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AZOT ATOMLARINING TURLI XIL HARORATDAGI UGLERODLI NANOTRUBKALARGA TA'SIRI

ВЛИЯНИЕ АТОМОВ АЗОТА НА УГЛЕРОДНЫЕ НАНОТРУБКИ ПРИ РАЗНЫХ ТЕМПЕРАТУРАХ

THE INFLUENCE OF NITROGEN ATOMS ON CARBON NANOTUBES AT DIFFERENT TEMPERATURES

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Annotatsiya

Azot qo‘shilgan uglerod nanotubalari noyob xususiyatlari va potentsial qo‘llanilishi tufayli materialshunoslik sohasida katta e’tiborni tortmoqda. Shu sababli, ushbu tadqiqotda ikki qavatli uglerod nanotrubka (IQUNT) ga azot atomlarining adsorbsiyasiga turli xil harorat (ya’ni, 300, 600 va 900 K) va bosim (1, 5 va 10 bar) ning ta’siri reaktiv o‘zaro ta’sir (ReaxFF) potentsialidan foydalangan holda molekulyar dinamika (MD) metodi yoradamida simulyatsiya qilish orqali o‘rganildi. Tadqiqotlar natijasi shuni ko‘rsatadiki, IQUNT sirtiga azot atomlarining yaxshi adsorbsiyasiga erishishda harorat va bosimning ta’siri yuqori bo‘lib, eng yaxshi adsorbsiya ko‘rsatgichi 300 K harorat va 10 bar bosmida bo‘lib, 79% ni tashkil qildi.

Ushbu tadqiqot IQUNT va azot atomlari orasidagi o‘zaro ta’simi tashqi parametrlarga bog‘liqligini tushunishga yordam beradi.

Аннотация

Углеродные нанотрубки, адсорбированные азотом, привлекают большое внимание в области материаловедения благодаря своим уникальным свойствам и возможностям применения. Поэтому в данной работе было исследовано влияние различных температур (т.е. 300, 600 и 900 К) и давлений (1, 5 и 10 бар) на адсорбцию атомов азота на двухслойные углеродные нанотрубки (ДСУНТ). Исследования были проведены методом моделирования молекулярной динамики (МД) с использованием потенциала (ReaxFF). Результаты исследований показывают, что влияние температуры и давления на достижение хорошей адсорбции атомов азота на поверхности ДСУНТ велико, а лучший показатель адсорбции был при температуре 300 К и давлении 10 бар, который составил 79 %. .

Данное исследование помогает понять взаимодействие ДСУНТ с атомами азота в зависимости от внешних параметров.

Abstract

Nitrogen adsorbed carbon nanotubes attract a lot of attention in the field of materials science due to their unique properties and application possibilities. Therefore, in this work, the influence of various temperatures (i.e. 300, 600 and 900 K) and pressures (1, 5 and 10 bar) on the adsorption of nitrogen atoms on double-layer carbon nanotubes (DSNTS) was investigated. The studies were carried out by the method of molecular dynamics modeling (MD) using the potential (ReaxFF). The results of the studies show that the influence of temperature and pressure on achieving good adsorption of nitrogen atoms on the surface of the DSNT is great, and the best adsorption rate was at a temperature of 300 K and a pressure of 10 bar, which was 79%. .

This study helps to understand the interaction of DSNTS with nitrogen atoms depending on external parameters.

Kalit so‘zlar: *ikki qavatli uglerod nanotrubka, azot adsorbsiyasi, molekulyar dinamika, chirallik.*

Ключевые слова: *двухслойная углеродная нанотрубка, адсорбция азота, молекулярная динамика, хиральность.*

Key words: *double-walled carbon nanotubes, nitrogen adsorption, molecular dynamics simulation, chirality.*

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KIRISH

1991-yilda S.Iijima tomonidan kashf etilgan[1] uglerod nanotrubka (UNT) lari fizika, kimyo, materialshunoslik kabi turli sohalarda katta qiziqish uyg‘otdi [2,3]. UNTlar kashf etilganidan buyon noyob xususiyatlari va potentsial qo‘llanilishi tufayli keng ko‘lamli tadqiq qilingan. UNT elektron qurilmalar [4,5,6], adsorbentlar [7,8,9] va boshqa ko‘plab imkoniyatlari tufayli keng o‘rganilib kelinmoqda. Bundan tashqari, UNTlar o‘zlarining noyob xususiyatlari tufayli turli sohalarda, jumladan elektronika, energiya saqlash [10] va biomeditsinada [11,12,13] keng qo‘llanilishi mumkin bo‘lgan materiallardan biridir.

