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Article

Vakuumdagi Ni va NiO nanozarralarining agregatsiya mexanizmlari

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Xulosa:
Eksperimental qurilmalar o'lchash imkoniyatlarining cheklangani nanozarralar agregatsiya jarayonlarini to'liq tushunishni murakkablashtirmoqda. Ayniqsa, Ni/NiO kabi nanokompozitlarining hosil bo'lishi va komposit nisbiy tarkibini nazorat qilish uchun ularning agregatsiya mexanizmlarini o'rganish dolzarbligicha qolmoqda. Shu jihatdan ushbu maqolada Ni va NiO nanoklasterlarining agregatsiya mexanizmlarini o'rganish uchun reaktiv molekulyar dinamika modellashtirishlaridan foydalanilgan. Natijalar shuni ko'rsatdiki, kislorod atomlari agregatsiya jarayoniga sezilarli ta'sir ko'rsatadi. Xususan, kislorod atomlari hisobiga NiO nanoklasterining barqarorligi yuqori bo'lib, kislorod atomlari NiO nanoklasteridagi nikel atomlarining boshqa nanoklaster atomlari bilan bog'lanishlar darajasini kamaytiradi. Natijada, Ni nanoklasterlari agregatsiya tufayli o'zaro kimyoviy bog' hosil qilgan holda barqarorlashishga intilsada, NiO nanoklasterlari zaif Van der Vaals kuchlari orqali agregatsiyaga kirishishga harakat qiladi. Umuman olganda, ushbu tadqiqot Ni va NiO nanoklasterlarining agregatsiya jarayonini atomar darajada yaxshiroq tushunishga yordam berib, kerakli xususiyatga ega metal/metal oksidi nanokompozitlarini ishlab chiqishga qaratilgan kelajak tadqiqotlari uchun muhim ahamiyat kasb etadi.

Kalit so'zlar: Ni va NiO nanoklasterlari, barqarorlik, agregatsiyasi, reaktiv molekulyar dinamika.

Aggregation mechanisms of Ni and NiO nanoparticles in vacuum

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Iqtibos: F.M. Safarov, F.A. Xaydarov, K.B. Egamberdiev, T.A. Ahmadjonov, U.B. Xalilov. Vakuumdagi Ni va NiO nanozarralarining agregatsiya mexanizmlari. **2024**, 1,1, 1. https://doi.org/

Olingan: 10.11.2024
Tuzatilgan: 18.11.2024
Qabul qilingan: 25.11.2024
Nashr qilingan: 30.11.2024

Abstract:
The limitations of the measuring capabilities of experimental devices complicate the complete understanding of nanoparticle aggregation processes. In particular, the formation of nanocomposites such as Ni/NiO and the study of their aggregation mechanisms to control the relative composition of the composite remain relevant. In this regard, this article uses reactive molecular dynamics modeling to study the mechanisms of aggregation of Ni and NiO nanoclusters. The results showed that oxygen atoms have a significant effect on the aggregation process. In particular, due to oxygen atoms, the stability of NiO nanoclusters is high, and oxygen atoms reduce the degree of bonding of nickel atoms in NiO nanoclusters with other nanocluster atoms. As a result, while Ni nanoclusters

tend to stabilize by forming mutual chemical bonds due to aggregation, NiO nanoclusters try to aggregate through weak van der Waals forces. Overall, this study provides a better understanding of the aggregation process of Ni and NiO nanoclusters at the atomic level and is important for future research aimed at developing metal/metal oxide nanocomposites with desired properties.

