

Atomistic Simulation of Ti₂C MXene Decoration with Ag Nanoparticles

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We report the numerical scheme that was developed within the framework of classical molecular dynamics methods for atomistic simulation of the deposition of Ag atoms onto the surface of two-dimensional (2D) titanium carbide Ti₂C (MXene) and the growth of silver nanoparticles (NP). Developed model adopts hybrid interatomic potential, where interactions between metal atoms and between metal-carbon are described within different methods. Proposed model can be used to study similar systems consisting of other metals, as well as two-dimensional carbides Ti_(n+1)C_n with $n = 2$ and 3. Experiments on simulation of the deposition of silver atoms onto the surface of two-dimensional titanium carbide Ti₂C with three different values of the growth surface area were performed. To investigate the peculiarities of nanoparticle formation and growth processes, two types of interaction between Ti₂C and Ag atoms with the metallic-type bonding and Van der Waals forces were considered. Considered cases simulate deposition onto hydrophilic and hydrophobic surfaces, respectively. It is shown that in case of hydrophilic-type of interaction Ag thin film growth on the substrate, while in case of hydrophobic surface, separate nanoparticles are formed. A modeled sample of the system with a silver nanoparticle formed on the surface of two-dimensional titanium carbide was obtained, and forces of interaction between the Ti₂C surface and NPs were calculated. In addition to the stationary case, the MXene-NP interaction was also considered under external loading. The friction forces between the nanoparticle and Ti₂C were calculated at three different magnitudes of the external load. It is shown that translational movement of the nanoparticle on the MXene surface observed in the case with largest magnitude of external load.

Keywords: MXenes, Molecular dynamics, Simulation, Nanoparticles, Decoration.

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1. INTRODUCTION

MXenes, being nitrides and carbides of a transition metals with a thickness of a few atomic layers are new class of two-dimensional materials, famous for their extraordinary properties [1]. Thus, recent studies reveal numerous possibilities of application of MXenes in electrochemistry, nanoelectronics, biophysics, and many other fields [1-7].

Besides two-dimensional materials, metal nanoparticles are also widely used in nanoelectronics to design novel devices with enhanced properties (see for example [8-9] and related references). Moreover, hybrid nanomaterials, including combination of different two-dimensional crystals, as well as decorating the surfaces of 2D materials with metal nanoparticles (NP) is one of the promising areas of modern nanotechnology [10]. For example, there is a large amount of research aimed at the chemical modification of graphene by methods of electrochemical deposition, photoreduction, etc. [10-12]. Such technologies make it possible to modify the properties of graphene with the purpose to improve its performance. In addition to graphene, surface decoration with metal nanoparticles also applicable to MXenes [13]. For example, study [14] reports synthesis of MXene/Ag composites for lithium-ion batteries, which demonstrate an increased charge rate and number of charge/discharge cycles. In particular, in [13] samples of MXenes decorated with silver, gold, or palladium nanoparticles were synthesized. The authors report on

the advantages of using their hybrid materials as a substrate for surface-enhanced Raman spectroscopy (SERS). The noble metal nanoparticles decorated MXenes demonstrate the high sensitivity of SERS detectors for the detection of methylene blue (MB) with estimated enhancement factors of the order of 10⁵. Overall, studies conducted in [13] open the way to expanding the use of hybrid materials based on noble metal nanoparticles and two-dimensional materials, including MXenes, in SERS systems of the visible range for sensors, detectors, as well as catalysis and biomedical applications.

Atomically thin structure of MXenes and diameter of few nanometres of NP make it difficult to study them on atomistic level. Such studies require special facilities like atomic force microscopy or similar, thus, additional theoretical investigations are conducted to get insights on physical processes that occur on an atomistic level.

In the proposed study, we report the computational model, developed for simulation of the process of deposition of Ag atoms onto surface of Ti₂C MXene and decorating it with silver nanoparticles. Our model based on a previously developed approach that was proposed for molecular dynamics (MD) simulation of the Ti_(n+1)C_n MXenes [7]. Here we introducing the deposition of Ag atoms into the simulated system to obtain the modelled samples of Ti₂C MXene with Ag coating as well as MXene decorated with silver NP or the ensemble of nanoparticles. We also describe the structure

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of obtained samples and calculate the interaction between Ag NP and Ti₂C MXene. Overall, proposed numerical scheme can be used in further synthesis and design hybrid materials for nanoelectronics.

