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COMPARISON OF ORDINARY AND UNUSUAL SURFACES IN GRAPHENE SYNTHESIS

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Abstract: Due to its electronic and mechanical properties and high chemical stability, research is being conducted on graphene growth by various methods. Among them, although CVD is one of the most effective methods, one of the main problems in graphene growing is the correct choice of the metal catalyst surface. For this reason, in this research paper, the probability of graphene growth on surfaces with a high Ni index(331) and a low Ni index (111) was estimated by the molecular dynamics (MD) method. The surface energy of the g-Ni(331) surface with graphene is higher than that of the g-Ni(111) surface, which is considered the most efficient for graphene growth (0.5 J / ^{m2}). it turned out to be lower. This means that graphene can be grown both on Ni(331) surfaces with a high index and on Ni(111) surfaces with a low index, which can be used to make nanodevices (nanotransistors, batteries, water filters, capacitors, etc.).

Key words: *Ni surfaces, chemical vapor deposition (CVD) of graphene, molecular dynamics, surface energy.*

Абстрактный

Благодаря его электронным и механическим свойствам и высокой химической стабильности проводятся исследования по выращиванию графена различными методами. Среди них, хотя CVD является одним из наиболее эффективных методов, одной из основных проблем при выращивании графена является правильный выбор поверхности металлического катализатора. По этой причине в данной исследовательской работе вероятность роста графена на поверхностях с высоким индексом Ni(331) и низким индексом Ni(111) оценивалась методом молекулярной динамики (МД). Поверхностная энергия поверхности g-Ni(331) с графеном выше, чем у поверхности g-Ni(111), которая считается наиболее эффективной при выращивании графена (0,5 Дж/м ^{2}). оказалось ниже. Это означает, что графен можно выращивать как на поверхностях Ni(331) с высоким индексом, так и на поверхностях Ni(111) с низким индексом, которые можно использовать для изготовления наноустройств (нанотранзисторов, аккумуляторов, фильтров для воды, конденсаторов и т. д.).).

Ключевые слова: *поверхности Ni, химическое осаждение из паровой фазы (CVD) графена, молекулярная динамика, поверхностная энергия.*

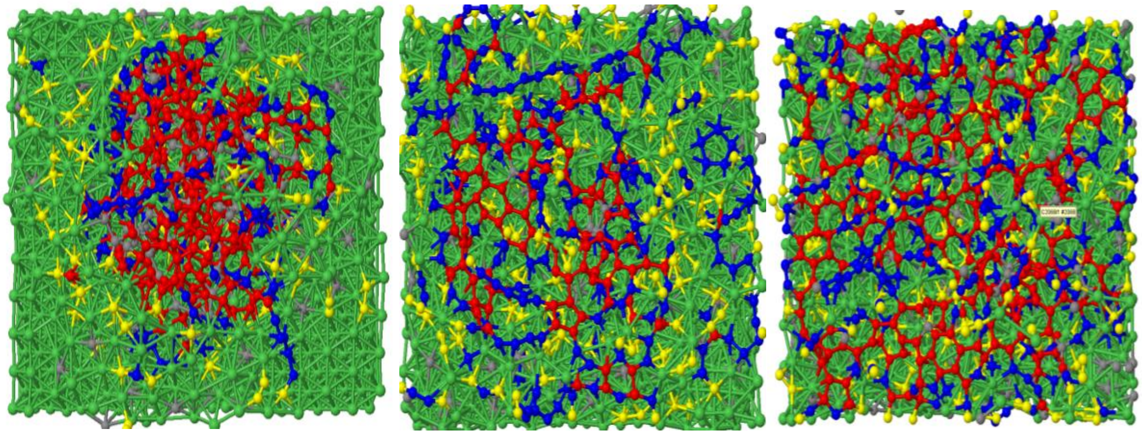
Enter. Graphene [1]is one of the nanomaterials with [7, 8]unique electronic [2, 3, 4]and mechanical [5]properties and high efficiency. chemical stability, which in recent years has been used in many areas [6]. In particular, [9, 10]it is used for various purposes in such areas as electrochemistry, energy storage [9, 11, 12], solar [5, 11, 12]and nanoelectronics . [5, 9]For this reason, the need for its synthesis has increased, and significant research works are being carried out in this direction [13].