Keywords: Ni and NiO nanoclusters, stability, aggregation, reactive molecular dynamics

Kirish

Nanoo‘lchamdagi zarrachalar sirtida joylashga atomlar ulushi mikro yoki makro o‘lchamdagi zarralarnikidan tubdan farq qiladigan darajada katta bo‘lib, turli xil sirt va kvant effektlarini keltirib chiqaradi [1]. Shu bois nanozarralarda noyob mexanik [2], optik [3], elektron [4], magnit [5] va katalitik [6] xususiyatlar kuchliroq namoyon bo’lishi zamonaviy nanotexnologiyaning jadal rivojlanishda muhim o‘rin tutmoqda. Hozirgi paytda nanozarralar ko‘plab sohalarda, jumladan, dorilarni yetkazib berishda [7], oqava suvlarni tozalashda [8], sensorlarda [9], yoqilg‘ilar ishlab chiqarishda [10], katalizatorlar olishda [11] keng qo‘llanilmoqda. Nanozarralardan foydalanishda nafaqat ularning xususiyatlariga balki narxining past bo‘lishiga ham alohida e’tibor qaratiladi [12–14].

Ayniqsa, Ni/NiO, Co/CoO, Fe/FeO kabi metal/metal oksid nanokompozitlar ushbu talabga javob beruvchi yangi material sifatida namoyon bo’lmoqda [15–17]. Ferromagnit va antiferomagnit fazalar tufayli ushbu nanozarralar yangi fizik xususiyatlarni namoyon qiladi [18]. Bu esa ularni turli sohalarda qo’llashga bo’lgan qiziqishni yanada orttirmoqda [19–22].

Hozirgi paytgacha ushbu nanozarralarni sof metalni qisman oksidlash, metal oksidini qisman qaytarish, bir qozonli sintez kabi ko’plab kimyoviy va fizik usullar orqali tayyorlangan [23,24]. Biroq qurilmalarning o’lchash imkoniyatlari cheklangani bois Ni/NiO kabi nanokompozitlarning hosil bo’lish mexanizmlarini tushunish qiyinligicha qolmoqda [23]. Jarayonlarni modellashtirish usullari, ayniysa, molekulayar dinamika usuli bu kabi qiyinchiliklarni hal qilishda, xususan nanozarralarning agregatsiya mexanizmlarini o’rganishda kuchli vositaga aylanib ulgurdi [25]. Bu usul orqali yadro/qobiq tuzilishga ega metal/metal oksid nanozarralarining sinterlanish (kimyoviy agregatsiya) mexanizmlarini o’rganish orqali kislorod atomlarining harakatchanligi ushbu nanozarralarning shakllanishi va barqarorligi uchun hal qiluvchi rol o’ynashi aniqlandi [26]. Yaqinda Rahbar va boshqalar 1000 va 1600 K oralig’ida Ni nanozarralarining agregatsiyasini o’rganilib, ularning strukturasi va barqarorligini baholadi [27]. Li va boshqalar esa mis nanozarralarining agregatsiyasiga isitish tezligining ta’sirini o’rganib chiqdilar [25].

Biroq bu tadqiqotlarning aksariyati yagona fazali nanozarralarning agregatsiyasiga qaratilgan bo’lib, turli fazali nanozarralarining agregatsiyasi bo’yicha tadqiqotlar juda kam, jumladan Ni va NiO nanozarralarining agregatsiyasi deyarli o’rganilmagan. Ni/NiO nanokompozitlarining noyob xususiyatlari ularning tarkibiga, morfologiyasiga, kristal fazalariga va donalarning o’lchamlariga bog’liq [28]. Ni va NiO nanozarralarining agregatsiya mexanizmlarini o’rganish Ni/NiO nanokompozitlarining qanday hosil bo’lishini tushunish imkonini beradi. Bu esa Ni/NiO nanokompozitlari sintezidagi asosiy muammo Ni va NiO ning nisbiy tarkibini nazorat qilish [24] da muhim rol o’ynashi mumkin. Shu maqsadda Ni va NiO nanoklasterlarining agregatsiya mexanizmlarini o’rganish uchun molekulyar dinamika simulyatsiyalarini amalga oshirdik. Bizning tadqiqotlar eksperimentatorlarga sintez jarayonini yanada optimallashtirish, kerakli xususiyatga ega nanozarralarni sintez qilishda foydali bo’lishi kutilmoqda.