2. SIMULATION SETUP

As it was mentioned in introduction, in our study we used previously developed model for MD simulation of MXenes, that are described in detail in [7]. Within proposed approach, interactions between carbon and titanium atoms in Ti₂C are described through empirical potential function, where energy of the system is presented as a sum of two- and three body terms [15]:

$$\Phi(r_1, r_2, \dots, r_N) = \sum_{i < j} U_{ij}(r_i, r_j) + \sum_{i < j < k} W_{ijk}(r_i, r_j, r_k), \quad (1)$$

while interactions between titanium atoms are calculated within Embedded atom method (EAM) [16]. Mentioned scheme was used to calculate forces between the atoms within MXene sample. At the same time, interactions between Ag atoms were described within EAM [16].

In our experiments we consider a system consisting of a sample of two-dimensional titanium carbide Ti₂C with lateral dimensions of 20 × 17 nm², onto the surface of which Ag atoms were deposited, as it shown in Fig. 1. The temperature of the Ti₂C sample was maintained at a 300 K using a Berendsen thermostat [17].

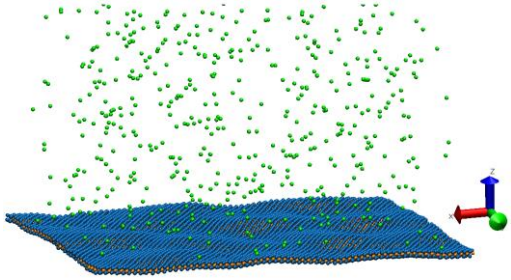


Fig. 1 – An example of the initial configuration of the studied system with a Ti₂C sample with dimensions of 20 × 17 nm² and silver atoms (shown in green) deposited on its surface

The deposition procedure was modelled as follows. Before the start of the experiment, the silver atoms were located at a height of 1.0 nm above the Ti₂C surface, while the x and y coordinates of each Ag atom were chosen randomly. The deposited atoms had only the normal component of the velocity directed towards the growth surface, the density of deposited atoms was chosen so, that the silver atoms did not interact with each other until approaching the Ti₂C surface at a cut-off distance of 1.0 nm. As soon as Ag atoms reach the cut-off distance to the surface, a thermostat was applied to them, and the atoms began to interact with each other, as well as with Ti₂C atoms, and as a result their velocities were changed according to the calculated forces of interatomic interaction.

In our study we considered three cases with different sizes of a surface areas on which silver atoms were deposited. As it was found out in the course of the experiments, the faster growth of one nanoparticle with a close to spherical shape occurred on a smaller area of the deposition surface. Therefore, in order to study the

formation of a separate silver nanoparticle, located on the surface of two-dimensional Ti₂C, experiments were also conducted with growth surface areas of 6.0 × 6.0 nm² and 3.0 × 3.0 nm². The configuration of atoms in these cases was chosen similarly to the general case shown in Fig. 1. A comparison of all initial configurations of the experiment is shown in Fig. 2.



Fig. 2 – Initial atomistic configuration of the system, consisting of Ti₂C MXene and Ag atoms with three different sizes of surface growth areas: 20 × 17, 6.0 × 6.0 and 3.0 × 3.0 nm² from left to right

Also, in order to investigate different types of interaction between Ti₂C and Ag atoms, deposited onto its surface, two cases were considered. Thus, in the experiments the forces between Ag atoms and two-dimensional carbide were calculated within both the EAM model, and the Lennard-Jones (LJ) potential. The EAM approach models the metal-type chemical bonding between the titanium atoms in Ti₂C and deposited silver atoms, while the LJ potential relates to the van der Waals forces between the nanoparticle and 2D MXene. In real conditions, the metallic bond relates to a pristine surface of Ti₂C without functional groups. The interaction within the LD potential models the general case of decoration without the formation of chemical bonds and can be related to the MXenes with various surface termination.

Another interpretation of the two considered cases can be the deposition onto “hydrophilic” (EAM potential) and “hydrophobic” (LJ potential) surface of MXene. It is worth to note, that hydrophilic or hydrophobic behaviour of a material is strongly influenced by the surface morphology of the material. The uneven surface of MXenes can lead to differences in the distribution of surface charges and functional groups, which can affect their hydrophilic and hydrophobic properties. For example, the presence of hydrophilic functional groups, such as -OH and -COOH, on the surface of MXenes can enhance their hydrophilicity, while the presence of hydrophobic functional groups, such as -F and -Cl, can enhance their hydrophobicity. Therefore, studying the interactions between nanoparticles and MXenes at nanoscale level is important for both hydrophilic and hydrophobic surfaces.

