi phase, driving a stoichiometric conversion toward the higher tetragonal manganese silicide Mn_4Si_7 according to the solid-state reaction:

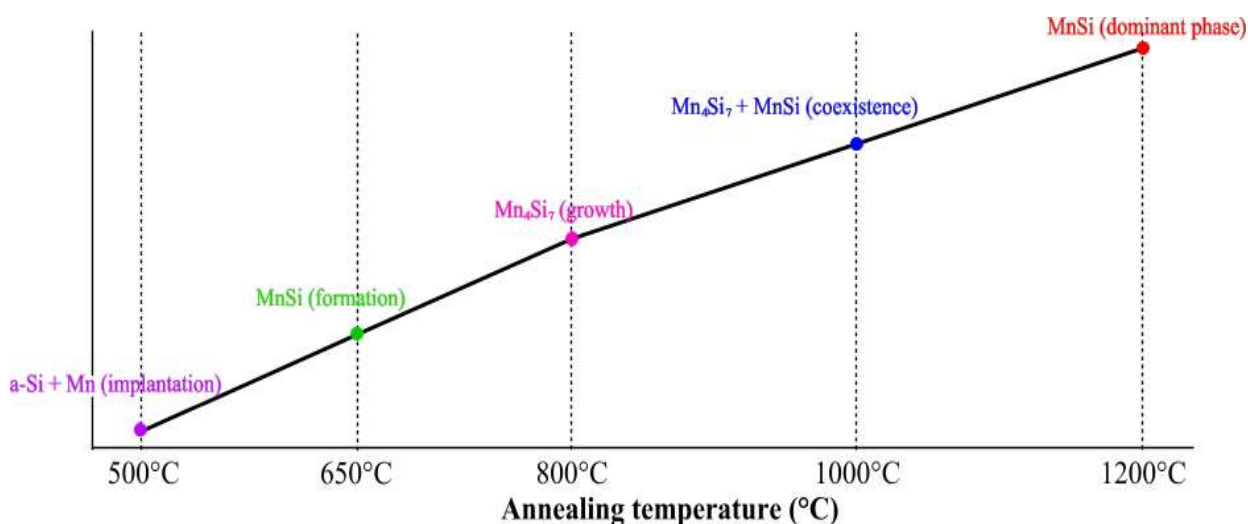


Fig. 2. Sequential stages of structural and phase transitions in the Si-Mn system as a function of thermal treatment temperature.

XRD profiles reveal sharp, intensified peaks corresponding to the (210), (211), (002), and (313) crystallographic planes. The notable enhancement in peak intensity combined with a marked contraction of the full width at half maximum (FWHM) values demonstrates coherent grain coarsening, yielding average crystallite dimensions of approximately 30 nm.

High-Temperature Disproportionation and Phase Evolution ($T > 900-1200$ °C). Beyond 900°C, average domain sizes grow further to 40-45 nm. Thermodynamic redistribution triggers localized phase separation: subtle diffraction signatures appearing at $2\theta \approx 43.2^\circ$ and 46.8° correspond to manganese-rich phases, primarily hexagonal Mn_5Si_3 .

Table 1. Temperature-dependent phase states, crystallographic parameters, and domain sizes in the Si-Mn system.

Annealing Temperature (°C)	Dominant Phase Composition	Crystallographic Symmetry	Characteristic XRD Peaks (2θ)	Average Crystallite Size (d)
≤ 600	a-Si + Mn clusters	Amorphous / Disordered	Broad diffuse halo at 28° - 29°	-
600–750	MnSi (monosilicide)	Cubic B20 ($P2_13$)	31.6° , 36.1° , 47.3° , 55.5°	15-20 nm
800–950	Mn_4Si_7 (higher silicide)	Tetragonal	27.5° , 33.8° , 41.2° , 44.6°	~ 30 nm
> 950–1200	MnSi + Mn_5Si_3 (disproportionation)	Cubic / Hexagonal	31.6° , 43.2° , 46.8° , 55.5°	40-45 nm

When temperatures approach 1100-1200°C, partial thermal dissociation of the Mn_4Si_7 phase takes place, resulting in the re-emergence and intensification of diffraction lines associated with the thermodynamically more resilient B20-MnSi phase [21].