Materiallar va usullar

Vakuumda joylashgan Ni va NiO nanoklasterlarining agregatsiya jarayonlarini modellashtirish reaktiv molekulyar dinamika usuliga asoslangan LAMMPS dasturiy to‘plamidan foydalangan holda amalga oshirildi [29]. Bunda model tizimlar sifatida o‘lchamlari (diametrlari) mos ravishda 1 nm va 1.2 nm atrofida bo‘lgan Ni_{55} hamda $Ni_{55}O_{55}$ (keyingi hollarda mos ravishda Ni hamda NiO ko‘rinishida beriladi) nanoklasterlardan tashkil topgan [30,31] Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftliklari tanlab olindi (1-rasm).

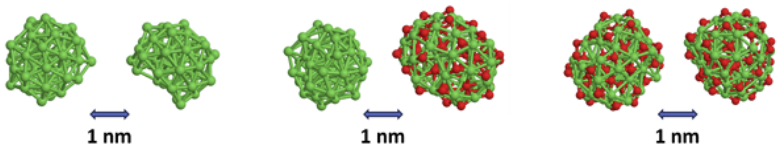

Figure 1. (**a**) NiNi, (**b**) NiNiO, and (**c**) NiONiO pairs of nanoclusters. Here, nickel and oxygen atoms are depicted in green and red, respectively.

Rasm 1. (**a**) Ni&Ni, (**b**) Ni&NiO va (**c**) NiO&NiO nanoklasterlar juftliklarining ko‘rinishi. Bu yerda nikel va kislorod atomlari mos ravishda yashil va qizil rangda tasvirlangan.

Modellashtirishlarda tizimdagi nikel va kislorod atomlari orasidagi o‘zaro ta’sirni ifodalash uchun Zou va boshqalar tomonidan ishlab chiqilgan parametrlarga asoslangan ReaxFF potensialidan foydalanildi [32]. Dastlab model tizimlardagi Ni va NiO nanoklasterlarining energiyasi keskin tushish va birlashgan gradient usullarini ketma-ket qo‘llash orqali minimallashtirildi. So‘ngra tizimning harorati NVT ansamblida Nose-Hoover termostati [33] yordamida 1 K/ps tezlik bilan 300 K gacha qizdirib olindi. Qizdirib olingan nanoklasterlardan iborat Ni&Ni, Ni&NiO va NiO&NiO juftliklar har biri alohida geometrik o‘lchamlari 4×4×4 nm3 ga teng bo‘lgan modellashtirish fazosiga joylashtirildi. Dastlabki holatda bu juftliklardagi Ni va NiO nanoklasterlarning sirtlarini bir-biridan bir xil ReaxFF o‘zaro ta’sir masofasida, ya’ni 1 nm masofada qilib joylashtirildi (1-rasm). Bu holatda har bir termodinamik tizim NVT ansamblda 2 ns davomida 300 K haroratda ushlab turildi. Modellashtirishlarda vaqt qadami 0.5 fs sifatida tanlab olindi.

Vakuumda joylashgan Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftliklarining agregatsiya/aralashish jarayonida hosil bo’lgan strukturalar, ya’ni, agregat yoki yangi klasterlar barqarorligini baholash quyidagi formula asosida Gibbs molyar erkin energiyasining o‘zgarishi (δG) [34] orqali amalga oshirildi:

$$\delta G = E_{\text{coh}} - \sum_i \chi_i \mu_i \quad (1)$$

bu yerda E_{coh} – tizimning har bir atomiga to‘g‘ri keluvchi bog‘lanish (kogesiya) energiyasi. χ_i va μ_i – tizimdagi i turdagi atomning konsentratsiyasi va uning kimyoviy potensiali bo’lib, Ni va O uchun kimyoviy potensial qiymatlari mos ravishda -4.45 eV va -2.8 eV ga teng [34].