3. RESULTS

3.1 Deposition onto Hydrophilic Surface

The atomistic configurations of the system during the deposition of silver atoms with the metallic type of Ag-Ti interaction and the area of the growth surface of 20 × 17 nm² are presented in Fig. 3.

The left and right panels of the figure show the configuration of the system with 512 and 1024 silver atoms on the Ti₂C surface, respectively. As it can be seen from the figure, silver atoms occupy places on the surface that relate to the minimum of interaction potential, thus forming atomic clusters of various sizes. The

size of such clusters increases as more silver atoms are deposited onto the surface. At the same time, the location of atomic clusters and individual atoms on the surface determined by the random uniform distribution of Ag atoms over the Ti_2C surface. As the number of deposited silver atoms increases, large percolation cluster of Ag atoms is formed on the surface of two-dimensional carbide, as shown in Fig.4.

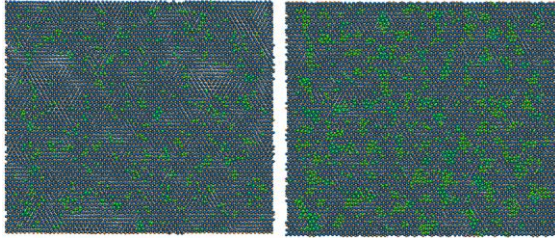


Fig. 3 – Atomistic configuration of a system with 512 (left) and 1024 (right) silver atoms on a Ti_2C surface with a deposition area $20 \times 17 \text{ nm}^2$

At the same time, obtained silver coating has a thickness of a single atomic layer. It can be expected that a further increase in the number of deposited atoms will lead to uniform coverage of the entire surface of Ti_2C with a thin film of silver while the formation of a separate nanoparticles was not observed.

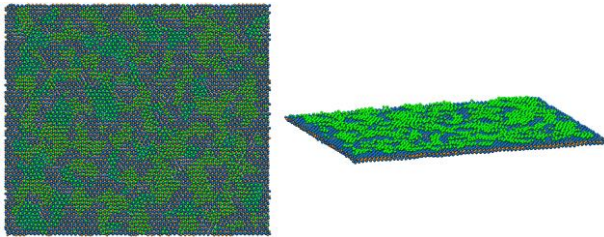


Fig. 4 – Atomistic configuration of a system with 2048 silver atoms on a Ti_2C surface with a deposition area $20 \times 17 \text{ nm}^2$. Top (left panel) and side (right panel) view

To investigate the possibility of the formation of a separate nanoparticle on the hydrophilic Ti_2C surface, an experiment with the size of growth surface area reduced to $3.0 \times 3.0 \text{ nm}^2$ (as shown in right panel of Fig. 2) also was performed.

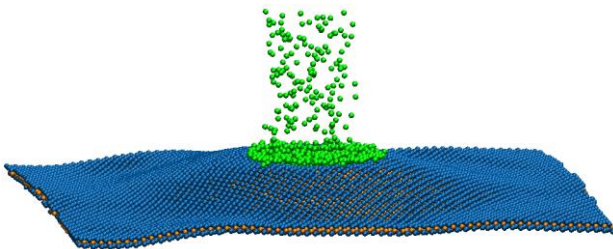


Fig. 5 – Atomistic configuration of a deposition process of 512 silver atoms onto a Ti_2C surface with a deposition area $3.0 \times 3.0 \text{ nm}^2$

The atomistic configuration of the system under the specified conditions with 512 silver atoms on the surface and a growth surface area of $3.0 \times 3.0 \text{ nm}^2$ is shown in Fig. 5. As can be seen from the figure, a similar behavior to the previous case with larger deposition area

is observed. With the difference that silver atoms cover the surface of Ti_2C by a several atomic layers, depending on the ratio of the number of deposited atoms and the growth surface area. At the same time, another feature of the experiment with a smaller area of the growth surface and the metallic type of Ag-Ti interaction is a noticeable curvature of the Ti_2C sheet in the z coordinate direction (see Fig. 1 for coordinate axes). This behavior can be caused by the fact that the forces of interaction between titanium atoms in the contact area and silver atoms above the surface reach sufficiently large values, which in total are strong enough to deflect the central region of the Ti_2C sheet. Concave shape of the two-dimensional titanium carbide sample is preserved even after the deposition of all silver atoms onto the surface.

