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# Carbon Nanotubes Use for the Semiconductors ZnSe and ZnS Material Surface Modification via the Laser-Oriented Deposition Technique

Natalia Kamanina <sup>1,2,3,\*</sup>, Andrey Toikka <sup>1,2,3</sup> , Bulat Valeev <sup>4</sup> and Dmitry Kvashnin <sup>4,5,6</sup>

- <sup>1</sup> Lab for Photophysics of Media with Nanoobjects at Vavilov State Optical Institute, Kadetskaya Liniya V.O., Dom 5, Korp.2/Babushkina Str., Dom 36, Korp.1, 199053 St. Petersburg, Russia; atoikka@obraz.pro
- <sup>2</sup> Photonics Department, St. Petersburg Electrotechnical University ("LETI"), Ul.Prof.Popova, Dom 5, 197376 St. Petersburg, Russia
- <sup>3</sup> Petersburg Nuclear Physics Institute, National Research Center «Kurchatov Institute», 1 md. Orlova Roshcha, 188300 Gatchina, Russia
- <sup>4</sup> Moscow Institute of Physics and Technology (National Research University), 9 Institutskiy per., Dolgoprudny, 141701 Moscow, Russia; bulat\_valeev@phystech.edu (B.V.); dgkvashnin@phystech.edu (D.K.)
- <sup>5</sup> Emanuel Institute of Biochemical Physics RAS, 4 Kosigina St., 119334 Moscow, Russia
- <sup>6</sup> Physics and Mathematics Department, Pirogov Russian National Research Medical University, Ostrovitianov Str. 1, 117997 Moscow, Russia
- \* Correspondence: nvkamanina@mail.ru; Tel.: +7-(812)-327-0095

**Abstract:** It is known that a material's volume and the surface structuring by the nanoparticles causes a significant change in the material's basic properties. In this aspect, the structuration of the surface of semiconductors is of interest, because their wide potential application in optoelectronics can extend the products' transparency, hardness, wettability, and other important parameters. This paper presents possible methods for the surface modification of zinc selenide and zinc sulfide when carbon nanotubes are deposited on the surface by the application of the laser-oriented technique. It also shows changes of the spectral, mechanical, and wetting characteristics of the considered materials. Using the molecular dynamic simulations, the possible process of the carbon nanotubes penetration into the considered surfaces is presented. The simulation results are partially supported by the obtained experimental data.

**Keywords:** ZnSe; ZnS; surface; carbon nanotubes; laser-oriented deposition; spectra; microhardness; wetting angle; MD



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## 1. Introduction

Among the different materials involved in general optoelectronics, semiconductor materials occupy a special place that is connected with the unique charge carrier mobility of the semiconductor structures and their operation in the visible and near-IR spectral range. These structures can be involved in the solar energy, gas storage, modulation, optical limiting, etc. schemes as well, and they can dramatically extend the applications of optoelectronics devices [1–4]. ZnSe and ZnS materials can be considered as perspective semiconductors to form the different detectors for the wide spectral range and to develop the mirrors and the optical limiting instruments [5–17]. Researchers have revealed the anti-reflective, luminescent properties of these materials and visualized the process of the nanoparticles' creation based on the ZnSe and ZnS structures and their introduction into the polymer matrices [8–11]. Treatment of these materials by femtosecond lasers has been explained as well [12,16].

Furthermore, it should be remarked that ZnSe and ZnS materials are widely used to make the electrically and optically addressed spatial light modulators (SLM), which operate in the blue and in the visible spectral range. This specific application is connected

with the high carrier mobility of these types of the materials. Thus, the response (switch-on and switch-off time) can be revealed with good speed. Indeed, the resolution of the SLM with the photo layers based on the ZnSe and ZnS structures is not so good. However, the compromise between the resolution and the speed can be found via the specific pulsed regime of the laser operations when the delay between the electric pulse and the light one can be varied [17,18].

Different types of classical methods and innovative approaches can be used in order to modify the interface and the surface of the semiconductor materials with the nanoparticles. As promising nano-objects used for this aim, carbon nanotubes (CNTs) [19–24] can be successfully proposed. The basic features of the carbon nanotubes are regarded to be their branched surface, their high conductivity, the strong hardness of their C–C bonds, the little value of the refractive index as well as their complicated and unique mechanisms of the charge carrier moving.