Har xil turdagi UNTlar orasida ikki devorli uglerod nanotrubkalari (IQUNT) barqarorligi va mexanik xususiyatlarining yaxshiligi tufayli keng miqyosda o‘rganilmoqda [14,15,16,17]. IQUNTlarning boshqa atomlar, xususan, bor (B) [18], azot (N) [19,20,21], kaltsiy (Ca) [22], palladiy (Pd) [23,24] va platina (Pt) [25] bilan o‘zaro ta’siri so‘nggi yillarda keng qamrovda o‘rganilmoqda. Ayniqsa bu elementlar orasida UNTlarga azot (N) adsorbsiyasi energiyani saqlash [26] va katalizator [27] kabi turli sohalarda qo‘llanilishi tufayli, unga so‘nggi yillarda katta e’tibor qaratilmoqda.

IQUNTlarga turli xil usulda N atomlarining adsorbsiyasi va doping qilish yordamida ularning mexanik, elektr va optik xususiyatlarini o‘zgartirish mumkinligi sababli, bular so‘nggi yillarda istiqbolli sohalar sifatida o‘rganilmoqda [19,20,21,28,29]. IQUNTlarda azotning adsorbsiya jarayonini tushunish gazni aniqlash va ajratish uchun samarali nanomateriallarni hosil qilish uchun juda muhim. IQUNTlarda azotning adsorbsiyasi naycha diametri va devor egriligi (chirallik) [19] kabi turli omillarga bog‘liq bo‘ladi. IQUNTga N atom va molekulalarining adsorbsiya bo‘yicha turli xil tadqiqotlar o‘rganilayotganiga qaramay ular orasidagi ta’sir mexanizmlarini o‘rganish bo‘yicha hali ham muammolar mavjud.

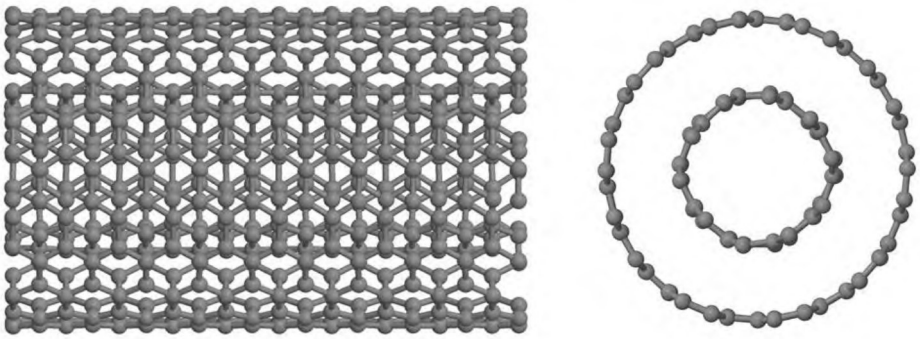
Ushbu tadqiqot molekulyar dinamika (MD) simulyatsiyalaridan foydalangan holda turli harorat va bosimlarda IQUNTlarda N atomlarining adsorbsiya mexanizmlarini o‘rganishdan iborat.

HISOBLASH USULLARI

Tadqiqotda jarayonlarni modellashtirish reaktiv molekulyar dinamika (MD) ga asoslangan LAMMPS dasturiy to‘plam orqali amalga oshirildi [30,31]. Simulyatsiyadagi atomlar orasidagi o‘zaro ta’sirni baholash uchun ReaxFF ptensiali [32] ishlatilgan. MD simulyatsiyalarida IQUNT modeli sifatida toza (5,5@10,10) nanotrubka tanlangan (1-rasm) bo‘lib, IQUNT diametri (D) quyidagi (1) tenglama yordamida hisoblangan:

$$D = \frac{\sqrt{3}}{\pi} R_{C-C}(a^2 + ab + b^2)^{\frac{1}{2}} \quad (1)$$

bu yerda $R_{C\text{-}C}$ – grafendagi uglerod atomlari orasidagi bog‘lanish uzunligi bo‘lib, 1,42 Å ga teng. *a, b* - xirallik indekslari.



1-rasm. (5,5)@(10,10) xirallikli kki qavatli uglerodli nanotrubka (IQUNT) modeli.

Tanlangan IQUNT diametrlari 6,78 Å va 13,57Å ni tashkil etib, eksperimental ravishda olingan nanotrubka diametrlari (6,3Å–7,9Å) va (13Å–16Å) [33] oralig‘ida. UNTning geometrik modellari tegishli o‘lchamdagi va bog‘lanish uzunligi 1,41Å [34] bo‘lgan grafen qatlami uchun olingan. Davriy chegara shartlari cheksiz uzunlikdagi IQUNTlarni z o‘qi bo‘yicha qo‘llanilgan.