In recent years [14] [14] [14] [15]Several methods have been used for graphene synthesis, including mechanical delamination, SiC decomposition, pulsed laser deposition (PLD), and chemical deposition from vapor phase detection (CVD). Despite the fact that theoretical and experimental [17]and model studies [18]on the preparation of graphene by these synthesis methods [16]are carried out, our knowledge of the type of substrates used for its growth and their stability [18]and the catalytic properties [19]are still insufficient. From this point of view, among these methods, although PLD and CVD methods are relatively more efficient, it is more convenient to control graphene formation in the CVD method than in the PLD method. Several conductive metals are used as the surface for graphene deposition, including: (Au [12], Cu [13, 14], Ni [23, 24], Co [25, 26], Fe [27], Pt [28], Pd [29], Ru [30, 31], Rh [32], Ir \l1033 [30]and their alloys are also used (Ni-Mo \l1033 [24], Cu-Ni [34, 35]). As a result of collaboration on graphene growth, the mechanisms of synthesis at the early stages of growth are not fully elucidated. Many studies have made great strides in growing graphene using conventional surfaces (Ni (111), Ni (100), Ni(110)...) using the CVD method. However, there is almost no information about the use of unusual surfaces (Ni(200), Ni(222), Ni(311), Ni(220)). As a result of studying the process on the basis of modeling, it is established that the formation of a carbon double bond on the selected surface leads to the formation of a carbon chain. In addition, it was shown that the formation of a carbon triple bond on the selected surface leads to the formation of a carbon ring, which is the first stage of graphene formation. The simulation results also showed that as the temperature increases during graphene formation, the defects (i.e., pentagon, heptagon, octagon, etc.) decrease, and the number of hexagonal graphene rings increases.

Among these surfaces, the Ni (100), Ni (110), and Ni (111) surfaces are catalytically active among conductive metals and can bind well to carbon atoms, making them some of the widely used metals for graphene growth [32, 33, 34, 35, 36, 37, 38]. However, effective control of graphene formation on the surface by correctly selecting the surface of the metal catalyst is still one of the main problems in graphene cultivation by the CVD method. Therefore, in recent years, along with these (low-index) surfaces, high-index surfaces have also attracted attention due to the fact that they have demonstrated sufficient thermal and chemical stability in chemical reactions. [19]. In particular, surfaces are used as catalysts (210), (331), (411), (630), (722), (730), (755), (830). However, the mechanisms of synthesis are not fully elucidated, since the synthesis of graphene through these surfaces is insufficiently studied.

Therefore, in this research paper, the properties of the Ni(331) surface with a high refractive index were evaluated by the molecular dynamics (MD) method in comparison with the Ni(111) surface with a low refractive index.

Modeling method and details . In this research paper, modeling of processes [39]was carried out using the LAMMPS software package based on the reactive molecular dynamics (MD) method. были The parameters [40]потенциала ReaxFF, разработанного Zou . [41]Crystals with the selected Ni(111) and Ni(331) [42]were created using the VESTA 3D program (Fig.*a*).



a) b) c)

Figure 1. Carbon nanostructures are formed by the transfer of carbon atoms to the surface of nickel at temperatures of 600 (a), 900(b), and 1200(c).

Periodicity $^{\text{conditions were}}$ applied for these (111) and (331) surface nickel crystals , respectively, and for both surfaces (x and y directions of space). Each layer of Ni crystals with surfaces (111) and (331) along the z direction consists of 120 and 60 atoms, respectively, and the number of layers on each surface is from 1 to 31. The distance between each layer in these surface crystals (along the z and b ' axes) is 2.03 and 0.8 Å, respectively . In addition, our calculations also used cases where a piece of graphene $_{48}$ H $_{18}$ (C48H18) was located parallel to both Ni surfaces (Fig. *1b*).

To calculate the surface energy of the selected model structures, their potential energies were minimized by the steep descent method and the combined gradient method. Before the energy minimization step, the structures were initially heated to 50 K in the NpT ensemble using a Noz-Hoover thermostat at a rate of 1 K / ps, and then the system was cooled to 0.1 K. During heating and cooling of the thermodynamic system, the system pressure was maintained at 0 atm. The surface energy of pure Ni crystals with minimal energy (i.e., Ni(331) and Ni(111)) was calculated using the following formula [43]:

$$\text{г} = \frac{1}{2A}\left(E_{slab} - \frac{N_{slab}}{N_{bulk}} E_{bulk}\right) \qquad (1)$$

where E_{slab} and E_{volume} are the energies of the base plate and ingots, respectively, N_{slab} and N_{volume} are the number of atoms in the base plate and ingot, respectively, *and A* is the surface area.