Conclusion and Recommendations

Comprehensive X-ray diffraction analyses verify a four-stage phase-formation pathway within the silicon-supported Si-Mn diffusion system. Following initial lattice perturbation and near-surface amorphization at lower temperatures, nucleation of the cubic MnSi phase occurs between 600°C and 750°C. Within the 800-950°C range, the silicon-rich tetragonal Mn_4Si_7 phase crystallizes, with grain dimensions expanding to around 30 nm. At temperatures exceeding 950°C, altered diffusion kinetics and

thermodynamic equilibria provoke phase disproportionation, yielding secondary Mn segregation alongside dominant re-stabilized MnSi. These systematic correlations offer a reliable processing foundation for the controlled synthesis of manganese silicide phases tailored for modern spintronic and nanoelectronic applications.

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UDC 538.971:539.12.04

SRIM/TRIM SIMULATION OF ION-BEAM MODIFICATION OF ZrO₂ - BASED CERAMIC MEMBRANES WITH Ag AND Au IONS

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Annotatsiya. Ushbu ishda energiyasi 50–2000 keV bo‘lgan kumush va oltin ionlarining sirkoniy dioksidi (ZrO₂) asosidagi keramik membranalariga implantatsiyasi SRIM/TRIM fizik asosidagi juft to‘qnashuvlar yaqinlashuvida Monte-Karlo usuli bilan modellashirildi. Tormozlanish qobiliyatlari, proyektiv yugurish yo‘llari (Ag uchun 19–338 nm, Au uchun 16–231 nm), vakansiyalar soni (6821 gacha), metall konsentratsiyasi va shikastlanish profillari hamda changlanish koeffitsiyentlari olindi. Nuqson hosil bo‘lishi atom siljishlari kaskadlari bilan boshqarilishi ko‘rsatildi: elektron va yadroviy tormozlanish tengligi Ag uchun 565 keV da, Au uchun 1921 keV da erishiladi. Nanoklasterlar hosil bo‘lishi uchun zarur flyuyenslar va membranalarni nurlantirish rejimlari aniqlandi.

Kalit so‘zlar: sirkoniy dioksidi, keramik membranalar, ion implantatsiyasi, kumush, oltin, SRIM/TRIM, radiatsion nuqsonlar.

Аннотация. Методом Монте-Карло в приближении парных столкновений на физической основе SRIM/TRIM рассчитана имплантация ионов серебра и золота с энергией 50–2000 кэВ в керамические мембраны на

основе диоксида циркония. Получены тормозные способности, проективные пробеги (19–338 нм для Ag и 16–231 нм для Au), число вакансий на ион (до 6821), профили концентрации металла и повреждения, коэффициенты распыления. Показано, что дефектообразование контролируется каскадами смещений: равенство электронной и ядерной тормозных способностей достигается при 565 кэВ для Ag и 1921 кэВ для Au. Определены флюенсы, необходимые для зарождения нанокластеров, и режимы облучения мембран.

Ключевые слова: диоксид циркония, керамические мембраны, ионная имплантация, серебро, золото, SRIM/TRIM, радиационные дефекты.

Abstract. Implantation of 50–2000 keV silver and gold ions into zirconia-based ceramic membranes was simulated by the Monte Carlo method in the binary collision approximation on the physical basis of SRIM/TRIM. Stopping powers, projected ranges (19–338 nm for Ag and 16–231 nm for Au), vacancies per ion (up to 6821), metal concentration and damage profiles, and sputtering yields were obtained. Defect production is governed by displacement cascades: electronic and nuclear stopping become equal at 565 keV for Ag and 1921 keV for Au. The fluences required for nanocluster nucleation and irradiation regimes for membranes were determined.

Key words: zirconia, ceramic membranes, ion implantation, silver, gold, SRIM/TRIM, radiation defects.

Introduction

Ceramic membranes occupy a special place among separation materials. Unlike polymeric membranes, they retain their performance at temperatures of several hundred degrees, in aggressive chemical media and under large pressure drops, which makes them indispensable in catalytic membrane reactors, high-temperature gas separation, water treatment and electrochemical devices. Zirconia-based membranes are widely used in ultrafiltration and nanofiltration, including aggressive media where polymeric materials fail, and stabilized ZrO_2 is the main electrolyte of solid oxide fuel cells [8, 12]. A typical ceramic membrane has an asymmetric structure: a coarse-porous support is

covered with one or several intermediate layers and, finally, with a selective layer 50–500 nm thick, which determines the separation properties of the membrane.