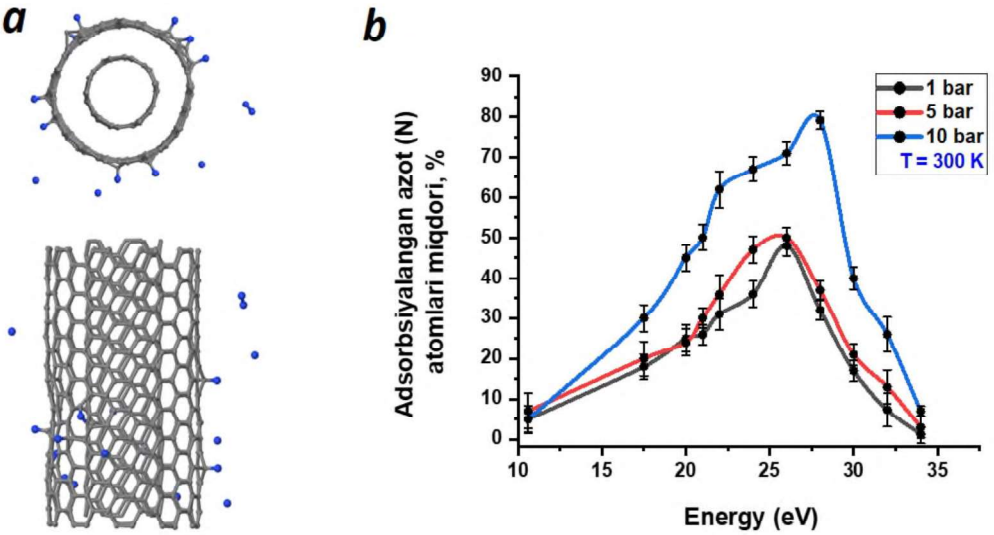
Tizimlarning harorati Berendsen termo-barostat (*NpT*) [35] yordamida 0,1 K/ps qizdirish tezligi bilan isitildi. Bu yerda *NpT* termobarostatidagi *N*-zarralar soni, *p*-bosim va *T*-harorat bo‘lib, ular doimiy ravishda saqlanadi. Tanlangan isitish tezligi oldingi tadqiqotlarda qayd etilgan qiymatlar

oralig‘iga (0,1-10,0 K/ps) mos keladi [36]. Keyin, bu isitilgan tizimlar (ya’ni, IQUNT) Bussi termostatida (*NVT*) 100 ps davomida ushlab turilgan. Bu yerda *NVT* termostatidagi *N*-zarralar soni, *V*-hajm va *T*-harorat bo‘lib, ular doimiy ravishda saqlanadi. Ushbu tadqiqotdagi simulyatsiyalar turli xil bosim (ya’ni, 1, 5 va 10 atm.) va harorat (ya’ni, 300, 600, 900 K) da amalga oshirilgan bo‘lib, *N* atomlari turli xil energiyada ushbu qizdirilgan IQUNT tizimlariga ixtiyoriy ravishda tashlandi. IQUNT (5,5@10,10) yuzasiga tushgan *N* atomlarining bosimi (2) tenglama yordamida har bir harorat uchun hisoblandi [37]:

$$p = J\sqrt{2\pi MRT}/N_A, \qquad (2)$$

Bu yerda, *J* - to‘qnashish oqimi ($nm^{-2}\cdot ns^{-1}$), N_A - Avagadro soni, *R* - universal gaz doimiysi, *M* - azot atomlarning molyar massasi va *T* - tizimning harorati.