Natijalar

1. Nanoklasterlarning agregatsiya/aralashish jarayoni

Klasterlarning agregatsiya/aralashish jarayoni Ni&Ni, Ni&NiO va NiO&NiO juftliklari orasidagi masofalarning o‘zgarishi orqali tahlil qilindi (2-rasm). Hisoblash jarayonlarida nanoklasterlar aniq sferik shaklda emasligi tufayli ularning diametrini aniqlashdagi xatolik ± 0.03 nm ni tashkil qiladi. Umuman olganda, ikkita nanoklasterning sirtlari orasidagi masofaning vaqt o‘tishi bilan o‘zgarishlarini tahlil qilish asosida agregatsiya/aralashish jarayonlarini uchta bosqichga bo‘lish mumkin: (i) yaqinlashish, (ii) agregatsiya va (iii) aralashish.

Shuni ta’kidlash kerakki, nanoklasterlar vakuumda joylashtirilgani bois ularning agregatsiya/aralashish jarayonida suvdagi agregatsiya jarayonidagiga o‘xshash Broun harakati kuzatilmaydi [35]. Birinchi (“Yaqinlashish”) bosqichda, nanoklasterlar sirtlari orasidagi masofa ularning diametridan kichraygan paytdan boshlab Van der Vaals va elektrostatik ta’sirlar natijasida sirtlari biri-biriga tekkuncha qisqarib boradi. Ikkinchi (“Agregatsiya”) bosqichda esa nanoklasterlarning sirtlari o‘zaro bir-biriga tekkan holda massa markazlari orasidagi o‘rtacha masofa vaqt o‘tishi bilan o‘zgarmay qoladi. Xususan, NiO&NiO nanoklasterlar juftligi uchun birinchi (“yaqinlashish”) bosqichi 0-139 ps vaqt intervallarida kuzatilib, 139-2000 ps vaqt intervalida, ya’ni “agregatsiya” bosqichida, nanoklasterlar sirtlari orasidagi masofa modellashtirish jarayonining oxirigacha o‘zgarmay qoladi (bu yerda 0.03 nm xatolik hisobga olinmaydi). Ni&Ni va Ni&NiO nanoklasterlar juftliklarida jarayonlar bir-birga o‘xshash bo‘lib, ular uchun “agregatsiya” bosqichi juda qisqa vaqt davom etadi. Ya’ni, bu vaqt qolgan ikki bosqich vaqtlariga nisbatan e’tiborga olmas darajada kichik bo‘ladi. Xususan, ushbu nanoklaster juftliklari uchun “yaqinlashish” bosqichlari mos ravishda 0-151 ps va 0-10 ps bo’lsa, ikkinchi bosqich ikkala holat uchun 1 ps dan ham qisqa

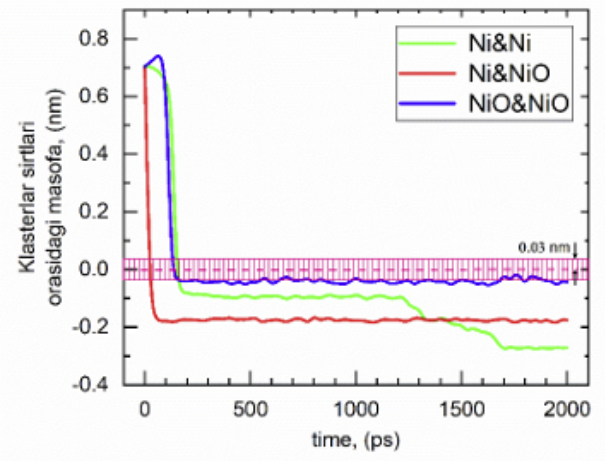

Figure 2. The change in the distance between the surfaces of nanoclusters in NiNi, NiNiO, and NiONiO pairs over time (the results for the pairs are presented in green, red, and blue, respectively).