The functionality of such a membrane can be substantially extended by incorporating noble metals into its near-surface layer. Silver and gold give the surface catalytic activity in oxidation reactions, produce localized surface plasmon resonance used in sensing and photocatalysis, and provide a pronounced antibacterial effect, which is important for water-treatment membranes. However, conventional methods of metal incorporation — impregnation, sol–gel coating and chemical or electrochemical deposition — give a poorly controlled depth distribution of the metal, and the deposited phase tends to accumulate at the pore mouths, reducing permeability and selectivity.

Ion implantation is free from these limitations. Unlike impregnation and deposition, ion implantation sets the depth of the metal by the ion energy and its amount by the fluence, and it does not block the pore space [11]. The process requires no solvents, proceeds far from thermodynamic equilibrium and allows metal concentrations well above the solubility limit to be reached. As a result, Ag and Au nanoclusters can be formed directly inside the near-surface layer; this approach has been studied in detail for silica glasses, sapphire and other dielectrics [11, 13], and it has been shown that subsequent ion irradiation can modify the size and spatial distribution of the embedded nanoparticles [18].

The price for these advantages is radiation damage of the matrix: every implanted heavy ion creates a cascade of atomic displacements that changes the local structure and the oxygen stoichiometry of the oxide. Zirconia is known as one of the most radiation-tolerant oxides: it does not amorphize even at doses of hundreds of displacements per atom and responds to irradiation by the accumulation of point defects, dislocation loops and phase transformations between the monoclinic, tetragonal and cubic modifications [9, 10]. Nevertheless, the depth of the damaged layer, the peak damage level and the loss of material by sputtering must be known in advance in order to choose an irradiation regime that does not degrade the transport properties of the membrane.

The SRIM/TRIM codes are the most widely used tool for such estimates [1, 2], but the calculated damage depends on the chosen options and threshold displacement

energies, and recommendations on their correct use are still being refined [6, 14, 15]. At the same time, systematic data on the ranges, damage profiles, sputtering and nanocluster nucleation threshold for Ag and Au ions in ZrO₂ over a wide energy range are practically absent in the literature. The aim of this work is to calculate the implantation of Ag and Au ions into ZrO₂ at energies of 50–2000 keV and to select irradiation regimes for membranes.

Research Methodology

The calculation was performed by the Monte Carlo method in the binary collision approximation (BCA) on the physical basis of the SRIM/TRIM codes [1–3, 16]. The target was treated as a homogeneous amorphous medium with a given atomic density. For polycrystalline ceramics with a grain size much larger than the ion range this is an adequate description, and channeling was therefore neglected. The ion trajectory was represented as a sequence of binary elastic collisions with target atoms, between which the ion continuously loses energy to the electronic subsystem.

Nuclear scattering was described by the universal Ziegler–Biersack–Littmark (ZBL) screened potential [1]. The scattering angle in each collision was calculated not by approximate formulas but by direct numerical integration of the classical scattering integral: a table of $\sin^2(\theta/2)$ was pre-computed for a grid of reduced energies (10^{-6} – 10^5) and reduced impact parameters using a 96-point Gauss–Legendre quadrature, followed by interpolation in logarithmic coordinates. The free flight path between collisions was taken equal to $N^{-1/3}$, and the maximum impact parameter $p_{\max} = (\pi N^{2/3})^{-1/2}$, where N is the atomic density. A control comparison of the mean energy transfer with the analytical ZBL nuclear stopping showed agreement within 2 % over the whole energy range. Electronic stopping was calculated in the Lindhard–Scharff approximation [4]. Since this approximation systematically underestimates the electronic losses of heavy ions, a single scaling factor $\xi = 2.2$ was introduced. Its value was determined by fitting to published SRIM/TRIM projected ranges for six reference systems (B, P and Sb ions in Si and Si ions in C at 14–120 keV). After calibration, the mean absolute deviation of the calculated ranges from the reference values is 7.7 %, and for five of the six systems it does not exceed 3.4 %. For the compound target, Bragg’s additivity rule was used.

