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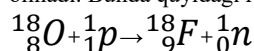
O'zRFA qoshidagi "Yadro fizika" instituti katta ilmiy xodimi, f.m.f.n. To'raqulov S. taqrizi ostida

$^{18}_{8}\text{O}_{(p,n)}\ ^{18}_{9}\text{F}$ REAKSIYALAR YORDAMIDA TIBBIYOTDA QO'LLANILADIGAN RADIONUKLIDNI SIKLOTRONDA OLINISHI

Annotatsiya

Butun jahon sog'liqni saqlash tashkiloti statistikasiga ko'ra, jahonda onkologik kasalliklardan o'lim ko'rsatkichlari yurak-qon tomir kasalliklaridan keyingi ikkinchi o'rinni egallaydi. Eng achinarlisi, bemorlarning deyarli 60 foizi kasallikning kechki III-IV bosqichlarida aniqlanayotganligidir. Onkologik kasalliklarni erta tashhislash va davolash bevosita Yadro tibbiyoti va Yadro fizikasiga chambarchas bog'liqdir. Bunday usul bizning O'zbekiston sharoitida birinchi bo'lib "New Life medical" nomli Yadro tibbiyot markazida qo'llanildi. Shunday radionuklidlardan biri $^{18}_{9}\text{F}$, kislorodning $^{18}_{8}\text{O}$ izotopi bilan boyitilgan suvni

$\text{H}_2\ ^{18}\text{O}$ siklotronning nishonlangan qurilmasida protonlar oqimi bilan nurlantirishda boradigan yadro reaksiyasiga asoslanib olinadi. Bunda quyidagi reaksiya sodir bo'ladi:



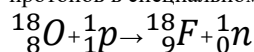
Kalit so'zlar: Siklotron, pozitron, $^{18}_{9}\text{F}$ [2] —FDG, proton, $^{18}_{8}\text{O}_{(p,n)}\ ^{18}_{9}\text{F}$, β^+ parchalanish, PET, gamma spektroskop.

ПОЛУЧЕНИЕ С ПОМОЩЬЮ ЦИКЛОТРОНА РАДИОНУКЛИДА, ИСПОЛЗУЕМОГО В МЕДИЦИНЕ В

$^{18}_{8}\text{O}_{(p,n)}\ ^{18}_{9}\text{F}$ РЕАКЦИЯХ

Аннотация

Согласно статистике Всемирной Организации Здравоохранения, смертность от онкологических заболеваний в мире занимает второе место после сердечно-сосудистых заболеваний. К сожалению, почти у 60% больных болезнь диагностируется на поздних III-IV стадиях заболевания. Ранняя диагностика и лечение онкологических заболеваний напрямую связаны с ядерной медициной и ядерной физикой. Одного из таких радионуклидов $^{18}_{9}\text{F}$ получают на основе ядерной реакции, происходящей при облучении воды $\text{H}_2\ ^{18}\text{O}$, обогащенной изотопом кислорода $^{18}_{8}\text{O}$, потоком протонов в специальном маркированном приборе циклотрона. Происходит следующая реакция:

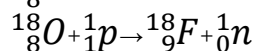


Ключевые слова: циклотрон, протон, $^{18}_{9}\text{F}$ -ФДГ, pozitron, $^{18}_{8}\text{O}_{(p,n)}\ ^{18}_{9}\text{F}$, β^+ распад, ПЭТ, гамма спектроскоп.

OBTAINING RADIONUCLIDES USED IN MEDICINE WITH $^{18}_{8}\text{O}_{(p,n)}\ ^{18}_{9}\text{F}$ REACTIONS USING CYCLOTRONS

Abstract

According to the statistics of the World Health Organization, the mortality rate from oncological diseases is the second highest in the world after cardiovascular disease. Unfortunately, almost 60% of patients are diagnosed in the late III-IV stages of the disease. Early diagnosis and treatment of oncological diseases is directly related to Nuclear Medicine and Nuclear Physics. One such radionuclide $^{18}_{9}\text{F}$ is obtained based on the nuclear reaction that takes place when water enriched $\text{H}_2\ ^{18}\text{O}$ with the isotope $^{18}_{8}\text{O}$ of irradiates with a stream of protons in a marked structure of a cyclotron. The following reaction occurs:



Keywords: cyclotron, $^{18}_{9}\text{F}$ [2] —FDG, proton, $^{18}_{8}\text{O}_{(p,n)}\ ^{18}_{9}\text{F}$, β^+ decay, PET, gamma spectroscopy.

Kirish. Fan va texnologiyalar rivoji yetuk cho'qqiga erishgan mana shunday davrda saraton kasalligi ko'pincha hali ham bedavo dard bo'lib qolmoqda. Saraton kasalligini erta davrlarida tashxislash bemorning hayotini saqlab qolish imkoniyatini beradi. Bugungi kunda O'zbekistonda onkologik kasalliklarga duchor bo'lgan 120 mingdan ziyod bemor qayd etilgan. Davlatimiz rahbari tomonidan tibbiyot sohasiga katta e'tibor qaratilmoqda. Prezidentimizning 2017-yil 4-apreldagi "2017-2021-yillarda O'zbekiston Respublikasida onkologiya xizmatini yanada rivojlantirish va aholiga onkologik yordam ko'rsatishni takomillashtirish chora-tadbirlari to'g'risida" gi Qarori yadro tibbiyoti sohasida kerakli chora-tadbirlarni ko'rishga muhim huquqiy asos bo'ldi.

2-fo'ra- ^{18}F -2-dezoksi-D-glyukoza (^{18}F [2] —FDG) pozitron emission tomografiyada (PET) da keng qo'llanilayotgan radiofarmasevtik diagnostik dori vositasidir.

^{18}F [2] —FDG xavfli o'smalarning joylashuvi, tarqalganlik darajasini aniqlashga, xavfli va xavfli bo'lmagan o'smalarni farqlashga va davo choralarining effektivligini aniqlashga yordam beradi [3].

PET klinik amaliyotida ^{18}F [2] —FDG ni limfomalar, melanomalar, sut bezlari saratoni, qizilo'ngach va ichaklar saratoni, qalqonsimon bez o'pka saratoni kabi kasalliklarni diagnostika qilishda qo'llaniladi. [1]

Tadqiqot metodologiyasi. Bu tadqiqot O'zbekistonda va Markaziy Osiyoda yagona bo'lgan "New Life Medical" Yadro Tibbiyot Markazida "GE MiniTrace Qilin (USA-Sweden)" rusumli siklotron yordamida ^{18}F [2] —FDG sintezi jarayonidagi xususiyatlarga asoslangan. O'zbekiston Milliy Universiteti Fizika fakulteti Yadro Tibbiyot Markazi bilan talabalarda amaliy ko'nikmalarni shakllantirish maqsadida 3 yillik shartnoma tuzgan.

Pozitron emission tomografiya (PET) tanadagi biokimyoviy va fiziologik jarayonlarni tasvirlashning kuchli diagnostik usulidir. PET anatomik tasvirni almashtirmaydi, balki tanadagi normal yoki shikastlangan to'qimalarda sodir bo'ladigan oddiy molekulyar jarayonlarni ko'rsatib beradi. Kompyuter tomografiya (KT) yoki Magnit rezonans tomografiya (MRT) anatomik nuqsonni ko'rish mumkin, lekin PET anormal to'qimalarning kimyoviy faolligi haqida ma'lumot beradi. PET tanada eng keng tarqalgan (C, N, O) elementlarning juda qisqa muddatda pozitron chiqaradigan nurlanishiga qarab anormal to'qimaning biokimyoviy reaksiyasini o'rganishga imkon beradi. Mazkur metod pozitronlarning elektronlar bilan annigilatsiya bo'lishi natijasida hosil bo'ladigan gamma-kvantlar juftligini qayd qilishga asoslangan. Pozitronning massasi va elektr zaryadining absolut qiymati mos ravishda elektron massasi va zaryadiga teng [4, 8].

Pozitron turg'un zarra hisoblanadi, lekin u modda elektronlari bilan ta'sirlashib annigilatsiya natijasida qisqa vaqt yashaydi. Masalan qo'rg'oshinda pozitron $5\cdot 10^{-11}\text{s}$ davomida annigilatsiyaga uchraydi. «Annigilatsiya» termini (annihilation) yo'q bo'lish, yo'qlikka aylanish ma'nosini beradi.

Pozitron bilan elektron to'qnashganda annigilatsiya hodisasi sodir bo'ladi [3]. Endi esa bu diagnostika qurilmasida ishlatiladigan ^{18}F —FDG radionuklidining fizik parametrlariga nazar solamiz.

^{18}F —FDG ga erishish uchun kimyoviy yondoshuvga, materialni tanlashga va ehtiyotkorlik bilan ishlashga e'tibor berish kerak. Bu izotopni deyarli ikki soatli yarim yemirilish davri, nisbatan kam energiyali gamma kvantlar chiqarishi uni PET radioizotopiga aylantirdi [6].

Parchalanish turi: ^{18}F —FDG 97 % o'zidan β^+ zarrachalar va 3% elektron qamrash yo'li bilan parchalanadi, pozitronning maksimal 653 keV energiya chiqarish bilan yakunlanadi. To'qimalarda pozitronning o'tacha yugurish masofasi 0.3mm. Bemor oladigan effektiv doza 7meV 10mCi (370 MBq). To'qimalar ichida ^{18}F —FDG keyinchalik ^{18}F —FDG-6-fosfatga aylanadi, to'qimalarda to'planadi va PET tekshiruvi davomida o'zgarishsiz holda qoladi [7].

1-jadval. ^{18}F dagi proton emmissiyasi

Qismaniy ulush	Maksimal energiya (MeV)	O'tacha energiya (MeV)
0.967	0.633	0.2498

2-jadval. ^{18}F dagi gamma kvantlar emissiyasi

Qismaniy ulush	Energiya(MeV)
1.93	0.5110
0.0307	0.000520

3-jadval. Turli yadro reaksiyalari yordamida ^{18}F ni olish usullari

Yadro reaksiyasi	Foydali energiya diapazoni (MeV)	Tabiiy boyitilganlik (%)
$^{18}\text{O}(\text{p}, \text{n})^{18}\text{F}$	14-4	0.2

$^{16}\text{O} (H^3, p) ^{18}\text{F}$	15–1	99.7
$^{16}\text{O} (\text{He}, n) ^{18}\text{Ne} : ^{18}\text{F}$	40–15	99.7
$^{16}\text{O} (\alpha, np) ^{18}\text{F}$	40–20	99.7
$^{16}\text{O} (\alpha, 2n) ^{18}\text{Ne} \rightarrow ^{18}\text{F}$	52–10	99.7
$^{20}\text{Ne} (d, \alpha) ^{18}\text{F}$	15–0	90.5
$^{20}\text{Ne} (p, 2pn) ^{18}\text{F}$	40–30	90.5
$^{20}\text{Ne} (H^3, \alpha p) ^{18}\text{F}$	40–10	90.5

^{18}F ni ishlab chiqarish usuli kichik hajmdagi (5 ml) $H_2^{18}\text{O}$ (boyitilgan suv) ni nishonga yaqin chegaralarda 3 Mev dan 20 Mev gacha energiyasi ortib boradigan protonlar bilan nurlantirishdan iborat. Suv nishoni bardosh bera oladigan nur oqimi kerakli suv hajmidagi bug'lanish darajasini aniqlash orqali topiladi. Hozirgi kunda maksimal nurlanish oqimi 60 mka ni tashkil qiladi. Bu kattalikni o'rtacha qiymati 20-40 mka ni tashkil qiladi. Nishonni yasash uchun quyidagi materiallar qabul qilingan: titan, kumush, oltin bilan qoplangan metallar (masalan nikel kabi), niobiy va tantalni o'z ichiga oladi [5].

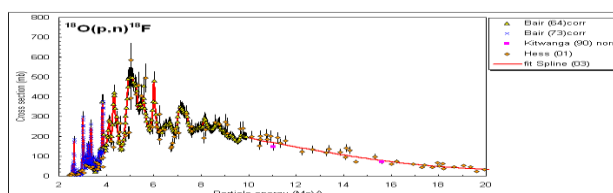
Tahlil va natijalar (Analysis and results)

4-jadval. Yuqori energiyali nishondagi $^{18}\text{O}_{(p,n)} ^{18}\text{F}$ ning chiqishi

Energiya diapazoni (MeV)	F-18 ni toyinganligi (mCi/mA)	F-18 ni to'yinganligi (GBq/mA)
20–2.5	395	14.6
18–2.5	373	13.8
15–2.5	327	12.1
11–2.5	230	8.5
8–2.5	132	4.9

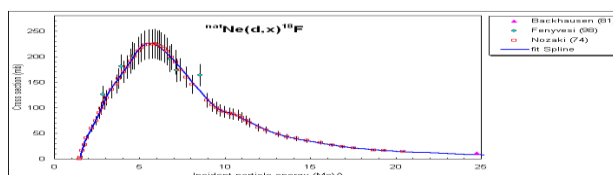
5-jadval. Yuqori energiyali nishondagi $^{nat}\text{Ne} (d, \alpha) ^{18}\text{F}$ ning chiqishi

Energy (MeV)	range	F-18 ni to'yinganligi (mCi/mA)	F-18 ni to'yinganligi (GBq/mA)
20–1.5		114	4.2
15–1.5		98	3.61
10–1.5		70	2.60
8–1.5		53	1.96
5.0–1.5		18	0.6



1-rasm. $^{18}\text{O} (p, n) ^{18}\text{F}$ reaksiya kesimini reaksiyadagi zarralar energiyasiga bog'liqlik grafigi

Yadro Tibbiyot Markazida hozirda ^{18}F —FDG ni olishning $^{18}\text{O} (p, n) ^{18}\text{F}$ reaksiya natijasida GE MiniTrace Qilin (USA-Sweden) rusumli siklotron yordamida olib kelinmoqda. Nurlanish davomida bosimi 35 bar bo'lgan "5.5" markali geliy gazi va bosimi 12 bar bo'lgan "5.0" markali vodorod gazi qo'llaniladi.

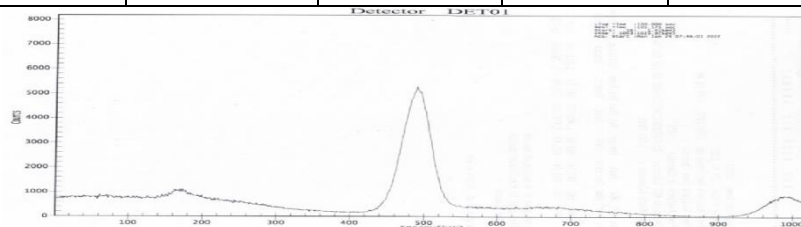


2-rasm. $^{nat}\text{Ne} (d, \alpha) ^{18}\text{F}$ reaksiya kesimini reaksiyadagi zarralar energiyasiga bog'liqlik grafigi

6-jadval. Siklotronida olib borilgan $^{18}_{8}\text{O}_{(p,n)}^{18}_{9}\text{F}$ reaksiyada tezlatkichning asosiy xarakteristikalar

Siklotronida olingan $^{18}_{9}\text{F}$ ni Fastlab 2 qurilmasi yordamida $^{18}_{9}\text{F}$ —FDG ga aylantiriladi. Nurlantirish uchun olinishi mo'jallangan radionuklid aktivligining kattaligiga qarab,

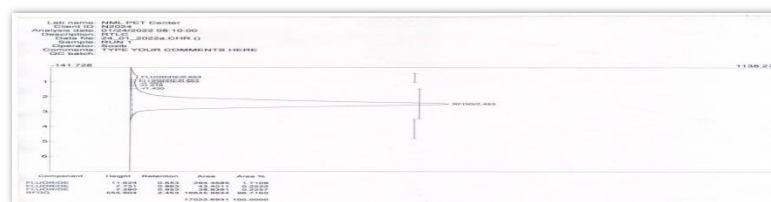
Ion manbasidagi tok(mA)	Ion manbasidagi kuchlanish (kV)	Magnitdagi tok kuchi(A)	Duantdagi kuchlanish (kV)	Vakumdagi bosim(mbar)	Oxirgi qilingan bosim (psi)	Nishondagi bosim (psi)
436	465	128.88	34.	1.4E-05	89.9	288.5



4-rasm. $^{18}_{9}\text{F}$ —FDG ning gamma spektrometrdagi olinan natijasi

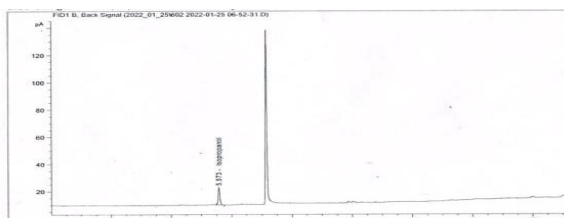
nurlantirish tok kuchi 60mkA dan katta bo'lmasligi kerak. Eksploatatsiya tajribalari ko'rsatishi bo'yicha maksimal aktivlikka nurlanish vaqti 120 daqiqa bo'lganda

5-rasm. $^{18}_{9}\text{F}$ —FDG ning Yupqa qatlamli xromotografiya natijasi.



erishiladi. Olingan $^{18}_{9}\text{F}$ —FDG ni quyida gamma spektrometr yordamida olingan tahlili keltirilgan: 4 va 5-rasmlarda olingan radionuklid $^{18}_{9}\text{F}$ —FDG ning tarkibi rostan ham $^{18}_{9}\text{F}$ —FDG dan tashkil topganligini ko'rsatuvchi gamma spektrometr natijalari keltirilgan.

Bunda grafikdagi cho'qqini tepasida olingan preparat haqiqatdan ham $^{18}_{9}\text{F}$ —FDG ligini va reaksiya 98.7% unum bilan borganini keltirib o'tilgan.



6-rasm. $^{18}_{9}\text{F}$ —FDG ning Gazli xromotografiya yordamida olingan natijalari.

6-rasmdagi tahlil natijasiga ko'ra $^{18}_{9}\text{F}$ —FDG preparat tarkibidagi qoldiq moddalar aniqlangan. Qoldiq moddalar qo'yilgan talablarga mos keladi. Bu izotop inson organizmiga tushganda tarkibidagi glukoza orqali saraton hujayrasiga yetib borib o'sha yerda o'rtnashadi va o'zidan β^+ zarralar chiqarishni davom ettiradi. Pozitron atom yadrosidan chiqariladi u qisqa masofani bosib o'tib energiyasi kamayadi, shu masofada atomlarni ham ionlashtiradi [9]. Pozitronlar shunda hosil bo'lgan erkin elektronlar bilan juftlashib 2ta zarra bir-biriga spirallanadi va soniyaning kichik bir qismida "pozitroniy" deb ataladigan ikki yadroli atomni hosil qiladi. Antizarralar o'zaro ta'sirlashganda ular keskin bir-birini yo'q qiladi. Har bir zarrachaning massasi to'liqligicha energiyaga aylanadi Eynshteyn formulasiga binoan annigilatsiya jarayonida bir biriga qarama-qarshi yo'nalgan $(180 \pm 0,3)$ 2 ta gamma kvant hosil bo'ladi [10].