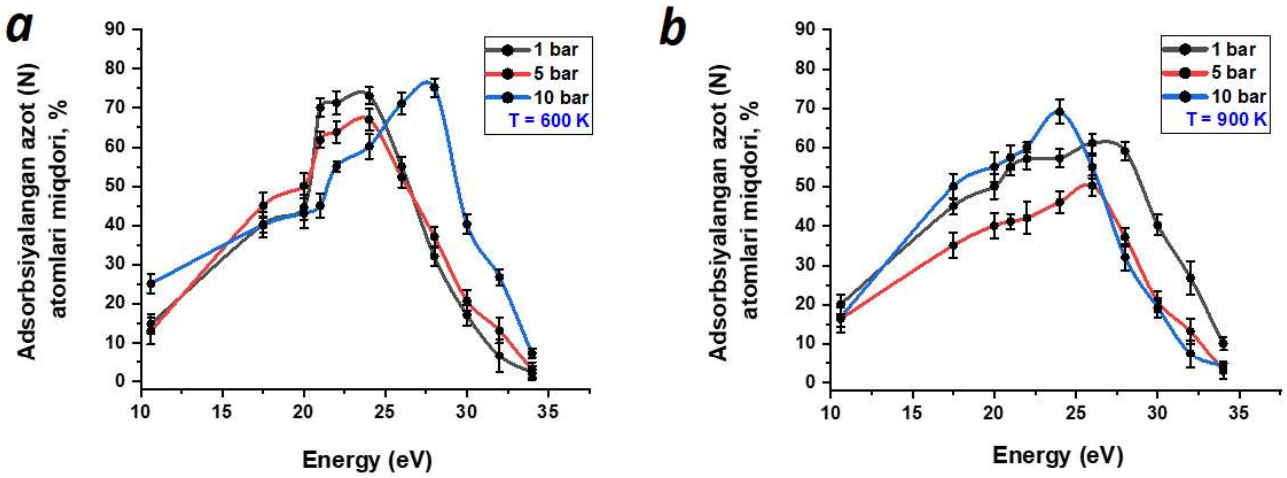
Simulyatsiyalarda IQUNT(5,5@10,10) sirtiga har bir *N* atomlari 10 ps oralig‘i bilan tashlangan va har bir *N* atom va model tizim o‘rtasidagi minimal masofa 10 Å qilib tanlangan. Barcha MD simulyatsiyalarida 2 ns umumiy simulyatsiya vaqti uchun 0,1 fs vaqt qadami ishlatilgan. Simulyatsiyalar har bir tadqiqot ishi uchun kamida 5 marta takrorlangan va yakuniy natijalar olingan qiymatlarni o‘rtacha hisoblash orqali olingan.



2 *a,b*-rasm. *a)* IQUNTga adsorbsiyalangan azot atomlarinng yon va tog‘ridan ko‘rinishi, *b)*IQUNT sirtiga adsorbsiyalangan atomlar miqdorining azot atomlari energiyasiga bog‘liqligi.

NATIJALAR VA MUHOKAMA

Ushbu simulyatsiya 1, 5 va 10 bar bosim bilan 300 K, 600 K va 900 K haroratda amalga oshirildi. 2- tenglama har bir haroratda doimiy bosim hosil qilishda boshlang‘ich sharoitlarda azot miqdorini aniqlash uchun ishlatiladi. Adsorbsiya jarayonining ikki turi mavjud bo‘lib, fizisorbsiya (van-der-Vaals kuchlari, elektrostatik qutblanish o‘zaro ta'sirning tabiatini aniqlaydi) va xemisorbtsiya (Kulon kuchlari va boshqalar) ga bo‘linadi [38,39]. Ushbu tadqiqotda IQUNT (5,5@10,10) yuzasida *N* atomlarining adsorbsiya darajasi tizimning temperaturasiga va sirtidagi atomlar bosimiga bog‘liq (2, 3, 4-*a,b*-rasm) holda hisoblangan. Natijalardan ko‘rish mumkinki, har xil haroratli (ya‘ni 300, 600, 900 K) tizimlar uchun turli bosimlarda (ya‘ni 1, 5, 10 bar) IQUNT yuzasiga adsorbsiyalangan *N* atomlar soni ham o‘zgargan. 300 K haroratda adsorbsiyalangan atomlar soni (bosim) ning ortishi bilan adsorbsiyalangan *N* atomlar soni mos ravishda ortdi (2*a,b*-rasm). Jumladan, 1 bar bosimda IQUNT ga adsorbsiyalangan N atomlarining miqdori (%) 4-48% oralig‘ida bo‘lsa, 5 va 10 bar bosimlarda mos ravishda 6-50% va 5-79% oralig‘ida bo‘ldi. Boshqacha qilib aytganda, nanotrubkada adsorbsiyalangan *N* atomlar miqdorining (%) maksimal qiymati 1, 5 va 10 bar bosimlarda mos ravishda 48%, 50% va 79% ni tashkil etdi.



3 *a,b*-rasm. IQUNT sirtiga adsorbsiyalangan atomlar miqdorining azot atomlari energiyasiga bog‘liqligi.