Thus, as the conducted experiments show, in the case when interaction between titanium atoms on the surface of Ti_2C and deposited silver atoms is modeled as a metallic-type bonding, the formation of individual Ag nanoparticles is not observed. At the same time, Ag thin film is formed on the surface of MXene.

3.2 Deposition onto Surface with Hydrophobic Properties

As it was mentioned above, the case when the interaction between silver atoms and Ti_2C sample is described through the Lennard-Jones pair potential, simulating deposition onto hydrophobic surface was also considered. We assume that for the formation of individual silver nanoparticles on the surface of a two-dimensional material it is necessary to simulate the conditions under which the contact angle of the surface silver atoms would be close to 180° (a situation corresponding to a hydrophobic surface) [18-20]. Since experiments with a metallic bond in the system led to a contact angle close to 0° (Ag atoms completely "spread" over the surface of Ti_2C), it can be expected that the required conditions of hydrophobicity will be observed when the forces of interaction between silver atoms will significantly exceed the Ag-MXene interaction. The results of a series of experiments with hydrophobic interaction are shown in Fig. 6 – Fig. 10.

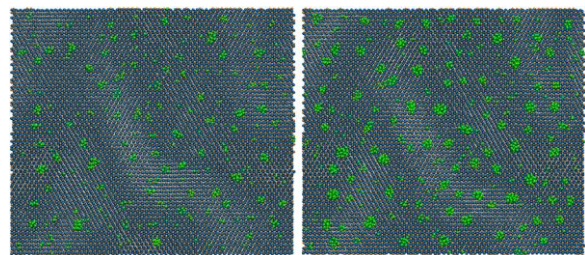


Fig. 6 – Atomistic configuration of a system with 512 (left) and 1024 (right) silver atoms on Ti_2C surface with a deposition area $20 \times 17 \text{ nm}^2$ and hydrophobic type of interaction

The left and right panels of Fig. 6 show the configuration of the system with 512 and 1024 silver atoms on Ti_2C surface, respectively, in the case of the "hydrophobic" Ag-MXene interaction (see Fig. 3 for comparison with the similar configuration in the "hydrophilic" case). As it can be seen from the figure, in contrast to the metallic-type of

Ag-Ti interaction, in the hydrophobic case, the so-called *island growth* of silver nanoparticles on the surface of Ti_2C is observed, instead of individual Ag atoms, mostly atomic clusters and nanoparticles of small sizes are present on the surface. When the number of deposited atoms increases, the nanoparticles growth in sizes as well, while at the same time new growth centres are formed on the surface.

The configuration of the system with 2048 silver atoms on the surface is shown in Fig. 7 (see Fig. 4 for comparison). We expect that with a further increase in the number of deposited atoms, individual nanoparticles of small sizes on the surface of Ti_2C will begin to overlap, which will lead to the formation of a single nanoparticle with dimensions proportional to the number of deposited atoms. Since conducting of such an experiment requires significant computational power, to optimize the time of the experiment and to obtain silver nanoparticles with a spherical shape on the surface of Ti_2C , the area of the growth surface was reduced to and $6.0 \times 6.0 \text{ nm}^2$. The configuration of the system after the deposition of 1024 silver atoms on the reduced area of the growth surface with hydrophobic-type of interaction is shown in Fig. 8. As can be seen from the figure, the reduction of the growth surface area allows to obtain several silver nanoparticles on the Ti_2C surface in a relatively short computational time, however, to obtain a single silver nanoparticle on the surface, a significant increase in the number of deposited atoms and therefore the time of the experiment is also required. Besides this, such configuration of the system is characterized by the presence of atomic clusters of small size, and individual Ag atoms that are located out of cut-off distance from each other, thus forming a separate center of growth of NPs.