Xulosa. Hozirgi texnika rivojlangan davrda insoniyatning sog'ligi eng yuqori o'rinlarga qo'yilmoqda. Saraton kabi bedavo dardni ham ilk bosqichlarda davolash mumkin. Kasallikning ilk bosqichini shu radioizotopni inson organizmiga kerakli miqdorda yuborgan holda PET qurilmasi yordamida aniqlanadi. Bu kasallikning turlari juda ko'p bo'lib, inson organizmining aynan qaysi organida, qanday chuqurlikda, tananing qaysi qismida joylashishiga qarab turli xil davolash choralarini ko'riladi. Lekin bu kasallikni davolashning asosida asosiy qurilma sifatida tezlatkichlar yotadi. Saraton kasalligini davolashda asosiy maqsad saraton hujayralari DNK larini yuqori energiyali zarrachalar yordamida buzishdan iborat. Bu kasallikni davolashda ishlatiladigan radioaktiv moddalar radioizotoplar deb atalib quyidagi asosiy xarakteristikalariga ega bo'lishi kerak: kam miqdorda radioaktivlikka ega bo'lishi, nisbatan kam yarim yemirilish davriga ega bo'lishi, parchalanishi davomida o'zidan massasi kichik zarrachalar chiqarib parchalanishi, izotopdan chiqqan zarrachalar muayyan yugurish masofasi va energiyani chiziqli uzatish

koeffitsiyentiga ega bo'lishi kerak. PET tanada eng keng tarqalgan (C, N, O) elementlarning juda qisqa muddatda pozitron chiqaradigan nurlanishiga qarab anomal to'qimaning biokimyoviy reaksiyasini o'rganishga imkon beradi. Mazkur metod pozitronlarning elektronlar bilan annigilatsiya bo'lishi natijasida hosil bo'ladigan gamma-kvantlar juftligini qayd qilishga asoslangan. 2-ftor- ^{18}F -2-dezoksi-D-glyukoza (^{18}F FDG) pozitron emission tomografiyada (PET) da keng qo'llanilayotgan radiofarmasevtik diagnostik dori vositasidir. ^{18}F FDG xavfli o'smalarning joylashuvi, tarqalganlik darajasini aniqlashga, xavfli va xavfli bo'lmagan o'smalarni farqlashga va davo choralarining effektivligini aniqlashga yordam beradi. ^{18}F FDG ning yarim yemirilish davri 109.75 daqiqa. ^{18}F FDG 97 % o'zidan β^+ zarrachalar va 3% elektron qamrash yo'li bilan parchalanadi, pozitronning maksimal 653 keV energiya chiqarish bilan yakunlanadi. Pozitronning to'qimada ruxsat etilgan o'rtacha yugurish masofasi ^{18}F FDG uchun 0.3 mm. Bemor oladigan effektiv doza tananing har 1 kg massasiga 7 meV 10 mCi (370 MBq). ^{18}F FDG ni olishda siklotronda quyidagi reaksiya borib ^{18}O (p,n) ^{18}F bu jarayonda siklotronda yoy razryadi orqali vodorod gazidan vodorod izotopi olinadi va u tezlatiladi. Vodorod izotopi bitta proton va bitta elektrondan iborat holda tezlashtirilib, 17-19 MeV energiyaga erishgungacha tezlashtiriladi va siklotronidan chiqishida elektroni ushlab qolinadi, proton esa nishon tomon harakatlanadi. ^{18}F yetarli aktivlikka (1.7 kyuri) 120 daqiqa davomida erishiladi.

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AB INITIO CALCULATIONS OF INTERMOLECULAR HYDROGEN BONDING IN TRIFLUOROACETIC ACID WITH WATER

Abstract

In this investigation, in order to further understand study the mechanism of formation of molecular clusters formed by trifluoroacetic acid with water molecules calculations were performed on the basis of the set of B3LYP/6-311++G(d,p) by the method of density functional theory (DFT). The stabilization of the cluster was determined by the increase in the number of water molecules in the molecular clusters, and the most stable cluster was the bicyclic structural cluster formed by four water molecules with trifluoroacetic acid. When the number of water molecules in a cluster exceeds four, a proton transition occurs between the molecules to form CF_3COO^- and H_2O^+ ions.

Keywords: trifluoroacetic acid, molecular cluster, H-bond, DFT method.

UCHFTORLISIRKA KISLOTASINING SUV MOLEKULASI BILAN MOLEKULALARARO VODOROD BOG'LANISHLARIDA NOEMPERIK HISOBLASHLAR

Annotatsiya

Ushbu ishda uchftorlisirka kislotasining suv molekulari bilan hosil qilgan molekulyar klasterlarining $[\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_n]$, $n=1-7$ shakllanish mexanizmini o'rganish maqsadida zichlik funksional nazariya (DFT) usuli va BLYP/6-311++G(d,p) funksiyalar to'plami asosida hisoblashlar olib borildi. Molekulyar klasterlar tarkibidagi suv molekularining soni ortishi bilan klasterning barqarorlashishi aniqlandi va eng barqaror klaster uchftorlisirka kislotasining to'rtta suv molekulari bilan hosil qilgan bisiklik strukturali klasteri ekan. Klaster tarkibidagi suv molekulari soni to'rttadan ortganda molekular orasida proton o'tish yuzaga kelib, CF_3COO^- va H_2O^+ ionlari hosil bo'lishi aniqlandi.

Kalit so'zlar: uchftorlisirka kislota, molekulyar klaster, H-bog'lanish, DFT usul.

НЕЭМПИРИЧЕСКИЕ РАСЧЕТЫ МЕЖМОЛЕКУЛЯРНОЙ ВОДОРОДНОЙ СВЯЗИ В ТРИФТОРУКСУСНОЙ КИСЛОТЕ И ВОДЕ

Аннотация

В данной работе приведены результаты исследования образования молекулярных кластеров, между молекулами трифторуксусной кислоты и воды методом теории функционала плотности (DFT) на основе набора B3LYP/6-311++G(d,p). Стабилизация кластера определялась увеличением числа молекул воды в молекулярных кластерах, причем наиболее устойчивым оказался бициклический структурный кластер, образованный четырьмя молекулами воды с трифторуксусной кислотой. Установлено что, когда число молекул воды в кластере превышает четыре, между молекулами происходит протонный переход с образованием ионов CF_3COO^- и H_2O^+ .

Ключевые слова: трифторуксусная кислота, молекулярный кластер, H-связь, метод DFT.

Introduction. Carbonic acids have a protonodonor group and two protonoceptor centers that can form various aggregates in the liquid state through hydrogen bonds [1-10]. The study of the structure, properties, and interactions of carbonic acids, including trifluoroacetic acid (CF_3COOH) with water molecules is important in solving problems related to aerosol and acid rain in the atmosphere [11-13].

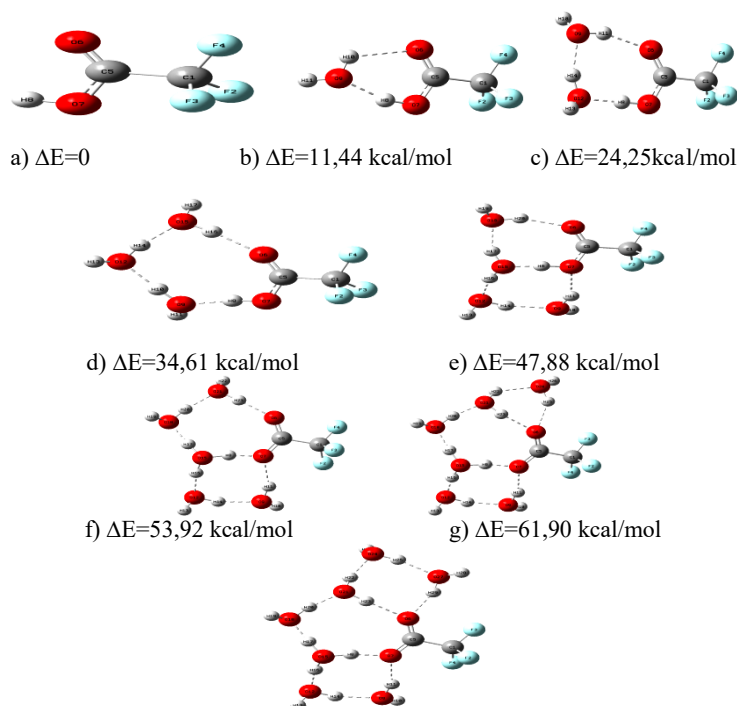
The interaction of CF_3COOH with water molecules was studied by V.D. Maiorov et al. [11,14], which showed that the peak displacement and intensity decrease of spectral bands, based on calculations, CF_3COOH anion is strongly hydrated by two water molecules. The optimal structure of the monomer and dimer of CF_3COOH through H-bonds with water was studied by E.G.Tarakanova et al [15] using the method DFT/(B3LYP 6-31++G(d, p)), in which the average hydrogen the bonding energy is ~ 9-10 kcal/mol and the DFT calculations obtained on the basis of 6-31++G(d,p) are consistent with the values in infrared (IR) and Raman scattering.

CF₃COOH acid was studied by IR spectroscopy in aqueous medium (D₂O). In the pure CF₃COOH, the maximum stretching vibration frequency of C=O is 1800 cm⁻¹, and in the aquatic environment it is observed that this peak shifts to the lower frequency side [16]. In this study, quantum chemical calculations were performed to study the interaction of trifluoroacetic acid, which belongs to the group of carbonic acids, with the simplest representatives of biologically active substances water molecules. The changes in the geometric and spectroscopic parameters of molecular clusters were analyzed using calculations.

Calculation methods. All calculations were performed in Gaussian 09 [17] on the basis set of 6-311++G(d,p) bases containing diffuse and polarization functions at the B3LYP level using the Density Functional Theory (DFT) method. The GaussView 5.0 graphical interface was used to visualize the calculation results.

Results and discussions. Figure 1 shows the optimal geometric structures of molecular clusters [CF₃COOH+(H₂O)_n, n=1-7] formed by the monomer of trifluoroacetic acid and water molecules. As can be seen, trifluoroacetic acid and water molecules form various molecular clusters using intermolecular hydrogen bonds.

Trifluoroacetic acid can form molecular clusters in different directions with a single water molecule, and the most stable of such clusters is the cyclic structural cluster (Figure 1, Table 1). The energy of the intermolecular interaction in the formation of such a cluster (CF₃COOH+H₂O) is 11.44 kcal/mol, and the average



h) $\Delta E=74,35$ kcal/mol

Figure 1. The optimal geometries of trifluoroacetic monomer and clusters with water molecules [CF₃COOH+(H₂O)_n, n=1-7]

energy required for each hydrogen bond is 5.77 kcal/mol. In the formation of this cluster, acid and water molecules act as both H-donors and H-acceptors. That is, the O-H functional group of the acid acts as an H-donor, and the C=O group acts as an H-acceptor. Also, in the formation of the cluster CF₃COOH+H₂O, the stretching vibration frequencies of the acid C=O and O-H relative to the monomer ($\nu_{C=O}=1860,5$ cm⁻¹, $\nu_{O-H}=3748,2$ cm⁻¹), and red-shifts were 39.6 cm⁻¹ and 463.3 cm⁻¹ respectively (Figure 3b). Also, the bond lengths of the C=O and O-H groups increase by 0.01 and 0.02 Å in cluster formation related to the monomer ($r_{C=O}=1,19$ Å, $r_{O-H}=0,97$ Å) (Figure 2). Changes in spectral and geometric parameters show that the O7-H8...O9 bond is stronger than the O9-H10...O6 bond.

The geometric structure of the most stable molecular cluster [CF₃COOH+(H₂O)₂] formed by two water molecules of trifluoroacetic acid is also cyclic (Figure 1c), with an intermolecular interaction energy of 24.25 kcal/mol. The average energy required for each hydrogen bond increases by 2.3 kcal/mol per cluster of CF₃COOH+H₂O. In the formation of such a cluster, the stretching vibration frequencies of the functional groups C=O and O-H of the acid molecule saw red-shift of 60 and 840 cm⁻¹, respectively, relative to the monomer state (Figure 3c), and the bond lengths increase by 0.015 and 0.01 Å (Fig.2).

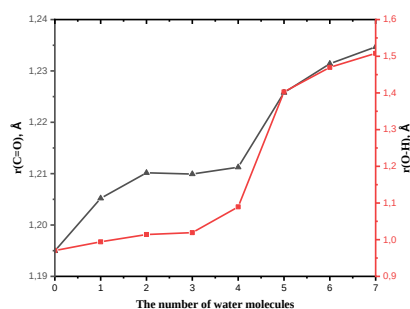


Figure 2. The dependence of C=O and O-H bonds distances on the number of water molecules in the molecular cluster

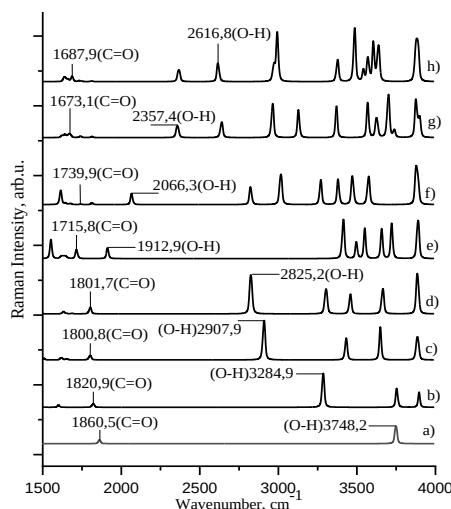
Similarly, the molecular cluster $[\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_3]$ formed by the three acids of water is also cyclic, with an intermolecular interaction energy of 34.61 kcal/mol. The average energy required for each hydrogen bond is 8.65 kcal/mol, which is 0.57 kcal/mol greater than $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_2$. This leads to further stabilization of the cluster.

The molecular cluster of trifluoroacetic acid formed by four water $[\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_4]$ is bicyclic. The energy of the intermolecular interaction in the formation of such a cluster is 47.88 kcal/mol. The average energy for each H-bond is 7.98 kcal/mol. The stretching vibration frequencies of the C=O and O-H groups of the acid range from 1715.8 and 1912.9 cm^{-1} , respectively.

Figure 3. The bands in an interval of 1500-4000 cm^{-1} of theoretical Raman spectra of molecular clusters: CF_3COOH (a), $\text{CF}_3\text{COOH}+\text{H}_2\text{O}$ (b), $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_2$ (c), $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_3$ (d), $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_4$ (e), $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_5$ (f), $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_6$ (g), $\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_7$ (h)

When the number of water molecules in the molecular cluster reaches five $[\text{CF}_3\text{COOH}+(\text{H}_2\text{O})_5]$, the proton belonging to the carboxyl group of the acid is transferred to the water molecule as a result of a strong electrostatic interaction and the $-\text{COO}^-$ anion and H_2O^+ cation are formed. As can be seen from Figure 3, the length of the O-H bond of the acid, i.e., the distance between the O7 and H8 atoms, increases sharply when the number of water molecules reaches five. This procedure also continued when the number of water molecules was higher than five (Fig.1 f, g, h). The spectral bands corresponding to the frequencies 2066.3 (f), 2357.4 (g) and 2616.8 cm^{-1} (h) shown in Figure 3 belong to the O-H vibrations of the H_2O^+ cation.

Table 1. Results of calculations of molecular clusters



The types of molecular clusters	The distance of hydrogen bond (Å)	Frequency of C=O vibration, cm^{-1} (Raman A4/AMU)	Frequency of O-H vibration, cm^{-1} (Raman A4/AMU)	Dipole momentum, (Debye)	Energy of intermolecular interaction (kcal/mol)	Average energy of hydrogen bonding (kcal/mol)
CF_3COOH	$r(\text{H}8 \dots \text{O}6) = 2.355$	1860.5 (11.8)	3748.2 (94.3)	2.36	-	-
$\text{CF}_3\text{COOH} + \text{H}_2\text{O}$	$r(\text{H}8 \dots \text{O}9) = 1.716$ $r(\text{O}6 \dots \text{H}10) = 2.271$	1820.9 (11.8)	3284.9 (152.0)	3.86	11.44	5,72
$\text{CF}_3\text{COOH} + (\text{H}_2\text{O})_2$	$r(\text{O}6 \dots \text{H}11) = 1.901$ $r(\text{H}8 \dots \text{O}12) = 1.588$ $r(\text{O}9 \dots \text{H}14) = 1.745$	1800.8 (14.7)	2907.9 (168.5)	3.51	24.25	8,08
$\text{CF}_3\text{COOH} + (\text{H}_2\text{O})_3$	$r(\text{O}6 \dots \text{H}16) = 1.856$ $r(\text{H}8 \dots \text{O}9) = 1.557$ $r(\text{H}10 \dots \text{O}12) = 1.688$ $r(\text{H}14 \dots \text{O}15) = 1.742$	1801.7 (19.0)	2825.2 (187.5)	3.54	34.61	8,65
$\text{CF}_3\text{COOH} + (\text{H}_2\text{O})_4$	$r(\text{O}6 \dots \text{H}20) = 1.925$ $r(\text{H}8 \dots \text{O}15) = 1.371$ $r(\text{O}7 \dots \text{H}11) = 2.025$ $r(\text{O}9 \dots \text{H}14) = 1.819$ $r(\text{O}12 \dots \text{H}16) = 1.754$ $r(\text{H}17 \dots \text{O}18) = 1.787$	1715.8 (22.9)	1912.9 (25.6)	2.08	47.88	7,98

CF ₃ COOH + (H ₂ O) ₅	$r(\text{O6} \dots \text{H23}) = 1.744$ $r(\text{H8} \dots \text{O7}) = 1.071$ $r(\text{O7} \dots \text{H11}) = 1.859$ $r(\text{O9} \dots \text{H14}) = 1.729$ $r(\text{O12} \dots \text{H16}) = 1.601$ $r(\text{H17} \dots \text{O18}) = 1.548$ $r(\text{H20} \dots \text{O21}) = 1.667$	1739.9 (1.1)	2066.3 (28.2)	4.66	53.92	7,7
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Conclusion. The results of the calculations showed that trifluoroacetic acid forms various H-bonded clusters with water molecules. As the number of water molecules in the cluster increases, the cluster stabilizes. The most stable of these clusters is the cluster [CF₃COOH+(H₂O)₄] formed by four water molecules of trifluoroacetic acid, which is bicyclic in shape. When the number of water molecules reaches five, one proton belonging to the carboxyl group of the acid is transferred to the water molecule and the –COO⁻ anion H₂O⁺ is formed.

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NUCLEAR REACTIONS UNDER THE EFFECT OF X-RAY IN NEUTRON STARS

Abstract

Observational measurements from X-ray satellites over the last decade have provided us with a wealth of information about possible nuclear reactions in neutron stars in high-density environments. Some of these processes have been studied in the laboratory by radioactive ion radiation from first-generation devices. In this article, I will report on experiments with radioactive rays from the ATLAS accelerator in Argonne.

Keywords: I-II type X-ray radiation, strong X-ray radiation, AstroSat, neutron star ocean ATLAS.

ЯДЕРНЫЕ РЕАКЦИИ ПОД ВОЗДЕЙСТВИЕМ РЕНТГЕНОВСКОГО ИЗЛУЧЕНИЯ В НЕЙТРОННЫХ ЗВЕЗДАХ

Аннотация

Наблюдательные измерения с рентгеновских спутников за последнее десятилетие предоставили нам огромное количество информации о возможных ядерных реакциях в нейтронных звездах в средах с высокой плотностью. Некоторые из этих процессов изучались в лаборатории с помощью излучения радиоактивных ионов от приборов первого поколения. В этой статье я расскажу об экспериментах с радиоактивными лучами на ускорителе ATLAS в Аргонне.

Ключевые слова: рентгеновское излучение I-II типов, сильное рентгеновское излучение, AstroSat, океан нейтронных звезд ATLAS.

NEYTRON YULDUZLARDAGI RENTGEN NURLARI TA'SIRIDAGI YADRO REAKSIYALAR

Annototsiya

So'nggi o'n yillarda rentgen sun'iy yo'ldoshlarining kuzatishdan olgan o'lchovlari bizga neytron yulduzlarining yuqori zichlikdagi muhitida sodir bo'lishi mumkin bo'lgan yadro reaksiyalari haqida ko'plab ma'lumotlarni taqdim etdi. Birinchi avlod qurilmalarining radioaktiv ion nurlari bilan laboratoriyada ushbu jarayonlarning ba'zilarini o'rganilgan. Ushbu maqolada men Argonnadagi ATLAS tezlatgichidan radioaktiv nurlar bilan o'tkazilgan tajribalar haqida xabar beraman.