In addition, the surface energy of Ni crystals with graphene ($_{48}$ H $_{18}$ C48H18) on the surface (i.e., γ-Ni(331) and γ-Ni(111)) was calculated by the following formula]:

$$\gamma_g = \frac{1}{A}\left(E_{slab} - \frac{N_{slab}}{N_{bulk}} E_{bulk}\right) - \text{г} \qquad (2)$$

here E_{slab} and E_{volume} are the energies of the base surface and casting, respectively, N_{slab} and N_{volume} are the number of atoms in the base surface and casting, respectively, *and A* is the surface area .

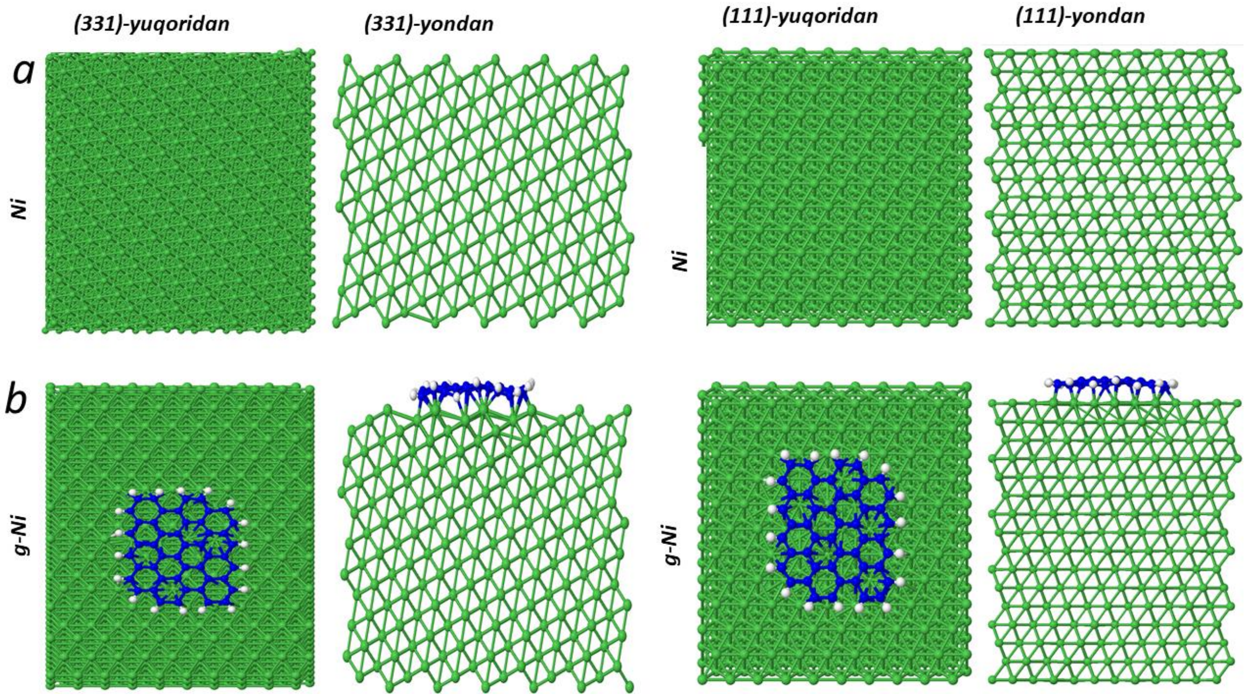


Figure 1. (a) Side and top views of pure (Ni) and (b) nickel surfaces with a parallel graphene layer on top (g-Ni). Here, the layers of Ni crystals with surfaces (111) and (331) are 16 and 26, respectively .

Results and their analysis. The results showed that the surface energy decreases with increasing number of layers in the Ni crystal (i.e., the number of atoms in the crystal and the thickness of each side). . In particular, Figure 2 shows the dependence of the surface energy of the Ni(331) and Ni(111) surfaces on the number of layers.