Radiation damage was calculated by the “quick” scheme corresponding to the Quick Damage option of SRIM, which is recommended for comparing irradiation regimes [6, 15]. For each recoil atom with an energy above the displacement threshold, the number of Frenkel pairs was determined by the Norgett–Robinson–Torrens model [5, 17], $N_d = 0.8T_{\text{dam}}/(2E_d)$, where T_{dam} is the damage energy, and was assigned to the depth of the collision. The threshold displacement energies were $E_d = 57$ eV for Zr and 27 eV for O. The damage in displacements per atom (dpa) was obtained as $D(x) = N_v(x)\Phi/N$, where $N_v(x)$ is the vacancy depth distribution per ion and Φ is the fluence; the metal concentration $C(x)$ was obtained in the same way from the distribution of stopped ions. The sputtering yield was estimated by Sigmund’s formula [7] with a surface binding energy of 6 eV. For porous membranes (porosity P), the effective atomic density $(1 - P)N$ was used, which gives $R_p(P) = R_p(0)/(1 - P)$. The target parameters for ZrO_2 were $\rho = 6.05$ g/cm³, $M = 123.22$ g/mol and $N = 8.87 \cdot 10^{22}$ cm⁻³. The calculations were performed for ion energies of 50, 100, 200, 500, 1000 and 2000 keV. The statistics were 1500 trajectories per regime for the energy scan and 6000 trajectories for the detailed depth profiles, which gives a statistical error of the projected range below 1 %. All calculations and data processing were carried out in Python (NumPy, SciPy).

Results and Discussion

Nuclear stopping (Fig. 1a) reaches 3.28 keV/nm for Ag at 200 keV and 6.10 keV/nm for Au at 500 keV. The equality $S_e = S_n$ occurs at 565 keV (Ag) and 1921 keV (Au); therefore, damage is cascade-dominated over the whole range. The projected range (Fig. 1b, Table 1) increases from 19.1 to 338 nm for Ag and from 16.2 to 231 nm for Au. Compared with CeO_2 , the ranges in ZrO_2 are 3–10% shorter because of the higher atomic density. The damage profiles (Fig. 2) are broader than the metal profiles and shifted towards the surface (centroid at a depth of 0.43–0.59 R_p); hence, the near-surface layer of the membrane is damaged more strongly than the region where the metal resides. The peak damage at $1 \cdot 10^{16}$ ions/cm² is 19–26 dpa for Ag and 34–44 dpa for Au. For a porous membrane, the profiles are stretched by a factor of $1/(1-P)$ while the peak values remain unchanged. Sputtering (2.1–5.8 atoms/ion) at fluences of $(3-5) \cdot 10^{16}$

ions/cm² removes from a few to tens of nanometres, which must be taken into account when choosing the energy.

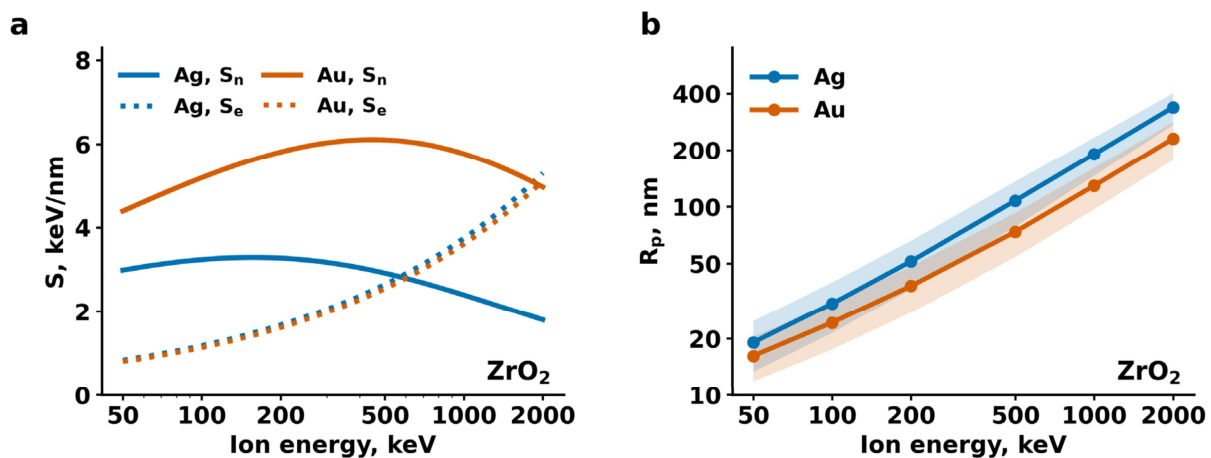


Figure 1. Stopping powers S_n , S_e (a) and projected range R_p (b) of Ag and Au ions in ZrO₂; bands show $\pm \Delta R_p$.