Kalit so'zlar: I-II tur rengen nurlanish, kuchli rengen nurlanish, AstroSat, neytron yulduz okeani ATLAS.

Kirish. Rentgen nurlari ta'siridagi yulduzlar portlashi koinotda tez-tez uchraydi. Misol sifatida, neytron yulduzlarni keltirish mumkin. Neytron yulduzi deyarli to'liq neytronlardan tashkil topgan astronomik ob'ekt bo'lib, uni o'ta zich qiladi. Uning zich moddasining tortishish kuchi boshqa yulduzdan, ko'pincha Quyosh kabi yulduz materiyasini uning yuzasiga tushib, uning atrofida disk hosil qiladi. Demak, bu Yerdagi biron bir laboratoriyada yaratib bo'lmaydigan ekstremal sharoitlarning tabiiy laboratoriyasidir. Ba'zan neytron yulduzi to'satdan rentgen nurlanishni chiqaradi, bu uning ichki qismini, sirtini o'rganish uchun muhimdir.

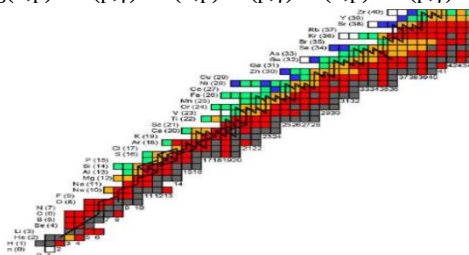
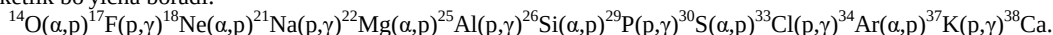
Hindiston Indore Texnologiya Instituti (IIT-Indore) astronomlari guruhi tomonidan ISRO'ning AstroSat ma'lumotlaridan foydalangan holda tadqiqotlar o'tkazadilar. AstroSat bir vaqtning o'zida bir xil astrofizik manbani kuzatuvchi beshta teleskopga ega. Astronomlar neytron yulduzining portlashlarini bir vaqtning o'zida ushlash uchun AstroSatning ikkita asbobidan, Yumshoq rentgen teleskopidan (SXT) va katta maydon rentgen proportsional hisoblagichidan (LAXPC) foydalanganlar. Bu kuzatuvda korishdiki, neytron yulduzi har to'rt soatda bir marta portlash chiqaradi. Bu portlashda rengen nurlanishi hosil bo'ladi[1].

Undan tashqari 1975 yilda ham kuzatilgan[2]. Ushbu tizimlardagi kuchli tortishish kuchlari materialning sirtga taxminan 200 MeV/u energiya bilan tushishiga ega, bu esa rentgen nurlarining uzluksiz oqimiga olib keladi. Agar etarli miqdorda material to'plangan bo'lsa, vodorod - geliy aralashmasi 10^{38-39} erg energiya chiqishi bilan portlaydi. Bu 10 soniyalardan bir necha daqiqagacha davom etadigan rentgen nurlari oqimining keskin o'sishiga olib keladi. Hozirgacha 100 dan ortiq shunday manbalar topilgan. Bu hodisani takrorlanish tezligi bir soatdan bir necha soatgacha bo'lganligi sababli, ushbu hodisalarning katta ma'lumotlar bazasi to'plangan [3]. Ushbu rentgen nurlanishini qisqaroq takrorlanish vaqti ya'ni 10 sekund ko'rsatadigan hodisalardan ajratish uchun I va II tur rentgen nurlanishiga bo'lingan. Bunda I turdagi rengen nurlanishi termoyadroviy reaksiya ketishlar va ularning turi bilan bog'liq. II turdagi rengen nurlanishi nurlanishning beqarorligi bilan bog'liq. Rengen nurlarining nurlanishlari koinotning kimyoviy evolyutsiyasi haqida so'zlamasa ham, lekin bizga juda zich yadro moddasida sodir bo'ladigan yadroviy jarayonlar haqida ma'lumotlarni beradi. Vaqt tuzilmalarining xilma-xilligi va nurlanish multipletlarining paydo bo'lishi turli guruhlar tomonidan o'rganilayotgan tadqiqot sohalriga misoldir[4].

Taxlil va natijalar. Kuchli nurlanishlar bir necha soat davom etadi va bu nurlanishda taxminan 10^{42} erg energiya ajralib chiqadi[5,6]. Taxminan bir yil takrorlanish vaqtiga ega bo'lgan bu kuchli nurlanishlar neytron yulduzining "okeanida" chuqurroq sodir bo'ladi. Bu beqaror uglerod yonishi va neytronga boy yadrolar orasidagi boshqa reaksiyalarni o'z ichiga olishi mumkin. I-turdagi rentgen nurlari nurlanishlarini o'rganish bizga neytron yulduzi atmosferasida sodir bo'ladigan yadro reaksiyalari haqida ba'zi ma'lumotlarni beradi. Bizning kuchli nurlanishlar haqidagi bilimiz ancha sodda va bu bilimizni boyitishimiz muhim.

Neytron yulduzlardagi (a,p) jarayondagi reaksiyalar. Argonna laboratoriyasidagi ATLAS og'ir ion tezlatgichida biz rentgen nurlarining protonga boy va neytronga boy tomonidagi nurlar yordamida I turdagi rentgen nurlari nurlanishlarini va kuchli nurlanishlarni tushunishimiz uchun muhim bo'lgan ba'zi reaksiyalarni o'rganilgan. Vodorod yoki deyteriy bilan to'ldirilgan ishlab chiqarish nishonini og'irroq massaga ega barqaror ion nurlari bilan bombardimon qilish orqali hosil qilingan.[7,8,9] Radioaktiv nurlar gaz xujayrasida teskari kinematikadagi reaksiyalar natijasida hosil bo'ladi, masalan, $^1\text{H}(^{10}\text{B},^{10}\text{C})n$, $^2\text{H}(^{32}\text{S},^{33}\text{Cl})n$ yoki $^2\text{H}(^{14}\text{C},^{15}\text{C})p$. Keyin bu ikkilamchi nurlar birlamchi nurdan 26° burchak ostida buruvchi magnit va magnitdan keyin joylashgan RF-supurgi bilan ajratiladi[10]. Ushbu radioaktiv nurlar bilan I turdagi rentgen nurlari nurlanishida (a,p) jarayonga taalluqli bo'lgan yadro reaksiyalari va kuchli nurlanishlarda muhim deb hisoblangan termoyadroviy reaksiyalar o'rganildi. Ushbu reaksiyalarning ba'zilari quyida batafsilroq muhokama qilinadi.

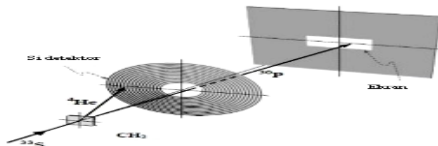
1-rasmdagi reaksiya yo'lidan ko'rinib turibdiki (a,p) reaksiyalar asosan A 40 massa diapazonida rol o'ynaydi va ko'p sonli ba'zan sekin b-parchalanishlardan qochib, reaksiya oqimida "qisqa yo'l"ni ta'minlaydi. ^{14}O dan boshlab (a,p) jarayon ketma-ketlik bo'yicha boradi:



1-rasm. Neytron yulduzdagi yadro reaksiya.

Ushbu reaksiyalarni eksperimental tadqiq qilish uchun teskari (p, n) yoki (d, n) reaksiyalar orqali ^{14}O , ^{17}F , ^{21}Na , ^{25}Al , ^{29}P , ^{33}Cl va ^{37}K nurlarini ^{18}Ne , ^{22}Mg nurlar bilan solishtirganda hosil qilish osonroq, ^{26}Si , ^{30}S , ^{34}Ar , ular (^3He , n) yoki (^{12}C , ^{10}Be) kabi ikki zarrali reaksiyalarini talab qiladi. Shuning uchun yuqorida qayd etilgan ko'plab tegishli (a,p) reaksiyalar barqarorlik vodiysiga yaqinroq bo'lgan radioaktiv nurlar yordamida vaqtga teskari (p,a) reaksiyasi orqali o'rganildi. Biroq, bu usul faqat asosiy holatning asosiy holatiga reaksiya kuchi haqida ma'lumot beradi, hayajonlangan holatlarning ta'sirini statistik model hisob-kitoblari yordamida olish kerak. So'nggi bir necha yil davomida o'tkazilgan bir nechta tajribalarda biz $^{22}\text{Mg}(\alpha,p)^{25}\text{Al}$, $^{26}\text{Si}(\alpha,p)^{29}\text{P}$, $^{30}\text{S}(\alpha,p)^{33}\text{Cl}$, $^{34}\text{Ar}(\alpha,p)^{37}\text{K}$ va $^{30}\text{P}(\alpha,p)^{33}\text{S}$ [11,13] reaksiyalari uchun vaqtga teskari ko'ndalang kesimlarini o'lchandi Birinchi to'rtta tizim radioaktiv ion nurlarini talab qiladi, oxirgi reaksiya esa eksperimental texnikani o'rganish uchun sinov holati sifatida barqaror ^{33}S nur bilan amalga oshirildi.

Tajriba qurilmani o'rnatish 2-rasmda ko'rsatilgan [12]. ATLAS tezlatgichining nurlari (^{25}Al , ^{29}P , ^{33}S , ^{33}Cl va ^{37}K) Enge Split-Pole spektrografining tarqalish kamerasiga o'rnatilgan CH_2 nishonlarini bombardimon qilgan. (p,a) reaksiyasidagi a zarralari $\theta_{\text{lab}} = 8^\circ - 25^\circ$ burchak diapazonini qamrab oluvchi ikki tomonlama halqasimon Si detektor tomonidan aniqlandi. $\theta = 1,5^\circ - 3^\circ$ burchak oralig'ida chiqarilgan reaksiya

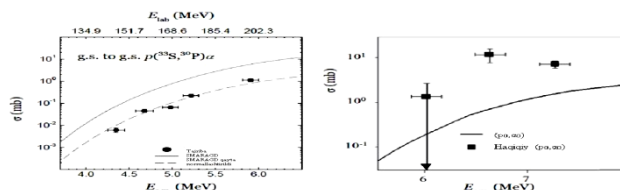


2-rasm. (p,a) reaksiyalarni o'lchash uchun ishlatiladigan tajriba qurilmaning sxemasi.

mahsulotlari ^{22}Mg , ^{26}Si , ^{30}P , ^{30}S , ^{34}Ar splitpole spektrografiga joylandi. Tizimni aniqlash samaradorligini oshirish uchun magnit gaz bilan to'ldirilgan rejimda ishladi[14].

Bunday sharoitda yadro zaryadi Z bilan tushadigan ionlar va azot gazi molekullari o'rtasidagi zaryad o'zgaruvchan to'qnashuvi magnit maydondagi ionlarning o'rtacha zaryad holatiga olib keladi $\langle q \rangle$ bu birinchi navbatda o'rtacha ion tezligiga $\langle v \rangle$ proporsionaldir. Natijada magnit qattqlik birinchi navbatda tezlikdan mustaqil bo'lib, natijada spektrometring fokal tekisligidagi ionlarning m/Z^2 qiymatiga ko'ra ajralishiga olib keladi. Ushbu texnika birinchi bo'lib 120-200 MeV energiya oralig'ida barqaror ^{33}S nurlari bilan $^{33}\text{S}(\text{p},a)^{30}\text{P}$ reaksiyasi uchun sinovdan o'tkazildi[12].

3-rasmda $^{33}\text{S}(\text{p},a)^{30}\text{P}$ va $^{33}\text{Cl}(\text{p},a)^{30}\text{S}$ reaksiyalarining qo'zg'alish funksiyalari 4-7 MeV diapazonida ko'rsatilgan[11,12]. Barqaror ^{33}S nurida mavjud bo'lgan yuqori intensivlik 10^8 zarracha/sek tufayli $^{33}\text{S}(\text{p},a)^{30}\text{P}$ reaksiyasining qo'zg'alish funksiyasi 5 μb ko'ndalang kesim mintaqasiga qadar o'lchanishi mumkin, $^{33}\text{Cl}(\text{p},a)^{30}\text{S}$ ning qo'zg'alish funksiyasi, taxminan 10 zarracha/sek nur intensivligi bilan o'lchangan reaksiyasi hozirgacha 5-10 μb reaksiya bilan cheklangan. 3-rasmdagi qattiq chiziqlar SMARAGD kodidan foydalangan holda statistik model hisob-kitoblaridan kelib chiqadi. [15]



3-rasm. Gaz bilan to'ldirilgan va magnit texnikasi bilan o'lchangan reaksiyasi ya'ni $^{33}\text{S}(\text{p},a)^{30}\text{P}$ chapda va $^{33}\text{Cl}(\text{p},a)^{30}\text{S}$ reaksiyasining qo'zg'alish funksiyalari o'ngda ko'rsatilgan.

3-rasmdan ko'rinib turibdiki, $^{33}\text{S}(\text{p},a)^{30}\text{P}$ reaksiyasining tajriba kesmalari statistik model taxminlaridan kichikroq bo'lsa, $^{33}\text{Cl}(\text{p},a)^{30}\text{S}$ reaksiyasi uchun buning aksidir. Shuni ta'kidlash kerakki, $^{33}\text{Cl}(\text{p},a)^{30}\text{S}$ reaksiyasining vaqtga teskari reaksiyasi yuqori darajalar bilan ikki tepalikli portlash strukturasini hosil qiladi. Biroq, ushbu simulyatsiyalarda kesma 100 faktorga o'zgartirildi, bu tajribada kuzatilganidan kattaroqdir.

Xulosa. Rentgen nurlanishlar bizga atmosferada va neytron yulduzlarining ichki qismida sodir bo'lishi mumkin bo'lgan keng spektrli yadro reaksiyalari haqida ma'lumot berishi mumkin. Ushbu yadro astrofizik ma'lumotlarda ishtirok etuvchi yadrolar massa vodiysining har ikki tomonidagi izotoplarni qamrab oladi.

So'nggi 10 yil ichida radioaktiv ion nurlarini yaratish bo'yicha butun dunyo bo'ylab olib borilgan sa'y-harakatlar bizga ushbu jarayonlarning ba'zilarini yerdagi laboratoriyalarida o'rganish imkonini berdi. Buning uchun kuchli radioaktiv nurlar va yuqori samaradorlikka ega detektor tizimlari kerak. Ushbu maqolada tasvirlangan faol maqsadli tizim yadro astrofizikasi uchun qiziq bo'lgan termoyadroviy va uzatish reaksiyalarining birinchi o'lchovlarini amalga oshirishga imkon berdi. Ushbu birinchi o'lchovlarda hisoblash hali ham taxminan 5k bilan cheklangan bo'lsada, MUSIC dan keyingilari uchun asos bo'lib xizmat qiladi.

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CO₂ GAZINI 1-ETIL-3-METILIMIDAZOLIY TETRAFTORBORAT ION SUYUQLIGIDA YUTILISHI

Abstract

Molekulyar dinamika simulyatsiyalari yordamida turli xil temperaturalarda CO₂ molekulalarining ekologik toza 1-etil-3-metilimidazoliy tetraftorborat ([EMIM][BF₄]) ion suyuqligida (IS) yutilishini tadqiq qildik. Mazkur ISning turli haroratlardagi zichligi va CO₂ gazini ISdagi erkin energiya profillari GROMACS dasturi yordamida hisoblandi va tanlangan ISning CO₂ molekulasini yutish potentsiali baholandi. Biz olib borgan tadqiqotlar atrof muhitga zararli bo'lgan CO₂ gazini samarador tutib qoluvchi muqobil manba sifatida [EMIM][BF₄] ion suyuqligi taklif etildi.

ABSORPTION OF CO₂ GAS IN 1-ETHYL-3-METHYLIMIDAZOLE TETRAFTORBORATE IONIC LIQUID

Abstract

Here, we investigated the absorption of CO₂ molecules at different temperatures in an environmentally friendly 1-ethyl-3-methylimidazole tetrafluoroborate ([EMIM][BF₄]) ionic liquid (IL) using molecular dynamics simulations. The densities of this IL at different temperatures and the permeation free energy profiles of CO₂ molecule into ILs were calculated using the GROMACS program package and the absorption potential of CO₂ in IL was estimated. Our study suggests that [EMIM][BF₄] ionic liquid can be used as an alternative source for efficient capturing CO₂ gas, which is harmful to the environment.

АБСОРБЦИЯ ГАЗА CO₂ В ИОННОЙ ЖИДКОСТИ ТЕТРАФТОРБОРАТА 1-ЭТИЛ-3-МЕТИЛИМИДАЗОЛА

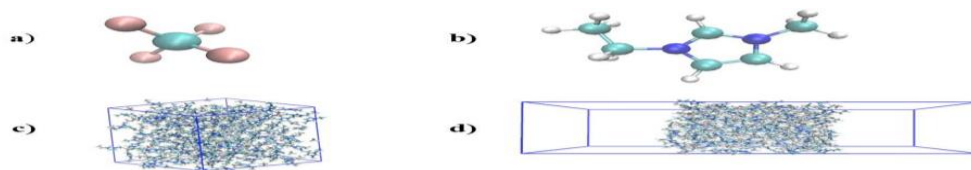
Абстракт

Здесь мы исследовали поглощение молекул CO₂ при различных температурах в экологически чистой ионной жидкости (ИЖ) 1-этил-3-метилимидазол-тетрафторбората ([EMIM][BF₄]) с использованием моделирования молекулярной динамики. С помощью пакета программ GROMACS рассчитаны плотности этой ИЖ при различных температурах и профили свободной энергии молекулы CO₂, а также оценен потенциал поглощения CO₂ в ИЖ. Наше исследование предполагает, что ионная жидкость [EMIM][BF₄] может быть использована в качестве альтернативного источника для эффективного улавливания газа CO₂, который вреден для окружающей среды.

Kirish. Atmosferada to'plangan issiqxona gazlari o'rtacha global temperaturaning ko'tarilishida asosiy sabab sifatida qaraladi. Qazilma yoqilg'i manbalarining yonishi natijasida atmosferaga katta miqdorda CO₂ gazi ajralib chiqadi [1]. CO₂ gazini turli xil usullar bilan tutib qolish orqali atmosferaga bo'lgan zararini kamaytirishi mumkin [2-4]. CO₂ ni erituvchilar yordamida tutib qolish keng tarqalgan iqtisodiy samarador usullardan biri hisoblanadi [5]. Misol uchun, alkanolamin eritmaları samarali CO₂ yutilish qobiliyatini ko'rsatdi, ammo ular past bug' bosimi, desorbsiya jarayonida erituvchining yo'qolishi va yuqori korroziya tezligi kabi kamchiliklarni keltirib chiqaradi [6, 7]. So'nggi yillarda ionli suyuqliklar kislotali gazlarni fizik va kimyoviy yutilish jihatdan muqobil erituvchilar sifatida foydalaniladi. ISlarning gazni ajratishdagi noyob fizik-kimyoviy xususiyatlari, kichik bug' bosimi, yuqori issiqlik barqarorligi va ekologik jihatdan tozaligi boshqa uslublarga nisbatan ustunlik beradi. ISning asosiy kamchiliklari ularning yuqori qovushqoqligi va narxidir. CO₂ turli ISlarda yutilishi eksperimental va nazariy jihatdan tekshirilgan [8, 9], ammo eksperimental tadqiqotlarining iqtisodiy jihatdan katta mablag' talab qilishi batafsil ma'lumot olishga to'sqinlik qiladi. Molekulyar dinamika (MD) simulyatsiya texnikasi molekulalar orasidagi fizik xususiyatlar, eruvchanlik va o'zaro ta'sirlarni o'rganish uchun eng qulay vosita sifatida ishlatilishi mumkin. Shuningdek, MD simulyatsiya ISdagi yutilish jarayonini yaxshiroq tushunishga ya'ni gazlar ion suyuqlik sirtida qoladimi yoki ichiga kiradimi degan savolga javob topishga imkon beradi. Buning uchun bizga molekulalar va atomlararo bog'langan va bog'lanmagan potentsial maydon ta'sir qiymatlari zarur bo'ladi. Koddermann va boshqalar tomonidan imidazoliy asosidagi ISlar ustida olib borilgan tadqiqotga ko'ra [10], simulyatsiya va eksperimentlar shuni ko'rsatdiki bug'lanish issiqligi, qovushqoqlik, diffuziya koeffitsientlari va yadro magnit-rezonansi (YMR) aylanish korrelyatsiya vaqtlari bo'yicha o'zaro bir-biriga yaqin bo'lgan natijalar olindi [11]. MD shuningdek, turli kuch maydonlari, hisoblash algoritmlari yordamida IS interfeysida sodir bo'ladigan molekulyar hodisalarni tekshirish uchun ham turli tadqiqotlarda foydalanilgan [9, 12, 13].