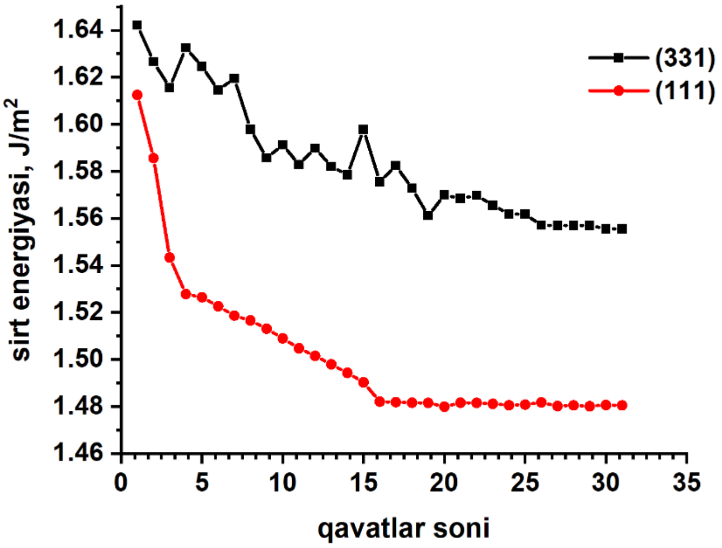


Figure 2. Dependence of the surface energy Ni (311) and Ni (111) on the surface thickness.

2 shows that the surface energy for the Ni(331) and Ni 111) surfaces in the first layer is 1.64 J / ^{m2} and 1.61 J/$^{m2, respectively}$, and as the number of layers increases, these energy values gradually decrease. slowly decreasing. Finally, the surface energies of Ni (331) and Ni(111) are 1.55 J/^{m2} and 1.48 from layers 26 and 16, respectively . J / m2 values ^{2} are reached, and these values remain unchanged with a further increase in the number of floors. This phenomenon is explained by the fact that the thermodynamic system has reached stability, and the stability of the system is expressed [44]by a change in the Gibbs molar free energy (ΔG) . In particular, the change in free energy consists of the sum of the (positive) surface energy and the (negative) energy of the rest of the crystal, and as the crystal thickens (the number of layers increases), its negative value increases, which means that the crystal surface also stabilizes \l1033 [44].

The results obtained were compared with the results obtained by other calculation/modeling methods for Ni(331) and Ni(111) surfaces (Fig.

In particular, CEM is the LMTO (2.36, 2.08) J / ^{m2} [45], EAM (1.97, 1.62) J/^{m2} [46], and MEAM (2.34, 2.04) J/^{m2} potential, and our results are slightly different, whereas EAM is CG (1.60, 1.36) J / ^{m2} [47], MC is EAM (1.91, 1.65) J/^{m2} [48], results obtained on the basis of EAM potentials (1.75, 1.49) J/m ^{2} [49]almost coincides with, for example, the calculated values of the surface energy for the Ni(111) and Ni(331) states differ by 0.80, 0.55 J/^{m2} and 0.20, 0.01 J/m2, respectively, compared to the results derived from the MEAM and EAM potentials.

Figure 4 shows that the surface energies of pure Ni (331) and Ni(111) are 1.55 and 1.48 J/^{m2}, respectively, whereas in the case of γ-Ni(331) and γ-Ni(111), these values are 0.95 and equal to 1.38 J/^{m2} These results show that when a piece of graphene is placed on the Ni(331) surface, the change in surface energy is greater than when a piece of graphene is placed on the Ni(111) surface, and it decreases by 0.5 J / ^{m2} . This result shows that [50]graphene can be grown similarly to a conventional surface (111), using the selected surface with a high index (331).