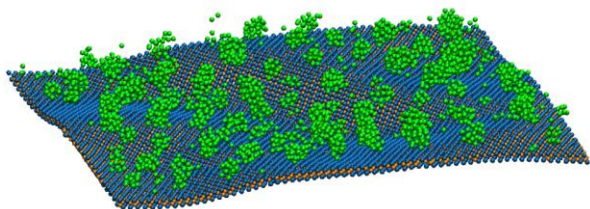


Fig. 7 – Atomistic configuration of a system with 2048 silver atoms on the surface of a Ti_2C surface with a deposition area $20 \times 17 \text{ nm}^2$ and hydrophobic type of interaction

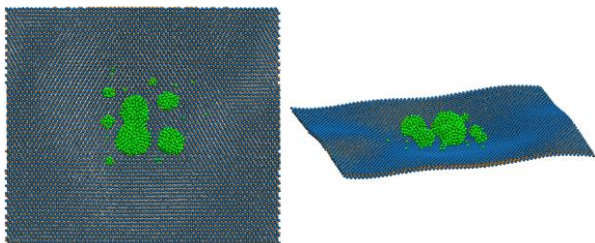


Fig. 8 – Atomistic configuration of a system with 1024 silver atoms on the surface of a Ti_2C surface with a deposition area $6.0 \times 6.0 \text{ nm}^2$ and hydrophobic type of interaction

This situation is undesirable at the beginning of the simulation, if the aim of an experiment is to obtain a single nanoparticle fixed on the Ti_2C surface, as it additionally requires computational power. One of the options for optimizing such a configuration can be the con-

tinuous extraction of isolated atomic clusters from the system during simulation.

However, this requires a separate algorithm to determine the isolated growth centre, as well as additional calculations. A much simpler solution is to reduce the growth surface area in such a way that, even at the beginning of the simulation, the additional NP growth centres will not appear. Example of such configuration is shown in Fig. 9.

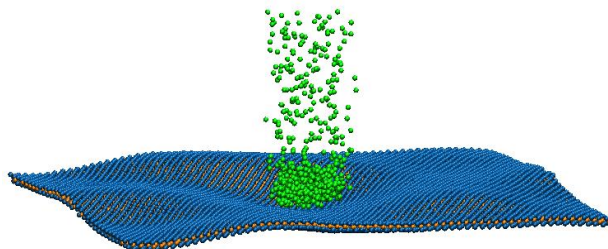


Fig. 9 – Snapshot of deposition of Ag atoms onto the surface of a Ti_2C surface with a deposition area $3.0 \times 3.0 \text{ nm}^2$

At the end of simulation, a silver nanoparticle on the surface of two-dimensional Ti_2C was obtained in a relatively short time, which is shown in Fig. 10.

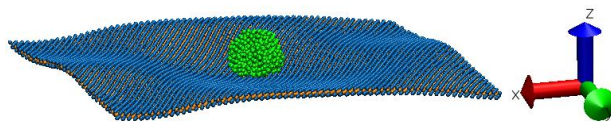


Fig. 10 – Single Ag nanoparticle at the surface of Ti_2C sample formed from the deposited atoms

Thus, as it follows from the conducted experiments, it can be concluded that in cases of deposition of Ag atoms onto hydrophobic and hydrophilic Ti_2C surfaces a qualitatively different growth mechanism is observed. Namely, growth of either the ensemble of nanoparticles or a thin silver film in the first and second cases, respectively. For comparison, Fig. 11 shows the atomistic configurations of the system with 2048 silver atoms on the Ti_2C surface with hydrophobic and hydrophilic interactions.

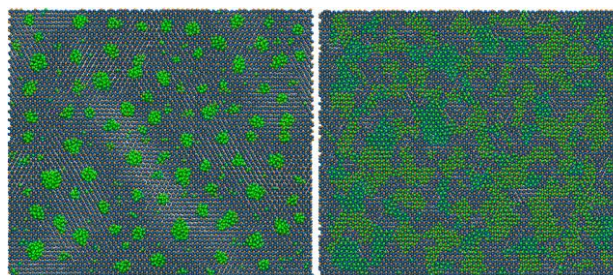


Fig. 11 – Comparison of atomistic configurations of a system with 2048 silver atoms on the surface of a Ti_2C surface with a deposition area $20 \times 17 \text{ nm}^2$ for hydrophobic (left panel) and hydrophilic (right panel) type of interaction

3.3 Interaction Between MXene and Nanoparticle

The formation of a separate silver nanoparticle with a close to spherical shape, (see Fig. 10) allows to calculate the interaction forces between the particle and Ti_2C sample in the stationary condition and under the exter-

nal force F_s , that can be applied to nanoparticle. Since the formation of a nanoparticle was observed only for the hydrophobic surface of Ti₂C, the further study of the interaction forces between a nanoparticle and two-dimensional Ti₂C will be carried out only for the hydrophobic type surface of MXene.