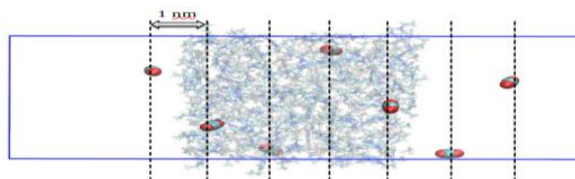
Ushbu tadqiqotda sof IS va CO₂/IS tizimlarining xarakteristikalarini MD modellash tirish yordamida o'rganildi. Biz MD simulyatsiyalarda GROMOS54a7 ta'sir potensialidan foydalandik [14]. Ushbu tadqiqotga turli haroratlarda CO₂ molekulasi ning [EMIM][BF₄] ISgida yutilish jarayonlari o'rganildi. Natijalar esa IS yordamida CO₂ yutilish potentsiali mavjud ekanligi isbotlab berildi.

Metod. Tizimlarni eksperimental tekshirishdagi qiyinchiliklar tufayli kompyuter simulyatsiyalari atomar darajada ma'lumot olish uchun eng qulay vositalardan biri hisoblanadi. Ushbu ishda MD simulyatsiyalari GROMACS 5.1.4 dasturiy paketi yordamida amalga oshirildi [15, 16]. EMIM, BF₄ va CO₂ molekulalarining boshlang'ich kordinatalarini hamda ta'sir potentsiallari www.atb.com saytidan (mos ravishda ID 22794, 268896, 12859) olindi. Ushbu ishda ISni hosil qilishda foydalanilgan kationlar va anionlarning molekulyar ko'rinishi 1a va b-rasmda tasvirlangan. Shundan so'ng teng sondagi 200 ta EMIM va 200 ta BF₄ ionlari olinib o'lchami 3.7 3.7 3.7 nm bo'lgan kubik boksqa PACKMOL dasturidan foydalanib joylashtirildi. Keyingi bosqichda sistema energiya minimizatsiyadan chiqarilib, qisqa NVT va NPT modellash tirish bajarildi. MD hisoblashlarda davriy chegara shartlarini hisobga olgan holda, 2 fs vaqt qadamidan foydalanib amalga oshirildi. Bog'lanmagan o'zaro ta'sirlarni hisobga olish uchun 1,0 nm cut-off radiusi qo'llanildi. Nose-Hover termostati [17] va Parrinello-rahman [18] harorat va bosimni nazorat qilish uchun qo'llaniladi. Davriy chegara shartlari barcha yo'nalishlarida qo'llanilgan. Shundan so'ng, 283 K, 313 K, 343 K va 363 K temperaturalarda [EMIM][BF₄] ISgi zichligini aniqlash uchun 40 ns MD simulyatsiya bajarildi (1c-rasmga qarang). Modellash tirishlar davomida 1 atm bosim qo'llanildi.



1-rasm. a) Tetrafluorborat (BF₄) molekulasini; b) 1-etil-3-metilimidazoliy (EMIM) molekulasini; c) [EMIM][BF₄] ion suyuqligining kubik boksda qo'rinishi; d) z-yo'nalishda vakum hosil qilingan IS ko'rinishi.

Ion suyuqlikda CO₂ molekulasi ni erkin energiya profilini hisoblash uchun muvozanat holatiga kelgan simulyatsiya kubik boksi (1c-rasmga qarang) o'zgartirilib [EMIM][BF₄] boks markaziga joylashtirildi (1d-rasmga qarang). Shundan so'ng tizim 303K, 353K, 403K va 453K temperaturalarda 1 atm bosimda NVT ansambli yordamida 20 ns simulyatsiya bajarildi. Ushbu modellash tirish sistemalari CO₂ molekulalarini boksqa joylashtirish uchun foydalanildi va energiya minimizatsiya hamda 5 ps NVT modellash tirish bajarildi. CO₂/IS tizimining interfeys qismini xususiyatlarini o'rganish uchun simulyatsiya boksi o'rtasida joylashgan ISni har ikki tomonda CO₂ bo'lgan ikki fazali boks tadqiq qilindi. Yettita CO₂ molekulalari vakumdan IS interfeysi va ichki qismiga 1 nm oraliq masofa bilan kiritildi (2-rasmga qarang). Shu tarzda 0.1 nm masofa bilan 7 ta CO₂ molekulalari -3.5 nm va 3.5 nm masofa oralig'ida o'zgaradi. Biz bitta erkin energiya profilini hisoblash uchun 10 ta simulyatsiya bajardik va 70 ta potentsial ta'sirlashuv ma'lumotlarini oldik. Bundan tashqari x va y o'qlari tekisligida turli xil nuqtalarda CO₂ ni hosil qilib yana qo'shimcha uch marta Soyabon namunalash usulida (SNU) modellash tirish bajarildi. SNU erkin energiya profilini hisoblash uchun keng qo'llaniladigan uslubdir. Molekulalarni membranalardan va oqsillardan o'tishi, dorilarni oqsillar bilan bog'lanishi va oqsillarni oqsillar bilan bog'lanishini ham baholashda ishlatiladi [19-23]. CO₂ erkin energiya profilini hisoblash uchun umumiy 4 ta SN uslubida 280 ta nuqtani o'z ichiga olgan 40 ta modellash tirish natijalari o'rtachalandi. Bunda CO₂ molekulasini harakati z-yo'nalishi bo'ylab $2000 \frac{\text{kJ}}{\text{nm} \cdot \text{mol}}$ bikirlik konstantasi yordamida cheklangan, molekulalarning qolgan ikki o'q (x va y) bo'ylab erkin harakatlanishiga ruxsat berilgan. Erkin energiya profilari SNU bilan 4 nsdan 160 ns davomida bajarildi va MD simulyatsiyasidan so'ng WHAM histogramma usuli [24] yordamida erkin energiya profili grafigi olindi (4-rasmga qarang) [25].



2-rasm. Soyabon namunalash usuli yordamida hosil qilingan [EMIM][BF₄]/CO₂ sistemasi ko'rinishi.

Natija va Muhokama. Molekulyar dinamika simulyatsiyani bajarish uchun sistemani tashkil qilgan molekulalarni bog'langan va bo'lanmagan ta'sir potentsiallarini to'g'ri tanlash muhim omil hisoblanadi. Sababi, model sistema real holatdagi tajriba natijalarini o'zida namoyon etishi zarur. Shuning uchun Automatic Topology Builder online serveridan olingan ta'sir potentsial parametrlari to'g'riligini tekshirish maqsadida 400 ta IS ionlarini o'z ichiga olgan tizim ustida 40 ns NPT modellash tirish bajarildi va turli temperaturalarda (283 K, 313 K, 343 K va 363 K) zichlik hisoblanib eksperimental ma'lumotlar bilan solishtirildi.

1-jadval va 3b-rasmdan yaqqol ko'rinadiki MD usulida olingan natijalar tajriba bilan yuqori aniqlikda mos keldi. Muvozanat vaziyatiga kelgan IS sistemasi vakum bilan IS yuzasini hosil qilish uchun modellash tirish boksi z o'qi bo'yicha kengaytirildi (1d-rasmga qarang). Vakum va IS yuzasida zichlik taqsimotini muvozanat holatiga keltirish uchun yana qo'shimcha NVT ansanblidan foydalanib 20 ns modellash tirish bajarildi. Z o'qi bo'ylab zichlik taqsimoti turli temperaturalarda hisoblandi (3a-rasmga qarang). Grafikga asosan IS markazidan 1.5 nm va 2.5 nm intervalda IS bilan vakum orasida zichlik taqsimoti hosil bo'ldi.

Harorat (K)	MD yordamida olingan zichlik (kg/m ³)	Eksperimental zichlik (kg/m ³)
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283	1301.3	1304.1
313	1281.5	1281.9
343	1258.0	1259.7
36	1241.1	1242.78

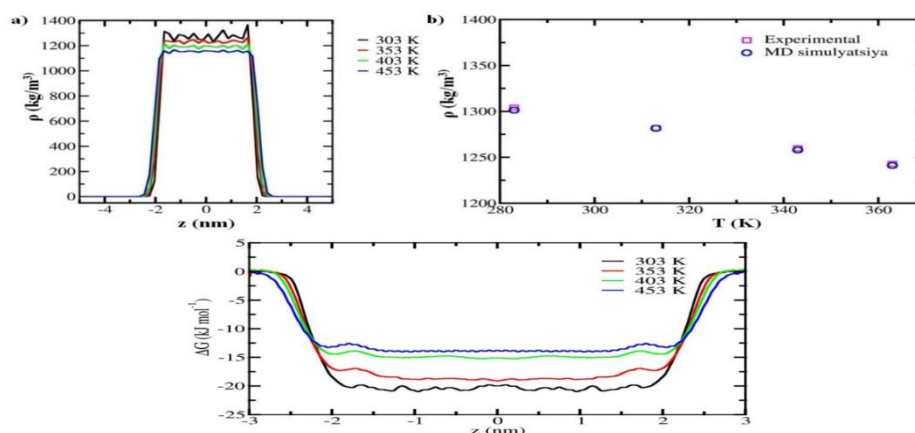
1-jadval. [EMIM][BF₄] ion suyuqligi zichligini temperaturaga bog'liqligini eksperimental va MD yordamida olingan qiymatlari.

Keyingi navbatda CO₂ molekulasi vakumdan IS ichiga kirishini eksperimental holatini modellashtirishda taqlid qilish uchun SNU yordamida MD simulyatsiyasi bajarildi.

3-rasm. a) z o'qi bo'ylab kengaytirilgan boksda zichlik o'zgarish grafigi; b) Turli temperaturalarda eksperimental va MD simulyatsiya natijasida olingan zichlik grafigi.

CO₂ molekulasi va IS orasidagi ta'sirlashuv potensialini baholash uchun CO₂ molekulariga tashqi kuch qo'yilib vakumdan IS markazigacha olib kiritildi. IS yuzasidan 1 nm masofadan uzoq bo'lganda hech qanday ta'sirlashuv mavjud bo'lmaydi. Tabiiyki erkin energiya profilida grafiklar nol qiymatni ko'rsatadi (4-rasmga qarang). CO₂ molekulasi ISga yaqinlashgan sari ta'sirlashuv potentsiali manfiy qiymatlarini ko'rsatmoqda va bu ta'sirlashuv IS ichki qismida minimum qiymatlarni qabul qiladi. Demak, vakumdan IS tomon harakatlangan CO₂ molekulasi IS ichki qismiga kirish ehtimoli juda yuqori. Temperatura oshishi bilan bu ehtimollik o'z navbatida kamayishi kuzatilyapti, lekin biz modellashtirish bajargan temperaturalarda CO₂ molekulasi IS ichiga kirish uchun hech qanday energetik to'siq mavjud emas. Erkin energiya minimum va maksimum qiymatlari farqi IS bilan CO₂ molekulasi bog'lanish erkin energiyasi beradi.

4-rasm 303K, 353K, 403K va 453K haroratlarda CO₂ molekulasi [EMIM][BF₄] ion suyuqligida erkin energiya profili grafigi ko'rsatilgan. Bu grafik biz tadqiq qilgan barcha temperaturalarda ISning 0.5 nm qalinlikdagi yuza qismida CO₂ molekulasi erkin energiya profili keskin o'zgarishini ko'rsatmoqda, lekin uning ichki qismida deyarli bir xil o'ratacha qiymatni tashkil qildi. Demak, CO₂ molekular IS sirtidan ko'ra ichki qismida stabil turishini taxmin qilish mumkin. Erkin energiya profili temperaturaga bog'liqligiga kelsak, temperatura ko'tarilishi bilan erkin energiya profili qiymati kamaydi va bu eksperimental olingan qiymatlarga mutanosib ekanligini ko'rsatdi [26]. 303K haroratda CO₂ molekulasi ion suyuqlikning ichki qismida qolgan temperaturalarga qaraganda eng kichik energiya farqlari qiymatini $\Delta G = -20$ kJ/mol qiymatga ega bo'ldi va aksincha 453K haroratdan eng maksimal $\Delta G = -13$ kJ/mol qiymatni qabul qildi.



4-rasm. CO₂ gazining turli temperaturalarda [EMIM][BF₄] ion suyuqligidagi erkin energiya profili.

Xulosa. MD simulyatsiyasi SNU foydalanib CO₂ molekularining turli temperaturalarda [EMIM][BF₄] ion suyuqligida yutilishini molekulyar mexanizmlarini tadqiq qildik. Natijalar shuni ko'rsatdiki CO₂ molekularini ion suyuqlikka kirish uchun potentsial to'siq yo'q ekan. Avval bajarilgan modellashtirish ilmiy ishlarini aksaryati gaz holatdagi CO₂ ni ba'zi ISlar bilan ta'siri o'rganilgan [27], lekin potentsial to'siqlar haqida batafsil ma'lumot mavjud emas. Shunday ekan [EMIM][BF₄] ion suyuqligini kelajakda CO₂ gazini tutib qolish uchun samarali manba sifatida foydalanish mumkin.

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INSON EPIDERMAL O'SISH OMILI OQSILIGA AZOTLANISH TA'SIRI: MOLEKULAR DARAJADAGI TADQIQOT

Abstrakt

Biz ushbu tadqiqotimizda Inson Epidermal O'sish Omili (IEO'O) oqsilini molekulyar dinamika uslubi yordamida modellashtirdik. Tabiiy, azotlangan tirozin hamda triptofan aminokislotalarini hosil qilib oqsilni 300 ns davomida dinamik evolyutsiyasi o'rganildi. Azotlanish ushbu oqsilda murakkab konformatsion o'zgarishlarni keltirib chiqardi. Asosan azotlangan aminokislotalar suv bilan ta'sirlashish oqsilni gidrofob qismlari tomon harakatlangan va tabiiy oqsilga nisbatan suvlanish darajasi kamaygan. Hisoblangan natijalar IEO'O oqsiliga azotlanish ta'siri va hujayrani molekulyar darajada boshqarish haqida yangi tushunchalar beradi.

Kalit so'zlar: Aminokislotalar modifikatsiyasi, inson epidermal o'sish omili (IEO'O), molekulyar dinamika (MD), konformatsion o'zgarish.

EFFECTS OF NITROSYLATION ON HUMAN EPIDERMAL GROWTH FACTOR PROTEIN: A MOLECULAR LEVEL STUDY

Abstract

In this study, we modeled the Human Epidermal Growth Factor (hEGF) protein using the molecular dynamics method. The dynamic evolution of the protein structures investigated during 300 ns by modifying of the natural amino acids such as tyrosine and tryptophan. The nitrosylation caused complex conformational changes in this protein. Basically, nitrosylated amino acids interact with water and move toward the hydrophobic parts the protein, reducing the solvent accessibility of the protein. The calculated results provide new insights into the effects of nitrosylation on the hEGF protein and assist control of the cell in molecular scale.

Keywords: Amino acid modification, human epidermal growth factor (hEGF), molecular dynamics (MD), conformational change.

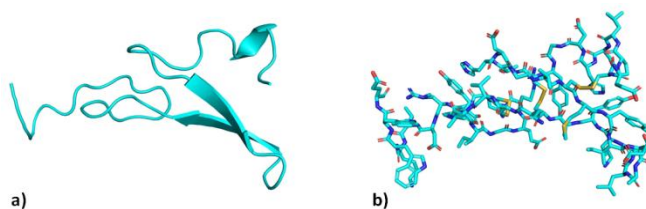
ВЛИЯНИЕ НИТРОЗИЛИРОВАНИЯ НА БЕЛОК ЭПИДЕРМАЛЬНОГО ФАКТОРА РОСТА ЧЕЛОВЕКА: МОЛЕКУЛЯРНОЕ ИССЛЕДОВАНИЕ

Абстракт

В этом исследовании нами смоделирован белок человеческого эпидермального фактора роста (hEGF) используя метод молекулярной динамики. Динамическую эволюцию белковых структур исследовали в течение 300 нс путем модификации природных аминокислот, таких как тирозин и триптофан. Нитрозилирование вызывает сложные конформационные изменения в этом белке. В основном нитрозилированные аминокислоты взаимодействуют с водой и перемещаются в сторону гидрофобных частей белка, снижая доступность белка для растворителя. Результаты расчетов дают новое представление о влиянии нитрозилирования на hEGF белок и помогают контролировать клетку в молекулярном масштабе.

Kirish. Tabiatdagi barcha organizmlar hujayralardan tuzilgan. Hujayra tarkibi oqsillar, nuklein kislotalar, lipidlar, uglevodlar kabi turli xil birikmalardan tashkil topgan. Hujayrada ularni barchasi ma'lum bir funksiyalarni bajaradi. Masalan, nuklein kislotalar irsiy axborotni saqlashi va avloddan avlodga o'tkazishi, lipidlar va uglevodlar energetik hamda hujayra devorida to'siq funksiyalarni, oqsillar tirik organizmlarning o'sishi, rivojlanishi, hujayrada sodir bo'ladigan barcha biokimyoviy jarayonlarni boshqarish va katalizator sifatida mazkur jarayonni jadal borishida ishtirok etadi [1]. Hujayrada turli signal o'tish jarayonlari ham mavjud bo'lib, bunday funksiyani bajaruvchi polipeptidlardan biri, Inson epidermal o'sish omili (IEO'O) oqsilidir. Epidermal o'sish omili hujayra darajasida o'z retseptori bilan bog'lanib hujayra o'sishini rag'batlantiradi, ya'ni hujayralarning bo'linishini tartibga soluvchi maxsus oqsildir [2,3].

Epidermal o'sish omili oqsili amerikalik biokimyogar Stanle Koen tomonidan 1962-yilda sichqon jag' osti bezida topilgan [4,5]. Keyinchalik, bu oqsil odamning so'lak bezida ham aniqlangan, shuningdek, fagotsitlarda, trombotsitlarda va qon plazmasida ham topilgan. IEO'O oqsili 51 aminokislotalardan tashkil topgan (1-rasm). Bu oqsil bilan retseptori orasidagi ta'sirni boshqarish orqali hujayrani ko'payish faktoriga molekulyar darajada ta'sir ko'rsatish mumkin [6].



1-rasm. IEO'O (PDB ID: 1IVO) oqsili kristall tuzilishi: (a) cartoon va (b) licorice ko'rinishi.

Tabiatda hujayralarga turli xil zararli ta'sirlar bo'lishi mumkin. Misol uchun, oksidlanish yoki shu bilan birga azotlanish zarari o'z ta'sirini ko'rsatishi natijasida bir qancha kasalliklarga sabab bo'lishi mumkin. Masalan, ko'krak bezi saratoni biopsiyasi tahlil qilinganda, azot oksidi (NO) konsentratsiyasi ko'pligi aniqlangan, bu esa oqsillarga ta'sir ko'rsatib saratonni tez rivojlanishiga olib kelishi mumkin [7]. Aktiv azot turlarining aminokislotalarda modifikatsiya keltirib chiqarishi (fenilalanin va tirozin nitrotirozinga, triptofan nitrotriptofanga) tajribalar yordamida aniqlangan [8].