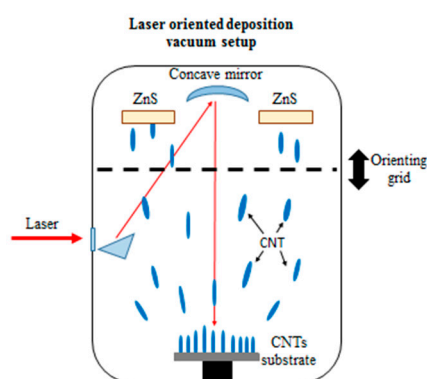
In the current paper, the laser-oriented deposition (LOD) approach, previously shown to treat inorganic crystals and metals, such as KBr [25], BaF<sub>2</sub> [26], and Al [27], is shown as the perspective instrument to modify the properties of the semiconductors based on ZnSe and ZnS. The possibility of the ZnS and ZnSe surfaces' modification via the vertically oriented CNTs deposition is shown. Modification leads to changes in the atomic structure of the surface as well as the mechanical and the optical properties. The obtained modified structures show prospects for an application as a basic element of the optoelectronics schemes, of the solar cells, and of the gas storage systems. Moreover, it can be useful for information technology and displays.

## 2. Materials and Methods

The matrix ZnSe and ZnS materials have been purchased from the “Alkor Technologies” company in Saint-Petersburg. The diameter of the substrate was 35 mm and the thickness of the ZnSe and ZnS structures was 5 and 3 mm, respectively.

To modify the properties of the semiconductor materials via their surface treatment, the single-wall carbon nanotubes (SWCNTs) type #704121 with the diameter placed in the range of 0.7–1.1 nm purchased from Aldrich Co. have been used. It is important in order to find the coinciding conditions between the dimensions of the CNTs directly with the elementary lattice of the material.

To modify the surface, the IR CO<sub>2</sub> laser with *p*-polarized irradiation at the wavelength of 10.6 μm and the power of 30 W has been used. The general view of the block scheme has been shown in [25]. It is shown that the laser system was connected with a vacuum hood, which contains the fixing unit samples and the device for depositing substances on the substrate. To explain the LOD technical process more clearly, the scheme is shown in Figure 1.



**Figure 1.** The scheme to show the LOD process used for the ZnS and ZnSe materials more clearly.

CNTs have been placed at the materials interface under the conditions of an additional applied electric field of  $100\text{--}600\text{ V} \times \text{cm}^{-1}$  in order to orient the nanotubes in the vertical

position during the applied process. It can be possible when, for example, the distance between the grid and the upper substrate can be varied. Some qualitative scheme of this process with the grid incorporated in the vacuum chamber was shown before as well [24]. It permits varying the velocity of the CNTs and forming the covalent bonding between the carbon atoms and the surface matrix materials with good advantage. Using such a scheme, the carbon nanotubes with a given diameter in the interstices of the lattice of the matrix material can be integrated. This procedure has been partially shown in several RU patents [28–30].

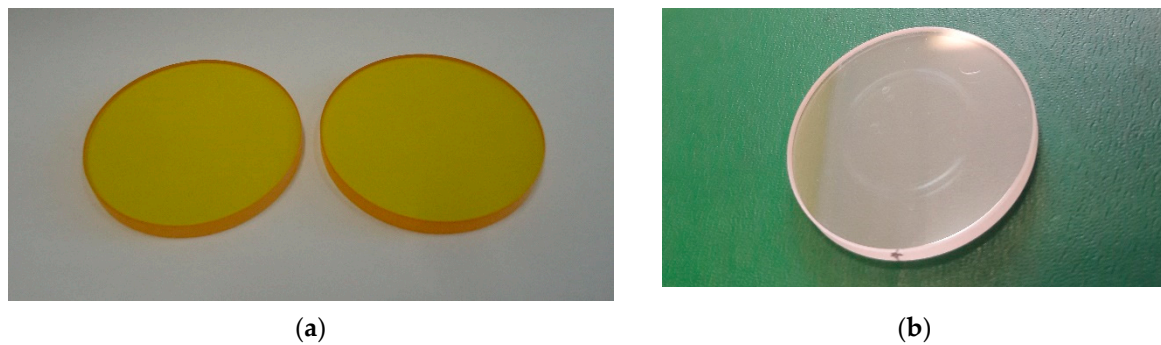
The spectra of the CNTs-treated materials have been obtained using the Furrier FSM-1202 instruments as well as using a VIS SF-26 spectrophotometer operated in the range of 250–1200 nm. The Polam-P312 microscope has been applied to make the image of the materials treated. The surface mechanical hardness (abrasive strength) has been revealed using the CM-55 instrument, and the microhardness has been measured via the PMT-3M device using; this device has been produced by “LOMO” (Saint-Petersburg, Russia) with the ability to vary indenter forces as well. The OCA 15EC device has been purchased from LabTech Co. (Saint Petersburg, Russia) and used to control the wetting angle change to predict the Lotus effect.