The configuration of the studied case within Cartesian coordinate box is shown in Fig. 10. During the simulation, the components of the forces acting on the nanoparticle from the titanium and carbon atoms of the Ti₂C sample were calculated. The time dependences of the normal and tangential components of the force acting on the nanoparticle in the stationary case are shown in Fig. 12. As it can be seen from the figure, the time dependence of the normal and tangential components of the force acting on the NP is characterized by a constant change of sign. At the same time, since the force does not reach a constant zero value, the nanoparticle does not leave the surface, which indicates the adsorption of NPs on the surface of MXene. The change in the direction of the force can also be affected by the constant fluctuation of the surface of the two-dimensional sample with the formation of wrinkles, as well as the changes in the average normal coordinate of the Ti₂C sheet in space.

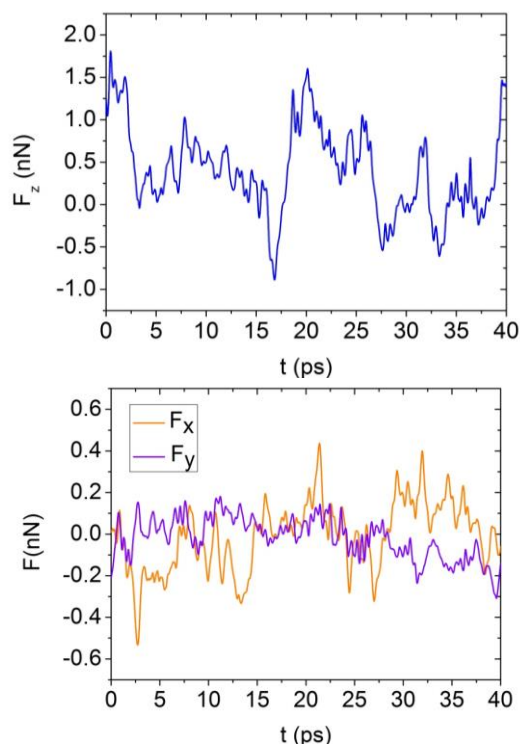


Fig. 12 – Time dependencies of the normal (top panel) and tangential (bottom panel) components of the force acting on Ag nanoparticle from the atoms in Ti₂C sample

The behaviour of the NP at the surface of MXene also was investigated at applied external load. Performed experiment allowed us to calculate effective adhesion forces between silver NP and Ti₂C sample, which can be used in further investigations of the tribological characteristics of the system and calculation of such parameters as friction coefficient between the NPs and the substrate, or similar. The initial configuration of the system before external shear loading is shown in Fig. 10. Stud-

ied system consist of silver nanoparticle obtained by the deposition of silver atoms and located in the center of the Ti₂C sample in a Cartesian coordinate box. In the next phase of experiment, an external shear load along the x axis was applied to silver NP. Three different magnitudes of the external load of 0.5, 10.0 and 50.0 nN were considered. The translational movement of the nanoparticle in the direction of the applied force was observed for the largest load magnitude. Related snapshots of the moving NP are it shown in Fig. 13.

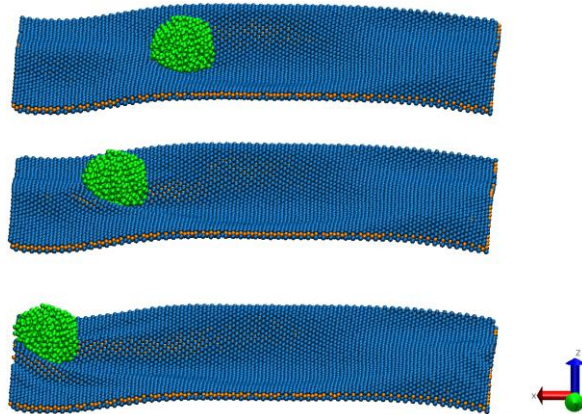


Fig. 13 – Snapshots of the sliding of Ag nanoparticles on the Ti₂C MXene at applied external load of 50 nN along the x axes