Biz ushbu tadqiqotimizda IEO'O oqsiliga azotlanish ta'sirini o'rgandik. Azotlanish tufayli oqsil strukturasi kuzatilishi mumkin bo'lgan konformatsion o'zgarishlarni molekulyar dinamika (MD) metodi yordamida tadqiq qildik.

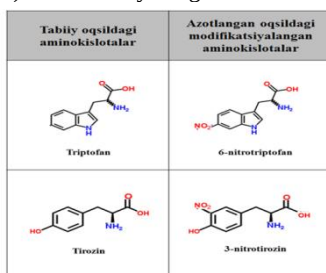
Usul. Azotlangan IEO'O oqsilida namoyon bo'ladigan o'zgarishlarni ifodalash maqsadida tabiiy holatdagi oqsil hamda NIT1 va NIT2 (1 va 2-jadval) azotlangan oqsillari uchun standard MD simulatsiyalarini bajardik va olingan natijalarni o'zaro taqqosladik. MD usuli biomolekulalarni o'zaro ta'sirlarini batafsil o'rganish uchun yuqori darajada aniqlikdagi mikroskop vazifasini bajaradi [9-14]. Jarayon vaqt bo'yicha modellashtrish trayektoriyalarini analizi yordamida batafsil ma'lumotlarni olish mumkin.

1-jadval. Modifikatsiyalangan aminokislotalar va azotlanish foizi.

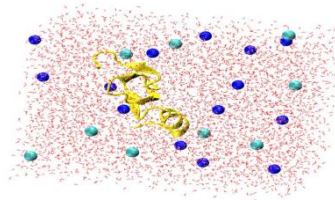
T/r	Oqsil	Modifikatsiyalangan aminokislotalar	Azotlanish (%)
1	NIT1	TRP49, TRP50	4%
2	NIT2	NIT1 + TYR13, TYR22, TYR29, TYR37, TYR44	14%

MD simulatsiyalarini bajarishda GROMACS dasturiy paketining 2020.1 versiyasidan foydalanildi [15]. IEO'O kristal tuzilishi boshlang'ich koordinatalari www.rcsb.org saytidan olindi (PDB kodi 1IVO). Model sistema suv bilan o'ralgan va 0.1 M konsentratsiyada NaCl ionlari qo'shilgan dodekaedr boksqa joylandi (2-rasm). Sistemadagi atomlararo ta'sirlashuvlarni ifodalash uchun GROMOS54A7 potentsiali [16], suv uchun SPC modelidan foydalanildi [17]. Bunday sistemalarni NIT1 va NIT2 uchun ham PTM server yordamida hosil qildik [18]. Dastlab "steepest descent" algoritmidan foydalangan holda sistemaning potentsial energiyasi minimallashtiriladi.

2-jadval. Azotlangan oqsillardagi (NIT1 va NIT2) modifikatsiyalangan aminokislotalar kimyoviy tuzilishi.



NPT (zarrachalar doimiy soni, bosim va harorat) sharoitida 300 ns MD simulatsiya qilganmiz. Hamma sistemalar ham xuddi shu bosqichlarda, bir xil fizikaviy parametrlardan foydalangan holda simulatsiya qilindi. Sistema zarrachalarning harakat tenglamalarini vaqt bo'yicha integrallashda "leap-frog" algoritmini qo'lladik va vaqt qadamini 2 fs qilib belgiladik.



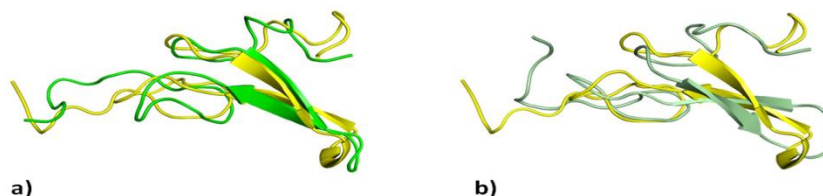
2-rasm. Suv va ionlar bilan o'ralgan IEO'O oqsili (qizil - suv molekullari; sariq - IEO'O oqsili; ko'k - natriy ionlari; binafsha - xlor ionlari).

Muvozanatlashni NVT (zarrachalar doimiy soni, hajm va harorat) bosqichida sistemaga 300 K temperatura berdik, V-rescale termostatidan foydalandik [19]. NPT 50 ps bosqichida Berendsen barostatida 1 atmosfera bosimi berildi. 300 ns NPT simulatsiyada esa sistemada izotropik doimiy bosimni ta'minlash uchun Parrinello-Rahman barostatidan foydalanmiz [20]. Barcha molekullararo ta'sirlashuvlarni hisoblashda zarrachalarning o'zaro ta'sir etadigan sferik radiusini (cutoff radius) 1.0 nm etib belgiladik. Keng doiradagi elektrostatik ta'sirlashuvlar PME (Particle Mesh Ewald) algoritmi orqali hisoblandi [21]. Boksning barcha vektorlari bo'yicha davriy chegara shartlari (Periodic Boundary Conditions) qo'llanildi. Oqsil atomlaridan boks devorlarigacha bo'lgan eng qisqa masofani 1.0 nm olganmiz. MD simulatsiyalardan olingan trayektoriyalar orqali sistemalarni analiz qildik. Azotlanish natijasida yuzaga kelgan oqsil zanjiridagi o'rtacha kvadratik og'ishlarni (RMSD—Root-mean-square deviation) hisobladik, shuningdek, oqsilning suv bilan qoplanish yuzasini (SASA—Solvent Accessible Surface Area), aylanish

radiusini (Radius of gyration) ya'ni oqsil atomlarining o'z o'qi atrofida taqsimlanishini, oqsilning har bir aminokislotasi harakatchanligining simulatsiya davomidagi o'rtacha kvadratik o'zgarishlarini (RMSF—Root-mean-square fluctuation) ham hisobladik. Analizdan olingan natija va grafiklarni o'zaro taqqosladik.

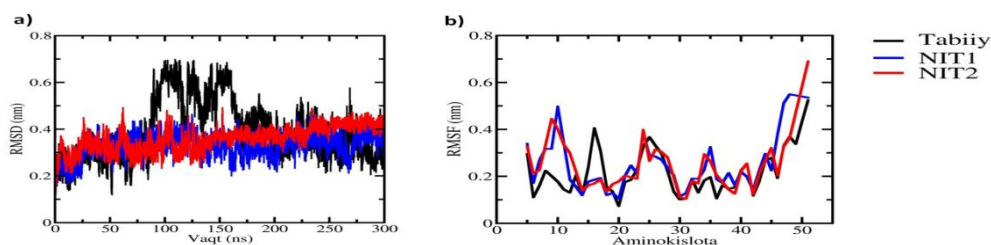
Natija va muhokama. Ushbu tadqiqotimizda IEO'O oqsiliga azotlanish ta'sirini MD modellashirish uslubi yordamida o'rgandik. Ma'lumki, oqsillar hujayrada turli xil vazifalarni bajaradi. Aynan, IEO'O oqsili o'z retseptori bilan bog'lanishi hujarani ko'payishiga sabab bo'ladi. Demak, IEO'O oqsilini retseptoriga bog'lanishini boshqarish orqali hujayra ko'payishini nazorat qilish mumkin. Avvalgi molekulyar darajadagi tadqiqotlar shuni ko'rsatadiki, IEO'Oni oksidlanish foizi oshishi o'z retseptori bilan bog'lanish erkin energiyasini kamaytirdi [21]. Ushbu holatda, hujayra ko'payishi bloklanishi mumkin, ya'ni oksidlanish zarari oshganda hujayralar o'sishdan to'xtaydi. Masalan, plazma tibbiyotida saraton hujayralarini shu yo'l bilan nobud bo'lishi qisman tushuntirilgan [22]. Agressiv saraton hujayralarida azot oksidi konsentratsiyasi normal hujayraga nisbatan yuqoriligi isbotlangan [23]. Azot oksidi faol azot zarralaridan bo'lib, tez reaksiyaga kirishadi. Aynan azot oksidi IEO'O bilan ham reaksiyaga kirishi ehtimoli mavjud. Takai va boshqalar sovuq plazma bilan suv aralashmali aminokislotalarga ishlov berilganda, nafaqat oksidlanish shuningdek azotlanish ham kuzatilgan [8]. Bunda asosan, tirozin, fenilalanin, valin, leysin va izoleysin aminokislotalarida azotlanish hosil bo'lgan. IEO'O oqsilida ham tirozin va triptofan mavjud. Yuqoridagi maqolaga asosan azotlanish turli aminokislotalarda ro'y berishi mumkin, lekin ularni ta'sirini umumiy tarzda molekulyar modellashirish bilan o'rganib bo'lmaydi. Sababi, hozircha faqatgina, fenilalanin, tirozin va triptofanni ta'sirlashuv potentsiallari ishlab chiqilgan [24]. Azotlanish ta'siri hozirgi kungacha molekulyar darajada yetarlicha o'rganilmagan. Shuning uchun ushbu ishimizda tirozin va triptofanga azotlanish ta'sirini tadqiq qildik. Bunda biz ikkita sistema, NIT1 va NIT2 hosil qildik (1 va 2-jadval).

Natijalar shuni ko'rsatdiki, azotlanishning ta'sirida aminokislotalardagi modifikatsiya oqsilning turlicha konformatsion o'zgarishlariga sabab bo'ldi. Bu strukturalardagi konformatsion farqlarni 3-rasmda ko'rishimiz mumkin. Shubhasiz, ular oqsilning tabiiy strukturasidan farq qilmoqda.



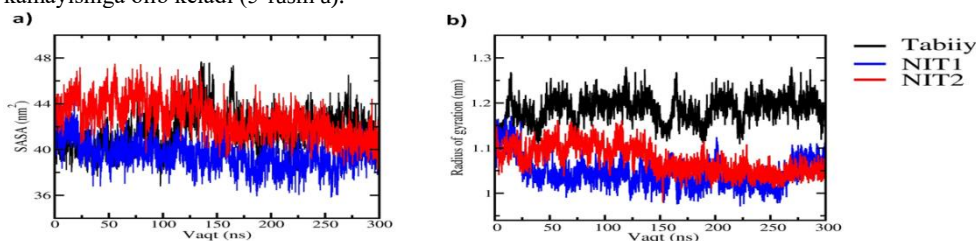
3-rasm. Tabiiy va azotlangan IEO'O konformatsion o'zgarishlarini taqqoslash: (a) tabiiy - sariq va NIT1 – yashil, (b) tabiiy va NIT2 – to'q yashil.

Tabiiy va azotlangan NIT1 va NIT2 oqsillari asosiy zanjiridagi o'rtacha kvadratik og'ishlarini hisoblab, ularni solishtirdik (4-rasm a). RMSDning hisoblangan o'rtacha qiymati azotlanishning kuchayishi bilan nisbatan ortadi, ya'ni NIT1ga nisbatan NIT2da o'rtacha kvadratik og'ishlar yuqoriroq (4-rasm). Bu azotlangan tuzilmalar moslashuvchan bo'lib, ularning konformatsiyasiga ta'sir qilishini ko'rsatadi (3-rasm). Oqsildagi har bir aminokislotalarning simulatsiya davomidagi o'rtacha kvadratik o'zgarishlarini ham hisoblab solishtirdik. Bunda azotlanish natijasida hosil bo'lgan aminokislotalardagi modifikatsiya o'zgarishlari tabiiy holdagi oqsil aminokislotalariga nisbatan kichik farq bilan yuqori ekanligini ko'rishimiz mumkin (4-rasm b).



4-rasm (a) Tabiiy, NIT1 va NIT2 oqsillari asosiy zanjiridagi o'rtacha kvadratik og'ishlari (RMSD); (b) Tabiiy, NIT1 va NIT2 aminokislotalarini o'rtacha kvadratik o'zgarishlari (RMSF).

SASA tahlili shuni ko'rsatdiki, azotlanishning ortishi, oqsilning suv bilan qoplanish yuzasi tabiiy oqsilga nisbatan avval ortib, so'ngra kamayishiga olib keladi (5-rasm a).



5-rasm. (a) Tabiiy, NIT1 va NIT2 oqsillarini suv bilan qoplanish yuzasi (SASA) va (b) aylanish radiusi.

Xulosa. IEO'O oqsiliga azotlanish ta'sirini MD simulyatsiyasidan foydalangan holda o'rgandik. Azotlanish murakkab konformatsion o'zgarishlarga olib keladi. Natijalar bir ma'noda shuni ko'rsatadiki, azotlanish darajasi NIT1 va NIT2 oqsillari konformatsiyasi va barqarorligiga ta'sir qiladi. Oqsillardagi aminokislotalarni modifikatsiyalanishi nafaqat strukturaviy balki hujayralarda signal o'tishini faollashtirishi yoki bloklashi mumkin. O'z izlanishlarimizda davom etib, IEO'O oqsilini uning retseptori bilan bog'lanishini kelgusi tadqiqotlarimizda o'rganamiz. Qo'lga kiritadigan natijalarimiz hujayrani molekulyar darajada boshqarish usullari haqida batafsil ma'lumotlar beradi.

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EXCITATION OF ISOMERIC STATES IN REACTIONS (γ, n) AND ($n, 2n$) ON ^{86}Sr NUCLEUS

Abstract

The cross sections for the formation of isomeric states in the reactions (γ, n) and ($n, 2n$) on the ^{86}Sr nucleus were measured by the induced activity method. The experimental results are compared with the data of other works and the TALYS-1.6 calculation.

Keywords: photonuclear reactions, isomeric ratios, bremsstrahlung, selenium isotopes, radioactivity, cross section, spin, neutron, activity, isomer, nucleus, nuclear reaction.

ВОЗБУЖДЕНИЕ ИЗОМЕРНЫХ СОСТОЯНИЙ В РЕАКЦИЯХ (γ, n) И ($n, 2n$) НА ЯДРЕ ^{86}Sr

Аннотация

Методом наведенной активности измерены изомерные сечения образований изомерных состояний в реакциях (γ, n) и ($n, 2n$) на ядре ^{86}Sr . Результаты экспериментов сравниваются с данными других работ и расчетом TALYS-1.6.

Ключевые слова: фотоядерные реакции, изомерные отношения, тормозное излучение, изотопы селена, радиоактивность, сечение, спин, нейтрон, активность, изомер, ядро, ядерная реакция.

^{86}Sr ЯДРОДАГИ (γ, n) ВА ($n, 2n$) РЕАКЦИЯЛАРДА ИЗОМЕР ҲОЛАТЛАР УЙҒОНИШИ

Аннотация

Кирилган активлик методи билан ^{86}Sr ядрога ($n, 2n$) ва (γ, n)-реакциялар изомер ҳолатлар ҳосил бўлиш кесимлари ўлчанган. Экспериментал натижалар бошқа ишларнинг маълумотлари ва TALYS-1.6 ёрдамида олинган ҳисоблаш натижалари билан таққосланади.

Калит сўзлар: фотоядро реакцияси, изомерлар нисбати, тормозланиш нурланишлари, селен изотопи, радиоактивлик, кесим, спин, нейтрон, активлик, изомер, ядро, ядро реакцияси.

Introduction. The study of the relative probabilities of excitation of the isomeric and ground states of the final nucleus in nuclear reactions is of fundamental and applied importance. Of great importance is the study of the formation of isomeric states of nuclei in nuclear reactions with various bombarding particles, which makes it possible to obtain information about the mechanisms of nuclear reactions and the properties of excited states of atomic nuclei [1,2].

Literature review. The cross sections and isomeric ratios of reactions of the (γ, n) type on the ^{86}Sr nucleus are poorly studied. There is only one work on the determination of the cross sections for the formation of $^{85\text{m}}\text{gSr}$ isomeric states in the energy range 12–18 MeV [1]. In this work, the isomeric ratios of the yields and cross sections of this reaction are also determined. The isomeric ratios of the yields of photonuclear reactions (γ, n) were also studied in [3–5] at a fixed energy. The energy dependence of the isomeric ratio of the reaction yields of the (γ, n) type on the ^{86}Sr nucleus has not been studied.

In the present work, the excitation cross sections of $^{85\text{m}}\text{gSr}$ isomers in the reactions (γ, n) and ($n, 2n$) on the ^{86}Sr nucleus in the energy range 13–35 MeV are studied.

Research Methodology. The neutron generator NG-150 of the Institute of Nuclear Physics of the Academy of Sciences of the Republic of Uzbekistan, which generates fluxes of fast neutrons with energies of 14 MeV, served as a neutron source. The initial experimental data on the reaction (γ, n) was an atlas of gamma spectra of radionuclides obtained in photonuclear reactions in the energy range of 10–35 MeV with a step of 1 MeV on the betatron bremsstrahlung γ -beam. High purity SrCO_3 (99.9%) in a natural mixture of bromine isotopes, pressed in the form of a disk with a diameter of 20 mm, was used as a target. Each SrCO_3 sample was placed between two copper foils (in the case of neutron irradiation of aluminum foil). The weight of the samples is 3–4 g. The time of exposure to a neutron flux with an energy of 14.1 MeV is 30–60 minutes.

The gamma activity of the targets was measured on a Canberra γ -ray spectrometer, consisting of a HPGe germanium detector (with a relative efficiency of 15%, resolution for the ^{60}Co 1332 keV line is 1.8 keV), a DSA 1000 digital analyzer, and a personal computer with the Genie 2000 software package for collection and processing of γ -spectra. The gamma spectra of the targets began to be measured after a pause of 5–60 min and were measured for 30–120 min.

The population of the isomeric and ground levels was identified by γ -lines: 231.4 keV (85mSr: $J\pi=1/2^-$, $T_{1/2}=68$ min) and 513.9 keV (85gSr: $J\pi=9/2^+$, $T_{1/2}=64$ days). The data on the decay scheme necessary for processing the measurement results were taken from [6]. The calculation of isomeric ratios of yields was carried out according to the ratios taken from [7]:

$$d = \frac{Y_m}{Y_g} = \left[\frac{\lambda_g F_m(t)}{\lambda_m F_g(t)} \left(C \frac{N_g I_g \varepsilon_g k_m}{N_m I_g \varepsilon_g k_g} - P \frac{\lambda_g}{\lambda_g - \lambda_m} \right) + P \frac{\lambda_m}{\lambda_g - \lambda_m} \right]^{-1} \quad (1)$$

where

$$F_m(t) = [1 - \exp(-\lambda_m t_i)] \exp(-\lambda_m t_p) [1 - \exp(-\lambda_m t_m)], \quad (2)$$

$$F_g(t) = [1 - \exp(-\lambda_g t_i)] \exp(-\lambda_g t_p) [1 - \exp(-\lambda_g t_m)], \quad (3)$$

Here, Y_m and Y_g are the yields of, respectively, the isomeric and the ground state; λ_m and λ_g are their decay constants; N_m and N_g are the numbers of detected events of decay of, respectively, the isomeric and the ground state; C is a coefficient that takes into account the miscounts of the detecting equipment and pulse positions; ε is the spectrometer efficiency; k is the coefficient of self-absorption in the sample; and t_i , t_p , and t_m are the times of irradiation, pause, and measurements, respectively.

Analysis and results. The obtained experimental results on the isomeric ratios of the yields and cross sections of the (γ, n) and $(n, 2n)$ reactions on the ^{86}Sr nucleus are given in Table 1 and 2. When determining the experimental errors, we took into account statistical errors, the error in determining the detector efficiency, the target measurement geometry, self-absorption of gamma rays, and coincidence.

The excitation functions of the (γ, n) -reaction were obtained from experimental isomeric ratios and total photoneutron reaction cross sections on [8]. The cross section was calculated by the Penfold-Liss method with a step of 1 MeV [9].