Rasm 2. Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftligidagi nanoklasterlar sirtlari orasidagi masofaning vaqt o‘tishi bilan o‘zgarishi (juftliklar uchun natijalar mos ravishda yashil, qizil va ko‘k ranglarda berilgan).

vaqtda sodir bo‘ladi va ular orasidagi masofa yanada qisqarishda davom etadi. Nanoklasterlar orasidagi masofa ularning sirtlari bir-biriga tekkandan so‘ng ham kamayishda davom etishi uchunchi (“aralashish”) bosqichining boshlanganidan dalolat beradi. Ushbu jufliklar uchun “aralashish” bosqichi 151-2000 ps va 10-2000 ps vaqt intervallarida kuzatiladi. Xususan, bu bosqichda, Ni&Ni nanoklasterlar juftligidagi ikkita nanoklaster sirtlari orasidagi masofa 1235-1680 ps vaqt intervalida kamayishda davom etgan bo‘lsa-da, Ni&NiO nanoklasterlar juftligi uchun esa nanoklasterlarining sirtlari orasidagi masofa 32-2000 ps vaqt intervalida deyarli o‘zgarmay qoladi. Ushbu hodisani (i) NiO nanoklasterining barqarorligi [36], yoki (ii) Ni nanoklasteridagi nikel atomlarining klaster bo‘ylab tartibli joylashishga bo‘lgan intilishi [27] orqali tushuntirish mumkin. Dastlabki natijalar shunga dalolat qiladiki, vakuumdagi Ni nanoklasterlari bir-biri bilan aralashib ketishga moyilroq bo‘lsa, NiO nanoklasterlari esa faqatgina zaif agregatsiyaga kirishishgagina harakat qiladi.

2. Nanoklasterlarning barqarorligi va ulardagi atomlarning bog‘lanishlar darajasi

Vakuumdagi Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftliklarining agregatsiya/aralashish jarayonida hosil bo’lgan strukturalar, ya’ni, yangi agregat yoki klasterlar barqarorligi 1-formula yordamida hisoblanadigan Gibbs molyar erkin energiyasining o‘zgarishi orqali baholandi. Har bir nanoklasterlar juftliklari uchun barqarorlikni o‘zaro solishtirish uchun Gibbs molar erkin energiyasi o‘zgarishi δG ning qiymatlari uning dastlabki δG_0 qiymatiga nisbatan olindi. Shuningdek, model tizimlardagi Ni hamda NiO nanoklasterlarining agregatsiya/aralashish jarayonida o‘zaro qanday bog‘lanishlar hosil qilgan holda ta’sirlashini tadqiq qilish maqsadida nanoklasterlardagi atomlarning bog‘lanishlar darajasi ham baholanib, ushbu kattaliklar qiymatlari ham dastlabki qiymatlarga nisbatan olindi. Xususan, Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftliklari uchun nanoklasterlari sirtlari orasidagi masofaning Gibbs molyar erkin energiyasi o‘zgarishlarining farqiga bog‘liqligi hamda klasterlardagi atomlarning bog‘lanishlar darajasining farqiga bog‘liqligi mos ravishda 3 a va b-rasmlarda ko‘rsatilgan.

Olingan natijalarni ko’rsatishicha, NiO&NiO nanoklasterlar juftligidagi ikkita NiO nanoklasterlar sirtlar orasidagi masofa agregatsiya/aralashish jarayonida kamayib borib so‘ngra o‘zgarmay qolgan butun vaqt mobaynida ularning molyar Gibbs erkin energiyasi o‘zgarishlaridagi farq hamda nanoklasterlar bog‘lanishlar darajasining farqi deyarli o‘zgarmaganligini ko‘rish mumkin. Bu esa NiO nanoklasterlari barqaror nanozarralar ekanligi [37] va ular agregatsiya jarayonida o‘zaro kuchsiz Van der Vaals kuchlari orqali bir-biri bilan ta’sirlashi hamda o‘zaro qo‘shilib ketishga moyil emas ekanligidan dalolat qiladi. Ni&Ni va Ni&NiO nanoklasterlar juftliklari holatida esa nanoklasterlar sirtlari orasidagi masofa agregatsiya/aralashish jarayonida kamayib borishi bilan ularning molyar Gibbs erkin energiyasi o‘zgarishlaridagi farq kamayib, bog‘lanishlar darajasining farqi ortadi. Bu shundan dalolat qiladiki, Ni klasterining barqarorligi juda past bo‘lib, boshqa Ni