The procedure for applying of the external force was implemented as follows. For all Ag atoms in nanoparticle, in addition to the interaction forces between Ag, Ti, and C atoms, calculated from the corresponding potentials, an external force was added by constantly increasing the x component of acceleration by a given value. During the experiments, the forces acting on the nanoparticle from the Ti and C atoms in Ti₂C MXene were calculated, as well as the time dependences of the average coordinates and velocities of the nanoparticle. Time dependences of the x components of the force acting from the Ti₂C on the silver nanoparticle in the three considered cases shown in Fig. 14. As can be seen from the figure, the behavior of the system in the cases with magnitudes of external load of 0.5 nN and 10.0 nN, are similar, while the case with 50 nN is qualitatively and quantitatively differs from the first two cases. The complete picture of the system behaviour becomes clearer after analysing the time dependences of the corresponding components of coordinates and velocities that are shown in Fig. 15. The average coordinates of the nanoparticle were calculated as the average values of the corresponding components of the coordinates of all Ag atoms. As it can be seen from the figure, the case with the smallest applied force 0.5 nN is characterized by the absence of translational motion of NP, and accordingly, the x component of the velocity is close to zero. The force acting on the nanoparticle is caused by the interatomic interaction between the nanoparticle and the substrate, and the external load has almost no effect on the behaviour of the system. When the external load increases to the value of 10.0 nN, x component of the NP velocity also increases, and nanoparticle moves for approximately 1.0 nanometre in the x direction during the considered simulation time. At the

same time, the contribution to the tangential x component of the force acting on the nanoparticle from the friction force during translational motion is barely noticeable without a detailed analysis, and the corresponding time dependence in Fig. 14 has a qualitatively similar form to the previous case.

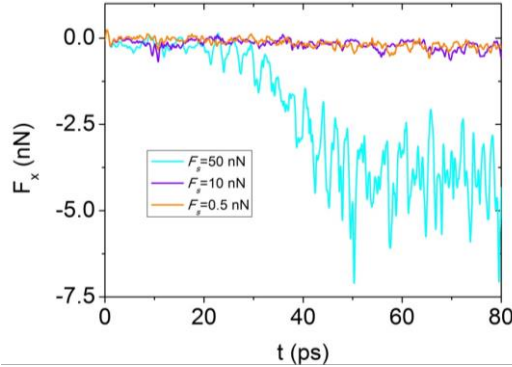


Fig. 14 – Time dependences of the x component of the force acting from the Ti_2C on a silver NP at applied external force (magnitudes of external force a denoted in the figure)

Increasing the external load to 50.0 nN leads to noticeable changes in the behaviour of the system. Thus, as Fig.14 shows, the corresponding dependence is characterized by a continuous growth of the tangential force with further fluctuations around the value of approximately -4.0 nN.

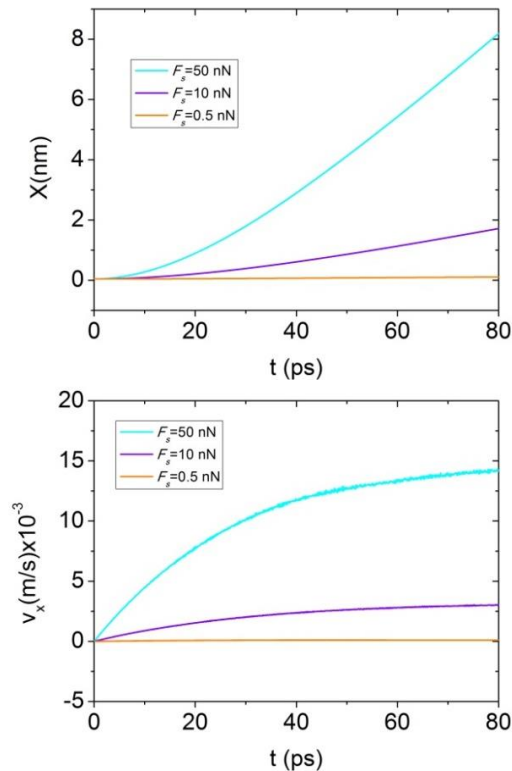


Fig. 15 – Time dependences of the average x coordinate (toppanel) and the corresponding velocity component (bottom panel) of a silver NP at applied external force (magnitudes of external force a denoted in the figure)

It is worth noting that the force acting from the Ti_2C on the silver nanoparticle has a direction opposite to the force of the external load, and can be interpreted as an effective friction force. The related dependences in Fig. 15 show the translational movement of the nanoparticle along the x axis with acceleration in the initial phase. Moreover, from the general form of the time dependence of the velocity, we expect that when a NP velocity reaches a certain value, the nanoparticle will continue to move without further acceleration.