The experimental dependence of the cross sections for the reaction $^{86}\text{Sr}(\gamma, n)^{85}\text{mSr}$ on the boundary energy of bremsstrahlung quanta was approximated by the Lorentz function, the parameters of which (the position of the maximum of the cross section E_m , the value of the cross section at the maximum σ_m , and the width of the distribution at half its height Γ) were determined by the least squares method from a set of experimental values. Approximation parameters and integral reaction cross sections are shown in Table 1. The errors are estimated based on the statistics of registered reports.

Table 1. Cross section for the reaction $^{86}\text{Sr}(\gamma, n)^{85}\text{mSr}$

Reaction	E_m , MeV	Γ , MeV	σ_m , mb	σ_{int} , MeV·mb	E_h , MeV	Reference
$^{86}\text{Sr}(\gamma, n)^{85}\text{Sr}$	$16,93 \pm 0,04$	5	174	1266 ± 82	22	[10]
$^{86}\text{Sr}(\gamma, n)^{85}\text{mSr}$	16,5	6	114	-	-	[1]
$^{86}\text{Sr}(\gamma, n)^{85}\text{Sr}^*$	$17,01 \pm 0,04$	$7,18 \pm 0,42$	162	2340 ± 230	22	This work
$^{86}\text{Sr}(\gamma, n)^{85}\text{mSr}$	$16,94 \pm 0,05$	$6,18 \pm 0,47$	98	1266 ± 151	22	This work

Note. *The cross sections were calculated using the TALYS-1.6 program, σ_{int} is the integral reaction cross section, E_h is the upper limit of integration.

To evaluate and compare the experimental results, we calculated the reaction cross section using the TALYS-1.6 software package [11]. The results of theoretical calculations are given in Table 1. As can be seen in Table 1, the value of the cross section at the maximum σ_m and the width of the distribution at half its height Γ in all works are consistent with each other within the measurement error. The energy position of the maximum of the $^{86}\text{Sr}(\gamma, n)^{85}\text{mSr}$ reaction cross section, within the error, coincides with the energy of the ^{86}Sr giant dipole resonance, determined by the empirical relation, which is equal to: 16.99 MeV which is consistent within the measurement error with the data in Table 2. At this energy, experimental value of isomeric ratios of cross sections, which is equal to: 0.56 ± 0.09 . Also, the isomeric ratios of reaction yields were calculated using the TALYS-1.6 software package, which is equal to: 0.56 at 25 MeV.

As can be seen from Table 1, information on the parameters of the giant dipole resonance is insufficient for a detailed analysis of these reactions. In [1], the reaction cross section $^{86}\text{Sr}(\gamma, n)^{85}\text{mSr}$ was determined in the energy range 12–18 MeV, i.e. does not completely cover the region of giant resonance. Our results on the width and position of the resonance coincide in the region of experimental errors with the data of [1] and the calculation results. The values of the maximum cross sections differ from each other.

In the case of the $(n, 2n)$ reaction, the experimental results on the cross sections for the formation of isomeric states and their ratios are given in Table 2.

To obtain the absolute values of the cross sections of the ground and isomeric states, methods were used to compare the yields of the studied and monitor reactions. $^{27}\text{Al}(n, \alpha)^{24}\text{Na}$ ($T_{1/2}=15$ h, $E_\gamma=1368$ keV) was used as a monitor reaction, the cross section of which is: $\sigma_m = 121.57 \pm 0.57$ mb at $E_n=14.1$ MeV [12].

As can be seen from Table 2, at 14.1 MeV, the values of the cross sections of isomeric states of all experimental works agree within the measurement errors. In the case of the cross sections of the formations of the ground state, the values are consistent with each other within the measurement errors, except for [14]. Also, using the TALYS-1.6 program, the total (total) cross sections were calculated, which are smaller than the experimental results obtained in [15].

The absolute error of the isomeric ratios of reaction cross sections is determined by the statistical error of counting in the photopeak of the measured γ -line, the efficiency of registration of γ -radiation, and the error in the values of the monitors cross sections.

Table 2. Cross section for the reaction $^{86}\text{Sr}(n, 2n)^{85}\text{m}, g \text{ Sr}$

E_n , MeV	σ , mb	σ_m , mb	σ_g , mb	σ_m/σ_g	Reference
14.1		227 ± 8	892 ± 53	0,25	13
14.6		253 ± 8	955 ± 57	0,26	13
14.1		227 ± 8	665 ± 65	0,34	14
14.6		253 ± 8	702 ± 79	0,36	14
14.1		221 ± 7	884 ± 62	$0,25 \pm 0,02$	This work

14.0	776*				This work
14.8	1129±58	219±14	909±56	0,24±0,02	15

Note. *The cross sections were calculated using the TALYS-1.6 program.

Conclusion/Recommendations. From the analysis of the data given in table. 1 and 2, it follows that experimental studies of the excitation of isomeric states in photonuclear reactions of the (γ, n) type were carried out mainly in the energy range of 10–25 MeV, i.e., in the region of giant dipole resonance. At energies above the giant resonance, the energy dependence of the isomeric ratios has been little studied. Thanks to these studies, it is possible to obtain information on the density of nuclear levels and on the contribution of direct processes to the mechanism of photonuclear reactions in a given energy range.

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MAGNETO-OPTICAL PROPERTIES OF YTTRIUM IRON GARNET ($Y_3Fe_5O_{12}$) WITH Ca AND Si IMPURITIES

Abstract

Magneto – optics is a branch of optics that studies phenomena resulting from the interaction of optical radiation with a substance in a magnetic field. Yttrium iron garnet $Y_3Fe_5O_{12}$ (YIG) - good studied ferrimagnetic compound, widely used taken in microwave and magneto-optical device. Their absorption spectra and the Faraday effect in the IR region, as well as the equatorial effect Kerr in the visible region of the spectrum. The spectra of absorption and magneto-optical effects are consistent with the corresponding spectra of single crystals. Based on the laws associated with magneto-optical effects, it became possible to create and improve devices for storing and transmitting information.

Key words: Magneto-optics, spectr, effect Kerr, effect Faradey, yttrium iron garnet, absorption spectrum, absorption coefficient.

МАГНИТООПТИЧЕСКИЕ СВОЙСТВА ЖЕЛЕЗО-ИТТРИЕВОГО ФЕРРИТ-ГРАНАТА ($Y_3Fe_5O_{12}$) С ПРИМЕСЯМИ ИОНАМИ Ca И Si.

Аннотация

Магнитооптика – раздел оптики, изучающий явления, возникающие в результате взаимодействия оптического излучения с веществом, находящимся в магнитном поле. Железо-иттриевый гранат $Y_3Fe_5O_{12}$ (ЖИГ) — хорошо изученное ферримагнитное соединение, широко применяемое в микроволновых и магнитооптических устройств. Измерены их спектры поглощения и эффекта Фарадея в ИК-области, а также экваториальный эффект Керра в видимой области спектра. Опираясь на законы, связанные с магнитооптическими эффектами, появилась возможность создавать и усовершенствовать устройства хранения и передачи информации.

Ключевые слова: Магнитооптика, спектр, эффект Керра, эффект Фарадея, железо-иттриевый гранат, спектр поглощения, коэффициент поглощения.

Ca VA Si IONLARI KIRITILGAN ITTRIY FERRIT-GRANATNING ($Y_3Fe_5O_{12}$) MAGNITOOPTIK XUSUSIYATLARI

Annotatsiya

Magnitooptika – optik nurlanishning magnit maydondagi modda bilan o'zaro ta'siri natijasida paydo bo'ladigan hodisalarni o'rganadigan optika bo'limi. Ittriy temir granat $Y_3Fe_5O_{12}$ (YIG) - yaxshi o'rganilgan ferromagnit birikma, mikroto'lqinli va magnitooptik qurilmalarda keng qo'llaniladi. Ularning infraqizil spektr sohasida yutilish spektrlari Faraday effekti, shuningdek ekvator effekti kuzatiladi. Spektarning ko'rindigan sohasida esa Kerr effekti, yutilish spektri va monokristallarning mos spektrlari bilan magnitooptik effektlar spektrlari o'rganiladi. Magnitooptik effektlar bilan bog'liq qonunlar asosida axborotni saqlash va uzatish qurilmalarini yaratish va takomillashtirish mumkin.

Kalit so'zlar: Magnitooptika, spektr, Kerr effekti, Faradey effekti, ittriy-ferrit granat, yutilish spektri, yutilish koeffitsiyenti.

Kirish. XX asrning 60-yillar oxiri 70-yillari boshlarida magnitooptika sohasining jadal rivojlanishini ko'rindigan va infraqizil spektr sohasiga yaqin bo'lgan sohalarda magnitooptik effektlarni ko'rsatuvchi yangi ferrodielektriklarning yaratilishi bilan izohlash mumkin. Bunday effektlarga misol qilib Faradey effekti, Kerr effekti va boshqalarni keltirish mumkin. Bunday materillarga misol qilib ferrit granatlar, ortoferritlar, ferrit shpinellar va boshqa shunga o'xshash magnit oksidlarni misol keltirish mumkin. Ushbu turdagi magnitlarning paydo bo'lishi fan va texnikaning turli sohalarida magnitooptik effektlarni qo'llash, birinchi navbatda, ular asosida ma'lumotlarni ko'rsatish, qayta ishlash va saqlash uchun prinsipial jihatdan yangi tizimlarni yaratish uchun keng istiqbollarni ochdi. Amaliy magnitooptikani rivojlantirishning hozirgi bosqichi yupqa magnit plyonlari yuzasi va hajmi bo'ylab tarqaladigan optik signallarni uzatish qayta ishlashni ta'minlaydigan optoelektronika va integral optikaning funksional qurilmalarini topologik elementlar va tuzilmalar yordamida yaratishning yupqa plyonka texnologiyasi va litografiya metodlari bilan bog'liq. Asosiy zamonaviy magnitooptik qurilmalarning ko'pchiligi epitaksial ferrit-granat plyonkalar yordamida tayyorlanadi. Shuning uchun ham bu tadqiqotlarni o'tkazishdan maqsad epitaksial ferrit-granat plyonkalari tarkibi va strukturalarini hamda ionlar bilan nurlantirilgan va legirlangan donor-akseptor kirishmalar kiritilgandagi o'zgarishlarni o'rganishdan iborat.

Tajriba va namunalar. Nodir-yer elementlari, siyrak-yer elementlari-Mendeleyev davriy sistemasining 111 guruhida joylashgan kimyoviy elementlar: ittriy (Y), lantan (La) va 14 ta lantanoidlar gruppasi hisoblanadi. Ba'zan skandiy (Sc) ham shu elementlar jumlasiga kiritiladi. Nodir yer elementlari tabiatda o'zaro birga uchraydi, kimyoviy xossalari ham bir-biriga o'xshash bo'ladi. Kumush kabi oq, havo kislorodi ta'sirida oksid parda hosil qilganligi sababli qorayadi. 2 guruhchaga bo'linadi: seriy guruhchasi (La, Ce, Pr, Nd, Sm, Eu) va ittriy guruhchasi (Y, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu). Noyob yer elementlari kimyoviy

va ayrim fizik xususiyatlarning katta o'xshashligini namoyon qiladi, bu ularning atomlarining tashqi elektron qobiqlarining deyarli bir xil tuzilishi bilan izohlanadi. Ularning barchasi kumush - oq metallar bo'lib, ularning barchasi shu kabi kimyoviy xususiyatlarga ega (eng xarakterli oksidlanish darajasi +3).

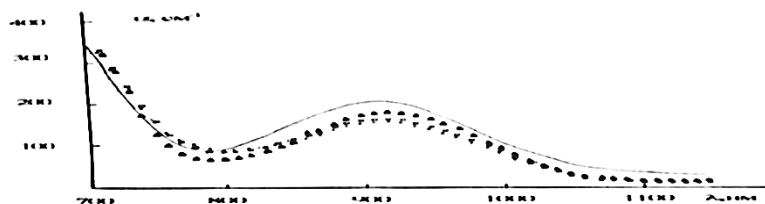
Nodir yer elementlari-metallar, ular tegishli oksidlar, ftoridlar, suvsiz tuzlarning elektrolizlari va boshqa usullar bilan tiklanadi.

Magnitoptika turli muhitlarning optik xususiyatlarining magnit maydon ta'sirida o'zgarishini o'rganadigan fizika bo'limi hisoblanadi. Bu sohada magnit maydonda joylashtirilgan jismlarda nurni chiqarish, tarqatish va yutilish xususiyatlari o'rganiladi. Magnit maydon, har qanday vektor maydoni kabi, fazoda ma'lum bir yo'nalishga ega bo'lib, unda optik anizotropiya (optik xususiyatlarning tengsizligi) paydo bo'ladi.

Ittriy-ferrit granat-kimyoviy tarkibi $\text{Y}_3\text{Fe}_2(\text{FeO}_4)_3$, yoki $\text{Y}_3\text{Fe}_5\text{O}_{12}$ bo'lgan sintetik granatlarning bir turi hisoblanadi. Bu elementning Kyuri temperaturasi 560K bo'lgan ferromagnetik material hisoblanadi. Ittriy temir granat - ittriy ferrit-granat, temir oksidi yoki ittriy oksidi sifatida ham ma'lum. Oxirgi ikki nom bu elementning kukunsimon shakllari bilan bog'liq. Temir ionlari fokus nuqtalarida har xil spinlarni hosil qiladi va natijada turlicha magnit holatlarni namoyon qiladi [2,5]. Ularning tarkibini boshqa elementlar bilan o'zgartirib, bu moddalarda turlicha qiziqarli magnit xossalarni olishimiz mumkin. Ittriy temir granat ($\text{Y}_3\text{Fe}_5\text{O}_{12}$) uchun Verd doimiysi katta qiymatga ega, bu Faradey effektining namoyon bo'lishiga olib keladi. Bundan tashqari mikroto'lqinli pechlarda chastotaning yuqori darajaligi, 1200 nm gacha bo'lgan infraqizil to'lqin uzunligi uchun past absorbsiya va elektron spinli rezonansda juda kichik chiziqli kengligiga ega. Bu xususiyatlar o'ta o'tkazgichlarda magnitoptik tasvirlash uchun juda muhimdir [4,6].

Ferritlar infraqizil spektridagi 1,3-5,5 mkm to'lqin uzunlik orasidagi sohalarida yuqori shaffoflik xususiyatini namoyon qiladi. Ferrit granatlar ferrit shpinellarga qaraganda yuqori shaffoflik bilan xarakterlanadi. Spektrning ko'rinadigan va yaqin infraqizil sohalaridagi ferrit granatalari yorug'lik magnitlanish vektori bo'yab tarqalganda sezilarli darajada Faraday effektini va magnitlanish vektoriga perpendikulyar tarqalganda taxminan bir xil Kotton Mouton moduli (magnit chiziqli ikki sinish) effektini ko'rsatadi [1,4]. Ittriy-temir granatni kuchli nazorat ostidagi sharoitlarda o'stirishda yutilish koeffitsiyentini $0,03\text{sm}^{-1}$ bo'lgan qiymatda kuzatishga erishilgan. Tolqin uzunligi $\lambda > 5,5$ mkm bo'lgan sohada ittriy ferrit granat optik yutilish ko'rsatkichgi kristall panjara tugunlarida yorug'lik fotonlari yutilishi bilan bog'liq. Optik yutilish $\lambda < 1,5$ mkm bo'lgan soha esa elektron yutilish chizig'ining cheti hisoblanadi. Xund qoidasiga ko'ra asosiy holatda bo'lgan Fe^{3+} ionining barcha d-elektron qobiqdagi 3d tashqi to'lmagan qobiqdagi elektronlarning spinlari parallel yo'nalgan bo'ladi. Shuning uchun Fe^{3+} ionining asosiy holatdagi to'la spini 5/2 ga va to'liq orbital momenti $L=0$ ga teng bo'ladi [3].

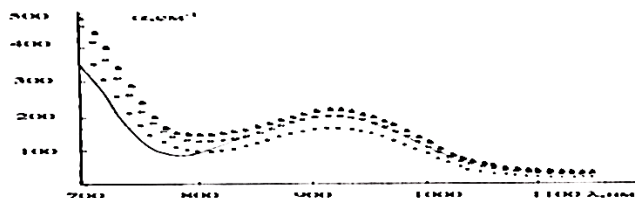
Taxlil va natijalar. Ittriy temir granatga Ca ionlari kiritilganda [10] o'tkazilgan tadqiqotlar quyidagi 1-rasmda keltirilgan. Grafikdan ko'rishimiz mumkinki, o'tkazilgan tadqiqotlarda 0,8-0,15mkm to'lqin uzunligi diapazonida optik yutilish koeffitsiyenti sezilarli darajada kamayganini ko'rishimiz mumkin. Bu holdagi yutilish spektrini sof holatdagi ittriy temir granati yutilish spektri bilan solishtirganda yutilish spektri markazi $\lambda \approx 0,96$ mkm ga siljiydi [3-4].



Rasm 1. Ittriy temir granatiga Cax ionlari kiritilgandagi yutilish spektri.

1. $-x=0$; 2. $\bullet-x=0,0025$; 3. $\circ-x=0,0049$; 4. $\blacktriangle-x=0,025$

Ittriy temir granatga Si ionlari kiritilganda o'tkazilgan tadqiqotlar quyidagi 2-rasmda keltirilgan. Si ionlari ittriy ferrit granatga kiritilgan holda grafikdan ko'rishimiz mumkinki, o'tkazilgan tadqiqotlarda kremniy ionlarining past konsentratsiyalarida 0,8-0,15 mkm to'lqin uzunligi diapazonida optik yutilish koeffitsiyenti sezilarli darajada kamayganini hamda $\lambda < 0,8\text{mkm}$ to'lqin uzunligi sohasida Si ionlarining konsentratsiyasi oshirilganda α yutilish koeffitsiyenti butun o'rganilayotgan spektr sohasi bo'yab qiymati sezilarli darajada oshganini ko'rishimiz mumkin. Bu holdagi yutilish spektrini sof holatdagi ittriy temir granati yutilish spektri bilan solishtirganda $\lambda \approx 0,96$ mkm to'lqin uzunligida yutilishning maksimumi



chiziqlari aralashuvini kuzata olmaymiz. [9]

Rasm 2. Ittriy temir granatiga Six ionlari kiritilgandagi yutilish spektri.

1. $-x=0$; 2. $\bullet-x=0,005$; 3. $\circ-x=0,009$; 4. $\blacktriangle-x=0,025$

Spektrning qisqa to'lqinlar sohasida esa Ca va Si ionlari kiritilganda yutilish koeffitsiyenti yanada ko'proq bu ionlarning konsentratsiyasiga bog'liq bo'lishi kuzatilgan. Ittriy-ferrit granat plyonkalatriga Ca va Si ionlari kiritilganda kuzatish mumkin bo'lgan yana bir asosiy xususiyat shuki, bu holda bu kristallning magnitoptik aslligi ham ortadi. Asosan $\lambda \approx 0,96\text{mkm}$ to'lqin uzunligi sohasida Ca ionlari kiritilganda magnitoptik asllik taxminan 30%gacha ortishini kuzatishimiz mumkin. Bundan tashqari Ca ionlari kirishmalari kiritilganda ittriy-ferrit granatning optik va magnitoptik xususiyatlariga ko'proq ta'sir ko'rsatishi tajribalarda ko'rilgan [1].

Xulosa. Ittriy temir granati mikroto'lqinli pechlarda, akustika, optika va magnitoptika sohalarida akustik uzatgichlar yoki o'zgartirgichlar sifatida keng foydalaniladi. 600 nm dan kattaroq bo'lgan yorug'lik to'lqin uzunliklari uchun shaffof.