600 K haroratda 1 bar bosimda 4-73% ga teng bo‘lgan bo‘lsa, 5 va 10 bar bosimda mos ravishda 3-67% va 25-75% oralig‘ida bo‘ldi (3*a*-rasm). Boshqacha qilib aytganda, nanotrubkada adsorbsiyalangan *N* atomlar miqdorining (%) maksimal qiymati 1, 5 va 10 barda 600 K uchun mos ravishda 73%, 67% va 75% ga teng bo‘ldi. 900 K haroratli tizim uchun 1 bar bosimda 4-67% ga teng bo‘lsa, 5 va 10 bar bosimda mos ravishda 5-50% va 3-69% oralig‘ida bo‘ladi (3*b*-rasm). Boshqacha qilib aytganda, nanotubkada adsorbsiyalangan N atomlar miqdorining (%) maksimal qiymati 1, 5 va 10 bar bosimdagi 900 K uchun mos ravishda 67%, 50% va 69% ni tashkil etdi.

IQUNTlari yuzasida azot atomlarining adsorbsiyasiga harorat ham bir necha jihatdan ta’sir qiladi. Yuqori haroratlarda tizim (IQUNT) ning issiqlik energiyasi (tebranish energiyasi) ortadi, bu adsorbsiyalangan azot atomlarining sirtdan desorbsiyasiga olib kelishi mumkin. Natijada bu yuqori haroratlarda nanotrubka yuzasida adsorbsiyalangan azot atomlari ko‘rsatgichi (%) pasayib ketishiga sabab bo‘ladi. Undan tashqari, IQUNT sirtiga tushayotgan azot atomlarining sonining ko‘payishi (ya’ni, Bosimning ortishi) hisobiga azot atomlarining nanotrubka yuzasiga tushish ko‘rsatgichi ortadi. UNT yuzasiga adsorbsiyalangan azot atomlariga sirtga tushayotgan boshqa azot atomlari ta’sir qiladi va birgalikda molekula sifatida qo‘shilib Langmuir-Hinshelvud rekombinatsiya mexanizmi tufayli desorbsiyalanishi (ya’ni, ikki sirt N atomlari bir-biriga kovalent bog‘lanib, azot (N_2) molekulasini hosil qiladi) sodir bo‘ladi [40]. Shuning uchun nanotrubka yuzasida azot atomlarining adsorbsiyasi tushayotgan N atomlari bosimi ortishi bilan tizim haroratiga mos ravishda o‘zgarishi mumkin, va bu natijada tizim haroratining o‘zgarishi (ortishi yoki kamayishi) nanotrubka yuzasida azot atomlarining yutilish energiyasiga ta’sir qilishi mumkin. Odatda, yuqori haroratlarda IQUNT dagi uglerod - uglerod (C-C) atomlari orasidagi bog‘lanish zaiflashadi va bu natijada adsorbsiya energiyasining pasayishiga olib keladi.

Uglerod nanotrubkalarida azot atomlari soni ortishi bilan ularning adsorbsion xossalari o‘zgaradi. Azot qo‘shilgan uglerod nanotrubkalari (N-UNT) sof UNTlarga nisbatan ma’lum gazlar uchun yuqori adsorbsiya qobiliyatiga ega ekanligi aniqlangan. Xususan, IQUNTlarda adsorbsiyalangan azot atomlari soni ma’lum bir azot adsorbsiyasiga qadar ortib borishi bilan adsorbsiya energiyasi ortib boradi. Adsorbsiya energiyasi maksimalga yetib borib, keyin kamayishni boshlashi kuzatilgan . Bu amin, piridin va pirrol azot kabi turli funktsional guruhlarning mavjudligi bilan bog‘liq. Ushbu azotli tizimlar sirt maydonini oshirish va nanotrubkaning elektron xususiyatlarini o‘zgartirish uchun nanotrubka sirtida faol joylarni ta’minlaydi.

Umuman olganda, haroratning IQUNT lari yuzasida azot atomlarining adsorbsiyasiga ta’siri yuqori haroratlarda diffuziya tezligining oshishi va adsorbsiya energiyasining kamayishi hamda adsorbsiyaning o‘zgarishiga bog‘liq bo‘ladi.

XULOSA

Ushbu MD simulyatsiyasi IQUNTda azot atomlarining adsorbsiya mexanizmini to‘gri tasvirlashga yordam beradi. Tizim harorati 300 K da IQUNT tomonidan azot adsorbsiyasi yuqori

haroratlarga (600 K va 900 K) qaraganda azot konsentratsiyasining yuqori miqdoriga ega bo‘ldi. Bir xil bosimda harorat ko‘tarilishi bilan, adsorbsiyalangan azot miqdori kamayadi. Adsorbsiyalangan azot miqdori doimiy haroratda bosimning oshishi bilan mos ravishda ortib boradi. Ushbu simulyatsiyada IQUNTda azot adsorbsiyasi uchun optimal harorat va bosim mos ravishda 300 K va 10 bar bo‘lib, adsorbsiya qiymati 79% ni tashkil qildi.

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