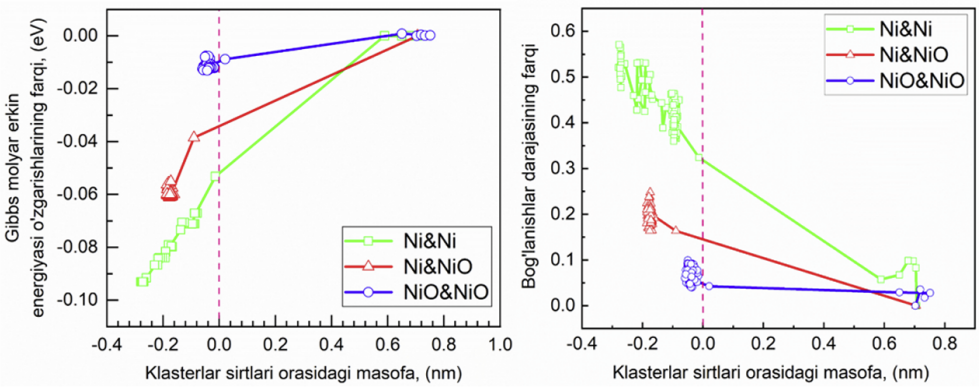

Figure 3. The dependence of the difference in the Gibbs molar free energy changes on the distance between the surfaces of nanoclusters and the difference in the bonding levels of atoms for NiNi, NiNiO, and NiONiO nanocluster pairs (the results for the pairs are presented with green squares, red triangles, and blue circles, respectively).

Rasm 3. Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftliklari uchun nanoklasterlar sirtlari orasidagi masofaning Gibbs molyar erkin energiyasi o‘zgarishlarining farqiga va ulardagi atomlarning bog‘lanishlar darajasining farqiga bog‘liqligi (juftliklar uchun natijalar mos ravishda yashil kvadrat, qizil uchburchak va ko‘k doiralar orqali berilgan).

yoki NiO nanoklasteri bilan o‘zaro birikib ketgan holda kimyoviy bog‘ hosil qiladi va natijada barqarorlashishga intiladi [38]. Agregatsiya/aralashish jarayonlaridagi Ni&NiO nanoklasterlar juftligidagi barqarorlikning Ni&Ni juftliklikdagi barqarorlikka nisbatan farqning yuzaga kelish sababi NiO nanoklasterlaridagi kislorod atomlari klasterdagi nikel atomlari bilan o‘zaro kimyoviy bog‘ hosil qilganligi tufayli nikel atomlarining boshqa klaster atomlari bilan kimyoviy bog‘lanishni kamaytirishi yoki susaytirishi hisoblanadi. Boshqacha aytganda, NiO nanoklasterlarining Ni nanoklasterlariga nisbatan anchagina barqaror bo‘lishi ularning boshqa klasterlar bilan agregatsiyasini kechiktiradi hamda ularning boshqa klasterlar bilan aralashib ketishidan saqlaydi.