Shuningdek Faradey burilishlarida qattiq jisimli lazerlarda ma'lumotlarni saqlashda hamda turli xil noxiziqli optika sohalarda ham qo'llaniladi

Magnitooptik effektlar telekommunikatsiyada keng qo'llaniladi va tez rivojlanmoqda. Ular axborotni qayd qilish va saqlash qurilmalarida, lazer nurlanishini boshqarish tizimlarida (deflektorlar, optik boshqariluvchi qurilmalar yaratish, yorug'likni modulyatsiya qilish va boshqalar), aniq magnetometrlarni yaratishda, lazer giroskoplarida, birlashtirilgan optik elementlar va boshqalarda keng qo'llaniladi.

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SUV ARALASHMALI SIRKA KISLOTASI VA ASETON SUYUQLIKLARINING DIELEKTRIK XOSSALARI

Abstrakt

Molekulyar dinamika simulyatsiyalari yordamida turli xil konsentratsiyalarda sirka kislota/aseton va suv molekularining aralashmalari tadqiq qilindi. Eritmalarning ortiqcha dielektrik singdiruvchanligi ϵ^E qiymatlari hisoblandi va konsentratsiyaga bog'liqligi GROMACS dasturiy paketi yordamida aniqlandi. Hisoblangan ortiqcha dielektrik konstanta qiymatlari sirka kislota va asetonning $x \sim 0.3$ mol konsentratsiyasida kuzatildi va ular sirka kislotasi va aseton – suv binar aralashmasida eng ko'p vodorod bog'iga ega bo'lgan geteromolekulyar klatrat strukturalar hosil bo'ldi.

Kalit so'zlar: sirka kislota, konsentratsiya, molekulyar dinamika.

DIELECTRIC PROPERTIES OF AQUEOUS SOLUTIONS OF ACETIC ACID AND ACETONE.

Abstract

The water solutions of acetic acid/acetone were investigated at different concentrations using molecular dynamics simulations. The excess dielectric constant ϵ^E of the solutions was calculated and the concentration dependence curve was determined using the GROMACS program package. The minimum values of excess dielectric constant were observed at concentration of $x \sim 0.3$ mol for acetic acid and acetone and it corresponds to the maximum number of heteromolecular clathrate structures by forming maximum number of hydrogen bond in these binary liquids.

Key words: acetic acid, concentration molecular dynamics

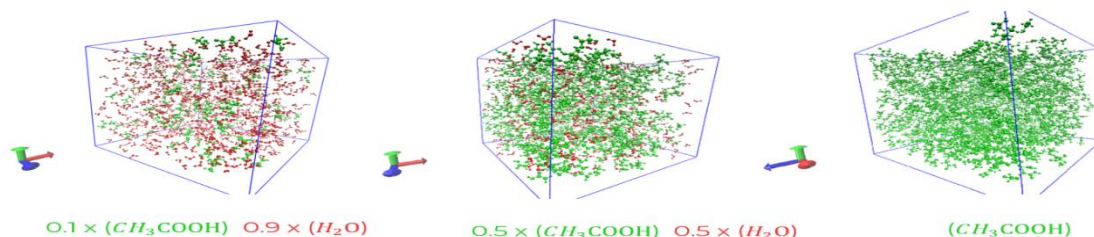
ДИЭЛЕКТРИЧЕСКИЕ СВОЙСТВА ВОДНОГО РАСТВОРА УКСУСНОЙ КИСЛОТЫ И АЦЕТОНА.

Абстракт

Исследованы водные растворы уксусной кислоты и ацетона при различных концентрациях с использованием моделирования молекулярной динамики. Расчёт избыточной диэлектрической проницаемости ϵ^E растворов и определение кривой концентрационной зависимости производились с помощью пакета программ GROMACS. Минимальные значения избыточной диэлектрической проницаемости наблюдались при концентрациях $x \sim 0.3$ моль для уксусной кислоты и ацетона, что соответствует максимальному количеству гетеромолекулярных клатратных структур, образующих максимальное количество водородных связей в бинарной жидкости.

Ключевые слова: уксусная кислота, концентрация, молекулярной динамики.

Kirish. Qayta tiklanuvchi energiya manbalarini rivojlantirish bugungi kunning asosiy masalasi sifatida qolmoqda [1]. Qayta tiklanuvchi energiya manbalari uzluksiz bo'lganligi uchun, bu energiyani saqlashga qaratilgan izlanishlarni olib borishnitaqazo etadi. Energiyani saqlash usullari uzluksiz elektr tarmog'iga bo'lgan talabni qondirish uchun ham zarur. Sayoramizda quyosh,



Rasm 1. Turli xil sondagi suv molekulari birlashib hosil qilish mumkin bo'lgan klatrat strukturalar.

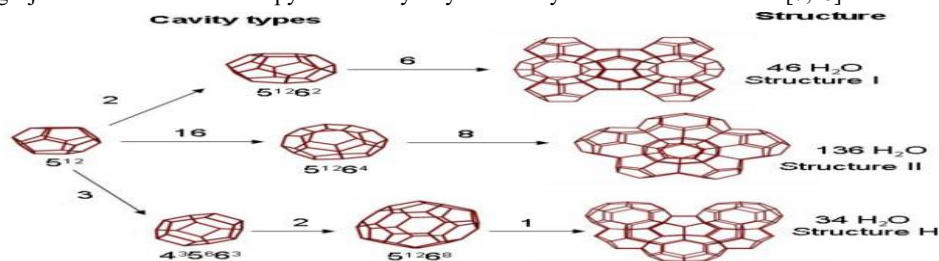
shamol energiyalaridan tashqari vodorod energiyasidan ham foydalanish imkoniyati mavjud [2]. Vodorod gazi yuqori bosim hosil qilishi sababli oddiy gaz balonlarida saqlash xavfli sanaladi.

Shuning uchun vodorodni past bosim ostida saqlash mumkin bo'lgan manbalarni izlash zarur. Shu manbalardan biri bu binar suyuqliklardir. Vodorodni suv va sirka kislota/aseton aralashmasi orqali saqlash bu ishning asosiy maqsadi hisoblanadi.

Tadqiqotlar shuni ko'rsatdiki, vodorodni saqlash juda ko'p muammolarni o'z ichiga oladi [3]. Vodorodni samarali saqlash uchun binar suyuqliklarni optimal konsentratsiyasini aniqlash zarur bo'ladi [4]. Suv yuqori bosim past temperaturalarda turli xil klatrat strukturalar hosil qilishi tadqiqot yordamida kuzatilgan [5].

Biz molekulyar dinamika metodi bilan turli xil konsentratsiyalarda binar suyuqliklarni dielektrik singdiruvchanligini aniqlanaymiz. Olingan natijalar esa suyuqlikni qaysi konsentratsiyasida eng ko'p klatrat strukturalar hosil bo'lganini ko'rsatadi. Natijada esa vodorodni saqlash mumkin bo'lgan optimal suv va sirka kislotasi/aseton aralashmasini prognoz qilamiz.

Simulyatsiyadan sistemalar va ularning tabiatini, ya'ni zamonaviy texnologiyalar yordamida erishib bo'lmaydigan nanoo'lchamdagi aniqlik bilan tushunish uchun foydalanish mumkin [6]. Agar bizda ba'zi sistemalarning eksperimental kuzatish asosida qanday harakat qilishini aytib beradigan ma'lumotlar mavjud bo'lsa, biz ushbu hodisalar qanday sodir bo'lganligi haqidagi savollarga javob berish uchun kompyuter simulyatsiyasidan foydalanishimiz mumkin [7, 8]. Bu esa o'z navbatida



sistemalarni optimal boshqarish imkonini beradi. Binar suyuqliklarda nisbatan past bosimda vodorodni saqlash mumkin. Bizni asosiy maqsadimiz – binar suyuqliklarni turli xil konsentratsiyasida dielektrik xossalarini tadqiq qilishdir. Biz molekulyar dinamika metodi bilan turli xil konsentratsiyalarda binar suyuqliklarni dielektrik singdiruvchanligini aniqlanaymiz.

Rasm 2: Yuqoridagi rasmda dastlab 0÷1 konsentratsiya miqdorlari oralig'idagi aralashma bokslaridan na'munalar keltirilgan.

Hisoblashlar Ubuntu sistemasida GROMACS dasturida amalga oshirildi [9]. Hisob-kitoblar Berendsenning termostatik nazorat algoritmlari yordamida sirka kislotasining turli konsentratsiyasida sirka kislotasi/aseton va suv molekullari bilan to'ldirilgan kubik qutidagi o'zgarish bosim va haroratda amalga oshirildi. Harakat tenglamasi 1,0 fs vaqt qadami bilan Verlet algoritmi yordamida yechildi [10]. Molekulalar orasidagi uzoq masofali Kulon kuchlari Ewald usuli yordamida $1 \cdot 10^{-6}$ kJ/mol aniqlikda hisoblangan. Sirka kislotasi-suv binar tizimining muvozanatiga 50 ns ichida erishildi. Hisoblash jarayoni xona haroratida ($T=300K$) eritmaning 0 ÷ 1 konsentratsiyalarida takrorlandi.

Suvning izotermik siqilish qobiliyati $4.5 \cdot 10^6$ Pa qiymatda olindi. Tuzilishdagi o'zgarishlar aralashmadagi qismlarning nisbatiga qarab suv molekullari va sirka kislotasi o'rtasida vodorod bog'larini hosil qilish uchun ta'sir jarayonlari tufayli yuzaga keladi. Aralashmadagi sirka kislotasi/aseton konsentratsiyasini oshirish bilan suv-suv, suv – eritma, eritma – eritma orasida vodorod bog'larining ketma ketligidagi o'zgarishlar sodir bo'ladi. Yuqoridagilarni tasdiqlash uchun molekulyar dinamika usuli yordamida sirka kislotasi – suv va aseton – suv aralashmalarining butun konsentratsiya oralig'ida dielektrik singdiruvchanligi o'rganildi. Buning ϵ^E ortiqcha dielektrik doimiyni qiymatlari (1) formula orqali hisoblandi [11].

$$\epsilon^E = (\epsilon_A - \epsilon_{A\infty}) - [(\epsilon_S - \epsilon_{S\infty})(1 - x) + (\epsilon_{Sk} - \epsilon_{Sk\infty}) \cdot X] \quad (1)$$

bu yerda A – aralashma S – suv, Sk – modda, X – modda konsentratsiyasi.

Natija va Muhokama. Eritmaning ϵ^E parametrlarining ortiqcha qiymatlari hisoblandi va sirka kislotasining $x \sim 0.3$ mol konsentratsiyasida o'zining eng past qiymatlarini qabul qildi, ular sirka kislotasi-suv binar aralashmasida vodorod bog'iga ega bo'lgan geteromolekulyar tuzilmalarning maksimal soniga to'g'ri keladi, bu suv hamda sirka kislotasi/aseton molekullari aralashishi natijasida hosil bo'ladi (1 – jadval va 3 – rasm). Sirka kislotasi-suv eritmasining ϵ^E parametrlari son qiymatlarining sirka kislotasi konsentratsiyasining oshishi bilan o'zgarishi eritmada sodir bo'layotgan tarkibiy o'zgarishlardan dalolat beradi.

1-jadval: Turli konsentratsiyalardagi suv va sirka kislotasi/aseton aralashmalarining dielektrik singdiruvchanlik ϵ va ortiqcha dielektrik singdiruvchanligi ϵ^E larning qiymatlari

Konsentratsiya	X_{Sk}	Y_s	ϵ	ϵ_s^E	ϵ_a^E
0	0	1000	71.09	0.00	0.00
0.1				100	900
0.2				200	800
0.3				300	700
0.4				400	600
0.5				500	500
0.6				600	400
0.7				700	300
0.8				800	200
0.9				900	100

1

1000

0

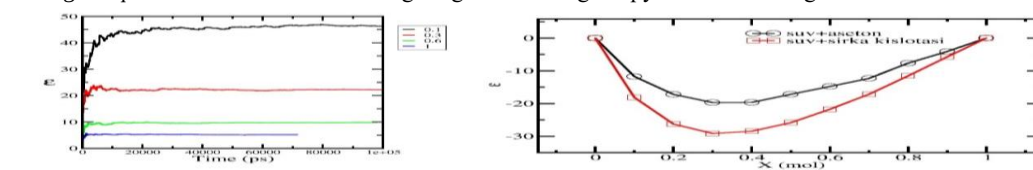
5.15

0.00

0.00

Bu yerda X_{Sk} – kirindi molekula va Y_s suv – suv molekulari soni

Eritmaning ε^E parametrining manfiy qiymati eritmadagi vodorod bog'larining tuzilishidagi o'zgarishlarni ko'rsatadi, bu bog'langan strukturalarning shakllanishiga olib keladi. Quyidagi rasmda (3 – rasm) tayyorlangan sirka kislotasi/aseton va suvli eritmalarining ortiqcha dielektrik o'tkazuvchanligining o'rtachalangan qiymatlari ko'rsatilgan.



Rasm 3: ε - dielektrik singdiruvchanlikning turli xil konsentratsiyalardagi 100ns davomida o'zgarishi. ε^E ortiqcha dielektrik doimiyni turli konsentratsiyada qiymatlarini o'zgarishi.

Model sistemaning dielektrik singdiruvchanlik qiymatlari simulyatsiya boshlanganda katta tebranishlar kuzatiladi (rasm 3). Bu sistemani muvozanat holatiga kelishi bilan bo'g'liq. Molekular muayyan vaqt o'tgandan keyin ta'sirlashuv potentsiallari taqdimlanadi va dielektrik singdiruvchanlik qiymati malum bir oraliqda kichik qiymatlarda tebranib turadi. Tizimda kirindi molekular konsentratsiyasi ortishi bilan bu tizim muvozanat vaziyatiga erishishi tezlashadi (rasm 3).

Xulosa. MD simulyatsiyasi yordamida olingan ε^E hisoblangan eritmalarining ortiqcha dielektrik singdiruvchanligi aralashma konsentratsiyasi o'zgarishi bilan qiymatlarini o'zgartirib bordi. Modellashtirish natijalari shuni ko'rsatdiki sirka kislotasi/asetonning $x=0.3$ konsentratsiyali suv aralashmada ε^E o'zining eng kichik qiymatlarini qabul qildi hamda aralashma eng ko'p vodorod bog'lar hosil qildi. Bu vodorodni saqlash mumkin bo'lgan eng optimal konsentratsiya deb topildi.

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THE INFLUENCE OF SURFACE POTENTIAL BARRIER ON PRIMARY KNOCK-ON ATOMS OF AG(110) SURFACE

Annotation

In the simulation surface potential barrier affection to the emission of knock-on atoms of silver single crystal surface is investigated versus monocrystal orientation. As a target has been used clean and oxygen O₂ covered surface of Ag(110). The azimuth angle of incidence (single crystal orientation) changed in the range $\xi=0-1800$ and counted from $\langle 001 \rangle$ direction. The code for incident ion and recoil trajectories calculation is based on the binary collision approximation (BCA). Geometry of surface potential barrier can also change the direction of emitted particles. It is used planar potential barrier, leaving knock-on atom can overcome the barrier only due to normal component of velocity. The provided calculations showed original characteristic points in dependences of reflection processes.

Key words: Computer simulation, BCA method, primary knock-on atoms (PKA), surface potential barrier, monocrystal orientation, reflection, aggregation.

ВЛИЯНИЕ ПОВЕРХНОСТНОГО ПОТЕНЦИАЛЬНОГО БАРЬЕРА НА ПЕРВИЧНО ВЫБИТЫЕ АТОМЫ ПОВЕРХНОСТИ AG(110)

Аннотация. Моделировано влияние поверхностного потенциального барьера на атомов отдачи серебра в зависимости от ориентации монокристалла. В расчетах использована чистая и покрытая молекулами O₂ поверхности Ag(110). Азимутальный угол бомбардировки (ориентация монокристалла) изменяется в интервале $\xi=0-1800$ и отсчитывается от $\langle 001 \rangle$ направления. Расчетная программа основана на приближении парных столкновений (ППС). Геометрия поверхностного потенциального барьера также влияет на направления, в которых вылетают выбитые частицы. Применена модель плоского барьера, параллельный поверхности мишени, вылетающий атом может преодолеть его только за счет нормальной компоненты скорости. Проведенные расчеты показали оригинальные характеристические точки в зависимостях процесса отражения.

Ключевые слова: Компьютерное моделирование, метод ППС, первично выбитые атомы (ПВА), поверхностный потенциальный барьер, ориентация монокристалла, отражение, скопление.

СИРТИЙ ПОТЕНЦИАЛ ТЎСИҚНИНГ AG(110) КРИСТАЛИ БИРЛАМЧИ ТУРТКИ АТОМЛАРИГА ТАЪСИРИ

Аннотация

Сиртий потенциал тўсиқнинг кумуш кристалли туртки атомларига таъсири монокристалл ориентациясига боғлиқ равишда моделлаштирилди. Ҳисобларда тоза ва O₂ билан қопланган Ag(110) сиртдан фойдаланилди. Азимутал бомбардимон бурчаги (монокристалл ориентацияси) $\xi=0-1800$ интервалда ўзгаради ва $\langle 001 \rangle$ йўналишдан ҳисобланади. Ҳисоблаш дастури жуфт тўқнашувлар яқинлашиши (ЖТЯ) га асосланган. Сиртий потенциал тўсиқнинг геометрияси ҳам туртки заррларнинг йўналишига таъсир қилади. Монокристалл сиртига параллел ясси барьер модели қўлланилди, туртки атом бу тўсиқни фақат тезликнинг нормал ташкил этувчиси ёрдамида енгиб ўтиши мумкин. Ўтказилган ҳисоблар тўсиқдан қайтиш жараёнидаги боғланишларда оригинал характеристик нукталар борлигини кўрсатди.

Калит сўзлар: Компьютерда моделлаштириш, ЖТЯ методи, бирламчи туртки атомлари (БТА), сиртий потенциал тўсиқ, монокристалл ориентацияси, тўсиқдан қайтиш, тўпланиш.

Introduction. Measuring energetic, angular and space distributions of sputtered and desorbed particles from crystal surfaces, considering these dependences with computer simulation results allows create methodical bases for diagnostics of composition and structure of crystal surfaces.

In [1-3] the sputtering of Cu (100) and (110) surfaces at Ar⁺, E₀=30 keV and Ne⁺, E₀=15 keV ion bombardment in 600< β <87,50 incident angle interval was investigated ($\beta=900-\psi$, ψ —grazing angle). In [3] the incident plane of ion beam was parallel to the close-packed surface row $\langle 110 \rangle$, forming surface semichannel. With β angle increasing sputtering yield S(β) is grow up, passing through max and then decrease. In the area of grazing incident angles (800< β <87,50) the curves have peculiarities (local minimums and steps). In [4, 5] angular dependences and the mechanisms of poly and monocrystal sputtering of Cu targets were investigated in binary collision approximation at Ar⁺ $\beta=0-87,50$ beams. In these works, until measurements [1] the dependences of sputtering yield S(β) at $\beta > 750$ were presented.

In [6, 7] it is shown via computer simulation the possibilities of recoil atom spectroscopy for the determining of location of adatoms on crystal surfaces with a submonolayer coverage. It is observed that angular and energetic distributions of knock-on adatoms have characteristic pikes, the location of that gives information about geometry of adsorbed atoms on crystal surfaces.

Calculation method. In the simulations [8, 9] as a target has been used clean and oxygen O₂ covered surface of Ag(110). According to the data from [10] the height of center of mass of O₂ above the surface plane is 0.94 Å, O-O bond length is 1.55 Å, binding energy E_b of O₂ with a surface is 0.53 eV and molecular binding (dissociation) energy is 5 eV.

The number of incident ions is 2x10⁴. The incident ions and the recoil atoms were followed throughout their slowing-down process until their energy falls below predetermined energy: 25 eV was used for the incident ions, and the surface binding energy was used for the knock-on atoms. The angle of incidence of the ion beam ψ was counted from the surface of target, the azimuth angle of incidence (single crystal orientation) changed in the range $\xi=0-180^\circ$ by target rotation around its normal and counted from <001> direction.