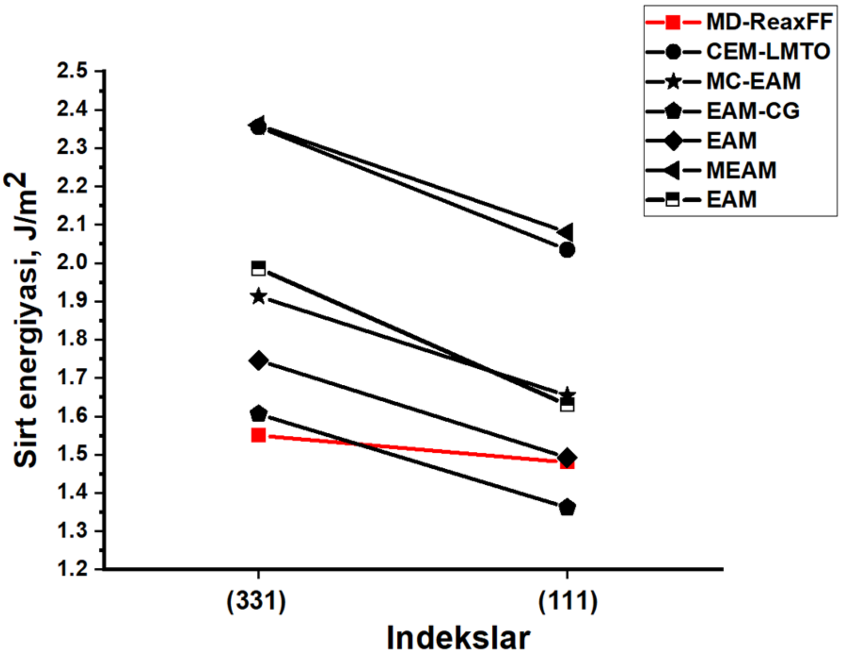


Figure 3. *Comparison of the surface energy values obtained for nickel (331) and Ni(111) surfaces with the results obtained by other calculation/modeling methods.*

Although the values obtained for the Ni(111) and Ni(331) surfaces do not coincide with the values obtained by other methods, the results obtained show that the surface energy of Ni(331) is greater than that of the Ni(111) surface. energy, similar to other results. To estimate the probability of graphene growth on Ni(331) and Ni(111)surfaces A piece$_{\text{of graphene}}$ (H $_{18}$ C48H18) was placed parallel to the surface of these surfaces and the change in surface energy was evaluated. In particular, Figure 4 shows pure Ni (331) and Ni (111) (*черный black) and* the surface energies of the surfaces γ-Ni(331) and γ-Ni (111) (*red), on which a piece of graphene is placed.*

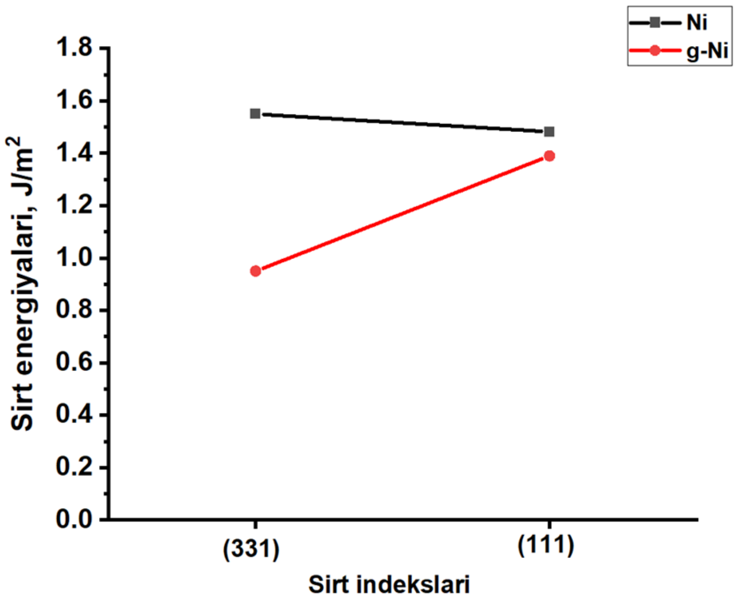


***Figure 4. Surface energy** of pure Ni crystals and graphene-coated Ni crystals.*

Brief content. In this research paper, the surface energies of high-index Ni(331) and low-index Ni(111) surfaces were investigated by computer simulation. The simulation results showed that an increase in the number of layers leads to a decrease in surface energy and surface stability. In particular, it is found that the surface energies of Ni(331) and Ni(111) are 1.55 J / ^{m2} and 1.48 J/^{m2}соответственно , respectively do not change from the 26th and 16th layers. The results obtained are almost consistent with the values of surface energies determined by other quantum mechanical methods . The calculation results also showed that the surface energy of the Ni (331) surface with graphene is 0.5 J/^{m2} lower than the surface energy of the Ni(111) surface with graphene. This means that graphene can be grown both on a high-index Ni(331) surface and on a normal Ni(111) surface.

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