Xulosa

Ushbu tadqiqotda vakuumdagi Ni va NiO nanoklasterlarining agregatsiya mexanizmlarini o’rganish uchun reaktiv molekulyar dinamika modellashtirish usulidan foydalanildi. Bunda Ni&Ni, Ni&NiO va NiO&NiO nanoklasterlar juftliklarining agregatsiya jarayonlari uchun modellashtirishlar amalga oshirildi. Olingan natijalar asosida kislorod atomlarining nanoklasterlar agregatsiyasiga sezilarli ta’sir ko’rsatishi aniqlandi. Xususan, Ni nanoklasterlari bir-biri bilan aralashib ketishga juda moyil bo‘lsa, NiO nanoklasterlari esa faqatgina zaif agregatsiyaga kirishishgagina intiladi. Bunga sabab NiO nanoklasterlari tarkibidagi kislorod atomlari nikel atomlari bilan o‘zaro kimyoviy bog‘ hosil qilishi evaziga nikel atomlarining bog‘lanishda ishtirok etadigan kimyoviy bog‘lar sonini kamayishidir. Buning natijasida NiO nanokalsteri yuqori darajada barqarorlashib, ularning agregatsiya jarayonlarida bir-biri bilan faqatgina o‘zaro kuchsiz Van der Vaals kuchlari orqali ta’sirlashishi kuzatiladi. Ikkita Ni nanoklasterlari esa juda reaktiv va beqaror bo‘lganligi tufayli bu nanoklasterlar qo‘shimcha kimyoviy bog‘lar hosil qilgan holda bir-biri bilan aralashib yanada barqarorlashishga intiladi. Ni hamda NiO nanoklasterlarining agregatsiya/aralashish jarayonida bir-biri bilan aralashishi kuzatilsada, bu aralashish qisman bo‘lib, bunga NiO nanoklasterlarining barqarorligi to‘sqinlik ko‘rsatadi. Umuman olganda, ushbu tadqiqot Ni va NiO nanozarralarining agregatsiya jarayonini atomar darajada yaxshiroq tushunishga yordam berib, kelajakda kerakli xususiyatga ega metal/metal oksidi nanokompozitlarini ishlab chiqish uchun o’z hissasini qo’shadi.

Mualliflarning hissalari

Konseptualizatsiya, F.S., K.E va U.X.; metodologiya, F.S. va F.X.; dasturiy ta’minot, F.S., K.E.; ma’lumotlarni kuratorlik qilish, K.E. va U.X.; original matnni yozish, F.S. va U.X.; vizualizatsiya, T.A.; loyiha boshqaruvi, U.X. Barcha mualliflar nashr qilingan qo‘lyozma versiyasi bilan tanish va u bilan rozi."

Authors' contribution

Conceptualization, F.S., K.E., and U.X.; methodology, F.S. and F.X.; software, F.S., K.E.; data curation, K.E. and U.X.; original draft writing, F.S. and U.X.; visualization, T.A.; project administration, U.X. All authors have read and agreed to the published version of the manuscript.

Moliyalashtirish

Mualliflar O'zbekiston Respublikasi Innovatsion rivojlanish agentligi (Grant № F-FA-2021-512) tomonidan moliyaviy yordam ko'rsatilganini e'tirof etadi.

Funding source

The authors acknowledge the financial support provided by the Innovation Development Agency of the Republic of Uzbekistan (Grant No. F-FA-2021-512).

Rahmatnomalar

Bizning barcha modellashtirishlar O'zbekiston Fanlar akademiyasi Ion-plazma va lazer texnologiyalari institutining superkompyuter klasteri yordamida amalga oshirilgani uchun institut ma'muriyatiga chuqur minnatdorchilik bildiramiz.

Acknowledgments

We express our deep gratitude to the administration of the Institute of Ion-Plasma and Laser Technologies of the Academy of Sciences of Uzbekistan for the use of their supercomputer cluster in all our modeling efforts.

Qisqartmalar

Ni/NiO	Nikel (Ni) va uning oksidi (NiO) ni anglatadi.
Co/CoO	Kobalt (Co) va Kobalt oksidi (CoO) ni ifodalovchi termin.
Fe/FeO	Temir (Fe) va Temir oksidi (FeO) ni ifodalovchi atama.

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