4. CONCLUSION

We presented the results of the computer simulations of decoration of two-dimensional Ti_2C MXene with Ag nanoparticles that were performed within the classical molecular dynamic methods. As our experiments shown, the formation of separate, spherically shaped nanoparticles was observed in the case (to which we refer above as hydrophobic case) when the interactions between deposited Ag atoms and MXene substrate were described by Lennard-Jones interatomic potential. While with metallic-type interaction between deposited Ag atoms and Ti atoms in the MXene substrate (hydrophilic case) the growth of Ag thin film was observed.

From performed simulation model of the sample of MXene decorated with single Ag nanoparticle of spherical shape was obtained. Obtained sample allowed us to investigate the tribological properties of the studied system and calculate effective values of the adhesive and friction forces between MXene substrate and Ag nanoparticle. As our experiments shown, the translational motion of the NP on the substrate surface was observed when the external load of magnitude 50.0 nN was applied to the NP. In general, critical value of the external force that initiates a translational movement of the NP in studied system may depend on many factors, like size of the nanoparticle, contact area between NP and substrate and a shape of the MXene sheet in the region where NP is located. Thus, as it can be seen in the Fig. 13, motion of the nanoparticle causes folding of Ti_2C nanosheet along the contact area NP-substrate in the direction of movement. Such folding of the 2D MXene and wrinkles on its surface may increase the external force needed to move the nanoparticle.

Even though we calculate the numerical characteristics of the NP-MXene interactions, obtained values can be considered only as effective parameters, that are valid within the studied system. To obtain the exact friction coefficient between Ag nanoparticle and Ti_2C MXene more detailed studies with experimental confirmation are needed. Nevertheless, presented results can be used in further investigations and design of the hybrid nanomaterials for application in nanoelectronics.

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Атомістичне декорування Ti₂C максену срібними наночастинкамиЯ.О. Кравченко^{1,3}, А. Таран², У.С. Швець¹, М. Кубах¹, В.М. Борисюк¹¹ Сумський державний університет, вул. Римського-Корсакова, 2, 40007 Суми, Україна² Національний науковий центр "Харківський фізико-технічний інститут", вул. Академічна, 1, 61000 Харків, Україна³ НаноБіомедичний центр, університет Адама Міцкевича, Wszehńnicę Piastowskiej 3, 61-614 Познань, Польща

Представлено комп'ютерну модель, розроблену в рамках методів класичної молекулярної динаміки, для атомістичного моделювання осадження атомів срібла на поверхню двовимірного карбиду титану Ti₂C (максену) та росту срібних наночастинок. В запропонованій моделі використовується гібридний міжатомний потенціал, де взаємодія між атомами металу та взаємодія метал-вуглець описується в рамках різних методів. Розроблена модель може бути використана для дослідження аналогічних систем, що складаються з атомів інших металів, а також двовимірних карбідів Ti_{(n+1)C_n} з n = 2 і 3. Проведені експерименти, що моделюють осадження атомів срібла на поверхню двовимірного карбиду титану Ti₂C з трьома різними значеннями площі поверхні росту. Для дослідження особливостей формування наночастинок та процесів росту також розглянуто два випадки взаємодії між Ti₂C та атомами срібла з міжатомними силами що відповідають утворенню хімічного зв'язку металевого типу та Ван дер Ваальсовими силами. Розглянуті випадки моделюють осадження на гідрофільну та гідрофобну поверхню відповідно. Показано що у випадку взаємодії підкладка-осаджені атоми гідрофільного типу на поверхні Ti₂C максену утворюється тонка плівка срібла, в той час як для гідрофобної взаємодії спостерігається формування окремих наночастинок. Отримано модельний зразок системи зі сформованою наночастиною срібла на поверхні двовимірного карбиду титану для якого були досліджені сили взаємодії між максеном і наночастиною. Окрім стаціонарного випадку взаємодії підкладка – НЧ була розглянута також при зовнішньому навантаженні. В останньому випадку були розраховані ефективні сили тертя між наночастиною та Ti₂C при трьох різних значеннях прикладеної зовнішньої сили. Показано що поступальний рух наночастинок по поверхні максену спостерігається лише у випадку максимальної зовнішньої сили.

Ключові слова: Максен, Молекулярна динаміка, Моделювання, Наночастинка, Декорування.