Table 1. Calculated implantation parameters for ZrO₂ (fluence $1 \cdot 10^{16}$ ions/cm²)

Ion	E, keV	R_p , nm	ΔR_p , nm	N_v , 1/ion	C_{max} , at. %	D_{max} , dpa	Y, atoms/ion
Ag	50	19.1	5.7	315	7.77	24	3.2
Ag	200	51.5	14.8	1012	3.16	26	3.5
Ag	500	107.8	28.9	2028	1.76	23	3.1
Ag	1000	190.6	43.8	3226	1.32	21	2.7
Ag	2000	338.4	64.2	4774	0.89	19	2.1
Au	50	16.2	4.3	331	10.29	34	4.2
Au	200	38.1	10.5	1132	4.36	42	5.6
Au	500	73.8	19.3	2447	2.58	44	5.8
Au	1000	129.4	32.0	4178	1.76	41	5.3
Au	2000	230.7	52.7	6821	1.12	38	4.9

The nanocluster nucleation threshold (≈ 8 at.%) at 500 keV is reached at $3.1 \cdot 10^{16}$ ions/cm² for Au and $4.5 \cdot 10^{16}$ ions/cm² for Ag, with peak damage of ≈ 136 and ≈ 105 dpa, respectively. Stabilized ZrO₂ does not amorphize even at hundreds of dpa, responding by point-defect accumulation and phase transformations [9, 10]; thus, such regimes are acceptable. Energies of 200–500 keV are recommended for a 50–100 nm layer and 1–2 MeV for a 200–300 nm layer.

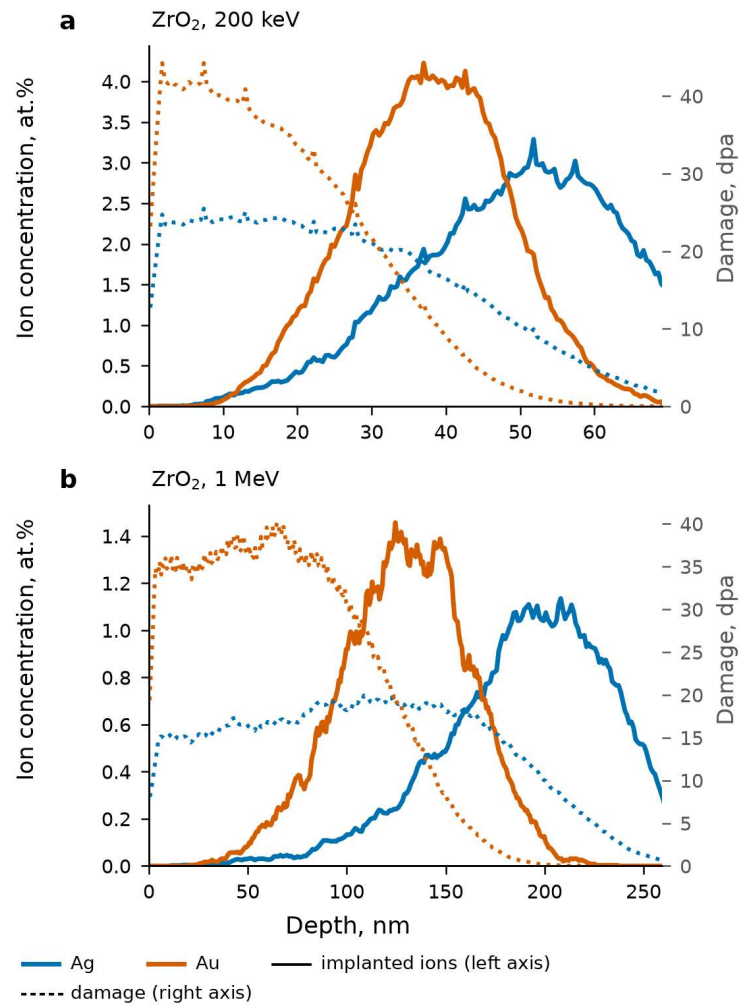


Figure 2. Depth profiles of implanted ions (solid lines) and damage (dotted lines) in ZrO₂ at 200 keV (a) and 1 MeV (b).

Conclusion and Recommendations

A complete set of implantation parameters for Ag and Au in ZrO₂ at 50–2000 keV has been obtained. Defect production is cascade-dominated over the whole range, and the damage maximum lies closer to the surface than the metal maximum. Nanoclusters form at $(3-5) \cdot 10^{16}$ ions/cm² and doses that do not amorphize ZrO₂. The results allow irradiation regimes to be chosen for the ion-beam modification of zirconia membranes.

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