The sputtering has been simulated in the primary knock-on regime. Only the primary knock-on recoil (PKR) atoms ejected from first, second and third layers have been considered. The present code for the ion and recoil trajectories calculation is based on the binary collision approximation (BCA). The particle interactions were described by the screened Coulomb potential with the Ziegler-Biersack-Littmark approximation to the Thomas-Fermi screening function. Some details of this binary code with repulsive potentials and its fitness for describing of glancing ion scattering have been described in [8, 9].

For calculations of non-dissociative desorption of adsorbed molecules from surface of single crystals the approach similar in "cut-off" model [11] used for description of the sputtered particles as dimers.

The presence of planar potential energy barrier with the height $U_s = 2.96$ eV for Ag atoms on the surface was taken into account. Geometry of surface potential barrier can influence to direction of emitted particles. In the case of planar potential barrier leaving knock-on atom can overcome only due to normal component of velocity (fig.1).

Consequently, during passing through the barrier trajectory of knocked-on atoms breaks and tilted from the surface normal. If the normal component of the velocity is small knock-on atom can be reflected to the surface.

If emitting particles with energy E_0 come to the planar barrier under angle θ_0 , after passing through surface barrier with height U_s , energy and direction of particle will be [12, 13]:

$$E = E_0 - U_s, \cos\theta = \left[\frac{E_0 \cos^2\theta_0 - U_s}{E_0 - U_s} \right]^{1/2}$$

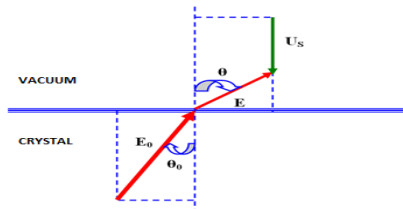


Fig 1. Planar surface potential barrier and deflection of trajectory of knock-on particle at passing through the barrier.

It is seen that a particle with energy less than $U_s/\cos^2\theta_0$ will reflect from the barrier and can't emit to vacuum, i.e. sputtering is not occurring.

In this work the influence of surface potential barrier to the emission and aggregation of knock-on atoms on silver single crystal surface was investigated versus monocrystal orientation.

Results and discussion. The number of dissociative and non-dissociative desorbed O₂ molecules before and after passing through the barrier in dependence to monocrystal orientation ξ at Ne⁺, $E_0=5$ keV, $\psi=100^\circ$ ion irradiation of O₂/Ag(110) surface is presented in Fig.2.

The barrier sensible decreases the number of as dissociative and non-dissociative desorbed particles, but forms of both dependences remain unchanged. This influence lead to the aggregation of silver atoms and oxygen molecules on the surface. The probability of the aggregation of reflected particles and their emission to vacuum at following collisions with incident ions is enough high.

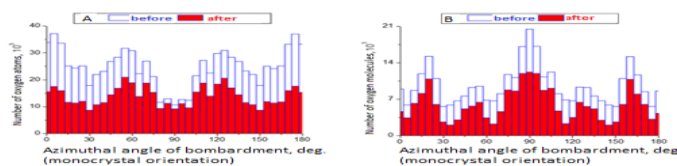


Fig.2. The number of dissociative (A) and non-dissociative (B) desorbed O₂ molecules before and after passing through the barrier in dependence to monocrystal orientation.

The character of the aggregation of reflected atoms and molecules strong depends on single crystal orientation. In this case of bombardment (Ne⁺, $E_0=5$ keV, $\psi=100^\circ$) maximal aggregation of oxygen molecules can occur in $\xi=150^\circ$, $\xi=90^\circ$ and $\xi=165^\circ$ orientations, especially in $\xi=90^\circ$ irradiation direction.

Comprehensive study of azimuth angular dependences knock-on particles showing the possibilities of the control of aggregating particles composition.

The affection of the barrier on the emission of silver atoms from clean and oxygen covered Ag(110) surface presented in fig.3. On the clean surface knock-on atoms mostly overpass the barrier (see fig.3A). The sensible reflection of Ag recoil atoms is possible only near $\xi=90^\circ$.

The simulation results show the unicity of $\xi=90^\circ$ direction (<110>), playing the special role in ion-atomic collision processes occurring on Ag(110) surface.

In the case of Ag(110) surface with adsorption O₂ layer the probability of the aggregation of knock-on particles between adsorption layer and monocrystal surface is high. The presence of submonolayer oxygen molecules on the surface lead to increasing the reflection of knock-on silver atoms back to the crystal.

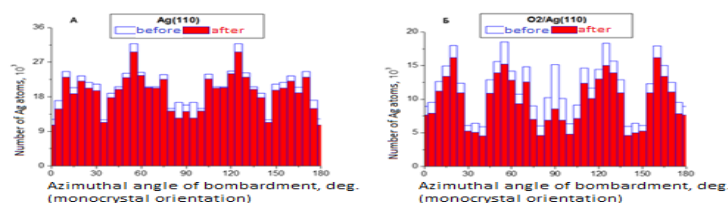


Fig.3. The number of knock-on atoms of silver crystal before and after barrier versus monocystal orientation ξ in the case of Ag(110) (A) and O₂/Ag(110) (B) surfaces.

Conclusion. From computer calculations data it is observed the reflection of the knock-on atoms of single crystal, adsorbed atoms and molecules (free particles) because of the presence of surface potential barrier and adsorbed layer on the crystal surface.

The simulation results show the possibility of the control of ion-collision processes occurring on single crystal surfaces.

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ВЛИЯНИЕ НАПЫЛЕНИЯ АТОМОВ Cs ЭЛЕКТРОННУЮ СТРУКТУРУ CoSi₂/Si(111)

Аннотация

С использованием методов ультрафиолетовой фотоэлектронной спектроскопии, спектроскопии поглощения света и истинно-вторичных электронов впервые изучены влияния напыления атомов Cs с толщиной $\theta \leq 1$ монослоя на плотность состояния электронов валентной зоны и зоны проводимости, параметры энергетически зон и квантовый выход фотоэлектронов. Установлено, что при напыление Cs ширина запрещенной зоны E_g плёнки не меняется, фотоэлектронная работа выхода Φ резко уменьшается, а квантовый выход фотоэлектронов увеличивается до 3 раза. Уменьшение Φ , в основном, объясняется уменьшением ширины зоны проводимости χ (средство к электрону). Показано, что при уменьшение χ до 3 эВ положение максимумов плотности состояния валентных электронов практически не меняется.

Ключевые слова: Электронные свойства, электронная оже-спектроскопия, ионная имплантация, нанопфаза, нанослой, силицид, эпитаксия, гетероплёнка, гетеросистема, морфология поверхности.

EFFECT OF DEPOSITION OF Cs ATOMS ON THE ELECTRONIC STRUCTURE OF CoSi₂/Si(111)

Abstract

Using the methods of ultraviolet photoelectron spectroscopy, light absorption spectroscopy and true secondary electrons, the effects of deposition of Cs atoms with a monolayer thickness of $\theta \leq 1$ on the density of state of electrons in the valence band and the conduction band, the energy band parameters and the quantum yield of photoelectrons have been studied for the first time. It has been established that, upon deposition of Cs, the band gap E_g of the film does not change, the photoelectronic work function Φ sharply decreases, and the quantum yield of photoelectrons increases up to 3 times. The decrease in Φ is mainly due to a decrease in the width of the conduction band χ (electron affinity). It is shown that as χ decreases to 3 eV, the position of the maxima of the density of states of valence electrons practically does not change.

Keywords: Electronic properties, Auger electron spectroscopy, ion implantation, nanophase, nanolayer, silicide, epitaxy, heterofilm, heterosystem, surface morphology.

CoSi₂/Si(111) ЭЛЕКТРОН ТУЗИЛИШИГА Cs АТОМЛАРИ ЧЎҚДИРИШНИНГ ТАЪСИРИ.

Аннотация

Ультрабинафша фотоэлектрон спектроскопияси, ёруғликнинг ютилиш ва ҳақиқий иккиламчи электронлар спектроскопияси усулларида фойдаланиб, бир қатлам қалинлиги $\theta \leq 1$ бўлган Cs атомлари чўқишининг валентлик зонаси ва ўтказувчанлик зонасидаги электронлар ҳолатининг зичлигига таъсири, фотоэлектронларнинг квант чиқиши ва энергетик зоналар параметрлари биринчи марта ўрганилди. Аниқланишича, Cs чўқтирилганда плёнканинг E_g тақиқланган зона кенлиги ўзгармайди, фотоэлектронларнинг чиқиш иши Φ кескин камайди, фотоэлектронларнинг квант чиқиши эса 3 мартагача ортади. Φ нинг камайиши, асосан ўтказувчанлик зонаси кенлигининг камайиши билан боғлиқ χ (электронга мойиллик). χ нинг 3 эВ гача камайиши билан валентлик электронларининг зичлик максимумларининг ҳолати амалда ўзгармаслиги кўрсатилган.

Калит сўзлар: Электрон хоссалар, оже – электрон спектроскопияси, ион имплантация, нанопазалар, нанокатлам, силицид, эпитаксия, гетероплёнка, гетеросистема, сирт морфологияси.

Введение. В последние годы получению и изучению состава, структуры и свойств тонких пленок силицидов, особенно CoSi₂, посвящено большое число работ [1-9]. Это в основном связано с широким применением их в создание ПДП и МДП структур для СВЧ транзисторов и интегральных схем, а также в создание светодиодов, детекторов излучения, других оптических и электронных приборов [10-14]. Известно, что осаждения на поверхность металлов, полупроводников и диэлектриков субмонослойных покрытий атомов металлов и газов (Cs, Rb, Ba, O, H и др.) приводит и существенному изменению их состава и физико-химических свойств [15-20]. В частности, в работе [15] показано, что

на поверхность CdTe при осаждение атомов бария с толщиной $\theta \leq 1$ монослой происходит уменьшение работы выхода и увеличение глубины зоны выхода истинно-вторичных и фотоэлектронов. В случае Si осаждение атомов Al, Ga, Pd, Cr приводил к образованию химической связи типа Me – Si и уменьшению ширины запрещенной зоны [16-18], а в случае GaAs напыление тонких пленок металлов и газов (Cs, Ca, Se, O и H) приводил к стабилизации положения уровня Ферми не зависимо от типа напыляемого вещества [16]. Однако до настоящего времени такие исследования для плёнок CoSi₂ практически не проводились.

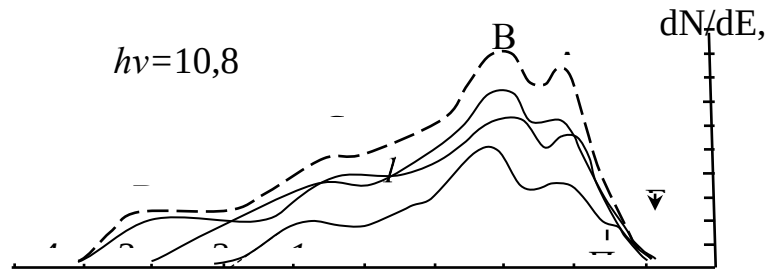
В данной работе впервые изучены влияние осаждение субмонослойных покрытий Cs на плотности состояния валентных электронов, параметров энергетических зон и оптические свойства плёнок CoSi₂/Si (111).

Методика. Исследования проводились с использованием методов ультрафиолетовой фотоэлектронной спектроскопии (УФЭС), спектроскопии истинно-вторичных электронов (ИВЭ) и спектроскопии поглощения света. В качестве объекта исследования использован МЛЭ пленки CoSi₂/Si (111) с толщиной $d = 500$ Å. Перед напылением Cs образцы очищались прогревом до $T \approx 950$ К в течение 2-3 часа при вакууме 10^{-7} Па. Прогрев мишеней, осаждение Cs и все исследование проводились в одном и там же сверхвысоковакуумном приборе. Состав поверхности контролировались методом оже-электронной спектроскопии. За 1 монослой принята толщина слоя Cs при которой значение работы выхода имеет минимум.

Результаты и их обсуждение. На рис. 1 приведены фотоэлектронные спектры пленки CoSi₂/Si(111) с субмонослойными покрытиями Cs в диапазоне $\theta = 0.2 - 1$ монослой. Энергия фотонов $h\nu$ составляла 10.8 эВ. По оси абсцисс отложена энергия связи E_{cv} электронов, отсчитанная относительно уровня потолка валентной зоны E_v . Здесь на всех кривых энергетического распределения (КЭР) фотоэлектронов использован один и тот же масштаб по вертикали, выбранной таким образом, что площадь под кривой пропорционально величине квантового выхода фотоэлектронов Y . Видно, что все кривые обладают явно выраженной тонкой структурой.

Рис. 1. Нормированное распределение фотоэлектронов по энергиям для плёнки CoSi₂/Si, с покрытиями Cs толщиной (в монослоях): 1-0; 2-0,2; 3-0,6; 4-1,0.

На спектре чистой плёнки CoSi₂ обнаруживается пики при $E_{cv} = -0.8$; -2.1 ; и -4.6 эВ, а также особенность при $E_{cv} \approx -0.4$ эВ. Анализ этого спектра и сравнение его со спектрами Si и Co даёт возможность предполагать, что пик A формируется вследствие гибридизации M_{23} состояния кремния и N_1 состояния кобальта, а пик B - вследствие гибридизации M_{23} состояния кремния и M_5 состояния кобальта, в то время как пик C образуется вследствие гибридизации M_1 -состояния кремния и M_4 -состояния кобальта. Появление особенности при $E_{cv} \approx -0.4$ эВ объясняется, наличием поверхностных состояний (ПС). При напыление Cs с ростом θ в интервале $\theta = 0.2 - 1$ монослоя интенсивности этих пиков увеличивается без заметного изменения их энергетических положений, а особенность при $E_{cv} = -0.4$ эВ исчезает. При этом ширина спектра ΔE и площадь под КЭР фотоэлектронов увеличивается, т.е. уменьшается фотоэлектронная работа выхода Φ , а квантовый выход фотоэлектронов Y увеличивается. При $\theta \geq 0.6$ монослой на КЭР появляется интенсивный пик D при $E_{cv} = -7.2$ эВ, по-видимому связанный возбуждением электронов из M_1 -состояния кремния. Наибольшие изменение спектра наблюдается при $\theta \approx 1$ монослой. Дальнейшее увеличение θ приводит к некоторому увеличению



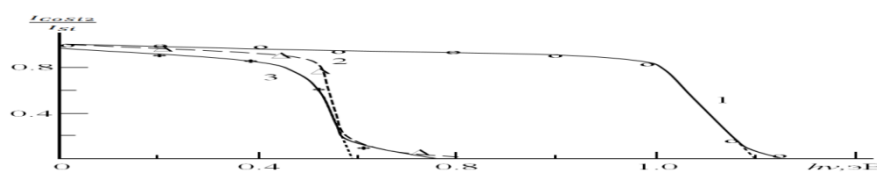
работы выхода. (КЭР фотоэлектронов, снятые при $\theta > 1$ монослой здесь не приводился.) Значение E_g определялось с использованием метода спектроскопии поглощения света.

На рис. 2 приведены спектры поглощения света (кривые зависимости I_{CoSi_2}/I_{Si} от $h\nu$) для Si (111), CoSi₂/Si и CoSi₂/Si с монослойным покрытием Cs. Экстраполяция правой части кривой I_{CoSi_2}/I_{Si} к оси $h\nu$ (рис. 2) даёт значение E_g исследуемого образца.

Рис. 2. Спектры поглощения света для: 1- чистого Si (111); 2- пленки CoSi₂/Si(111); 3- CoSi₂ с пленкой Cs толщиной 1 монослой

Где I_{Si} и I_{CoSi_2} – интенсивности проходящего света через Si (111) без и с пленкой CoSi₂ соответственно. Из рис. 2 видно, что E_g чистого Si равна 1.1 эВ, а CoSi₂ – 0.6 эВ. При напыление Cs с толщиной 1 монослой интенсивность проходящего света немного уменьшается во всей исследованной области $h\nu$, а значения E_g практически не меняется.

На основе данных рис. 1 и 2 нами определены основные параметры энергетические зон системы Cs/CoSi₂ (табл). В таблице также приведены значения Y . Здесь значение Φ определялся по формуле $E_v = \Phi = h\nu - \Delta E$, а значение сродство к электрону определялся по формуле $\chi = E_v - E_g$. Значение E_v относительно уровня вакуума равна фото – электронной



работе выхода[7].

Из таблицы видно, что уменьшения Φ плёнки CoSi_2 при осаждение Cs в основном, происходит вследствие уменьшения сродство к электрону χ .

Таблица

Параметры зон и значение Y для $\text{CoSi}_2/\text{Si}(111)$ с субмонослойными покрытиями Cs

θ_{Cs} в монослоях	Параметры зон, эВ			Y (при $h\nu = 10.8$ эВ)
	E_v	E_g	χ	
0	4.9	0.6	4.4	$4 \cdot 10^{-4}$
0.2	3.6	0.6	3.1	-
0.6	2.5	0.6	2	$9 \cdot 10^{-4}$
1	1.9	0.6	1.4	$1.1 \cdot 10^{-3}$

Таким образом спектры фотоэлектронов, полученные при $h\nu \approx 10 - 15$ эВ, хорошо отражает плотность состояния валентных электронов поверхностных слоев исследуемых образцов. Однако, до настоящего время не существует прямые методы оценки плотности состояния электронов зоны проводимости. При этом важное научное и практическое значение имеет получение информации о положении максимумов плотности электронных состояний в зоне проводимости. Экспериментально это можно осуществлять снятием энергетических спектров истинно-вторичных электронов $N(E_2)$ при низких энергиях первичных электронов E_p материала, контролируемо снижая работы выхода его поверхности [10].

На рис. 3 приведены спектры ИВЭ $N(E_2)$, снятые при $E_p = 5$ эВ, для чистого CoSi_2 и CoSi_2 со субмонослойной ($\theta \approx 0.6$) пленкой Cs. E_2 – энергия вторичных электронов. Нуль на оси E_2 соответствует уровню вакуума пленки CoSi_2 .



Рис. 3. Спектры ИВЭ пленки CoSi_2 и CoSi_2 покрытой Cs толщиной $\theta \approx 0.6$ монослой, измеренные при $E_p \approx 5$ эВ.

Видно, что после напыление Cs выход истинно-вторичных электронов в вакуум увеличивается, а начало спектра смещается в сторону меньших энергии на ~ 2.4 эВ, т.е. потенциальный барьер (сродство к электрону χ) уменьшается на 2.4 эВ. На этой части спектра обнаруживаются особенности при энергиях $E_{c1} = -0.8$ и $E_{c2} = -1.9$ эВ (относительно E_v при энергиях $E_{c1} = 3$ и $E_{c2} = 4.1$ эВ). Положения этих особенностей соответствуют максимумам плотности электронных состояний в зоне проводимости. Увеличивая толщины пленки Cs до 0.8 – 1 монослоев можно уменьшит χ на ~ 3 эВ. Однако при этом в спектре начинает появляться особенности, связанные с адатомами Cs.

Заключение. Показано, что при напыление Cs на поверхность CoSi_2 толщиной $\theta \leq 1$ монослой, значение E_g и положение максимумов плотности состояния валентных электронов практически не изменяется, работа выхода фотоэлектронов уменьшается до 3 эВ, квантовый выход фотоэлектронов увеличивается в 3 и более раза. При $\theta \geq 0.6$ монослой на спектре появляется новый максимум при $E_{c3} = -7.2$ эВ, характерный для кремния.

Впервые экспериментально определены положения максимумов плотности свободных электронных состояний в зоне проводимости CoSi_2 . Эти максимумы расположены при энергиях 0.8 и 1.9 эВ ниже уровня вакуума.

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