To describe the implantation of the CNT at an atomic scale, the molecular dynamic (MD) simulations were carried out using the LAMMPS package [31]. Interaction between the ZnS system and CNTs was described via the Tersoff interatomic potential [32], which was parameterized according to [33]. For the description of the C–C interaction, the Tersoff potential was parameterized according to the procedure [34]. To describe the interaction between the CNT and the ZnS substrate, the Lennard–Jones 12-6 potential was used. The interaction parameters were fit as:  $\epsilon = 0.0113$  eV,  $\sigma = 1.76$  Å. All the simulations were performed at room temperature. The behavior of an atomic under the finite constant temperature was estimated by use of the N ose–Hoover thermostat [35,36]. The total time of the simulation was 60 ps with the time step of 1 fs. The bottom layer of the ZnS substrate was fixed to avoid the displacement of the whole structure during an implantation process. To avoid the effective energy dissipation during the implantation, the boundary conditions with rescaling of the atomic velocities were applied. The initial velocities of CNTs were set up from 100 to 600 m/s.

### 3. Results and Discussion

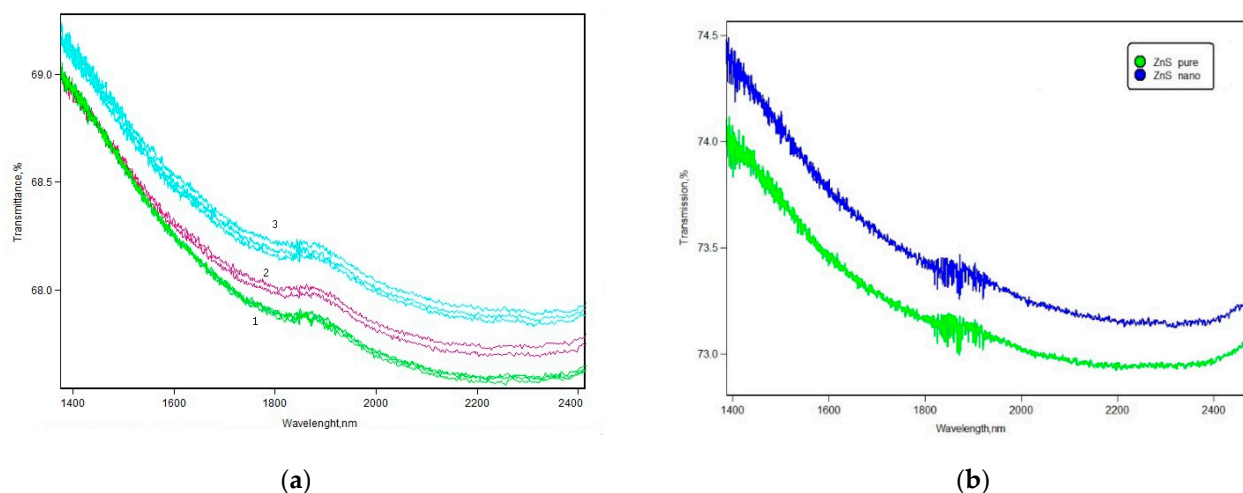
It is well known that the ZnSe and ZnS materials are the most promising key elements in the optical industry. ZnSe is used in X-ray detectors, in the development of the cores for the optical fibers, in the IR-laser techniques for windows of the CO<sub>2</sub> lasers, etc. ZnS is used as a suitable material for the phosphors and for the semiconductor laser technology, etc. The LOD procedure indicates some advantage of the modified properties of such materials. Why? It is connected with the fact that the refractive index of the CNTs is so small and close to 1.1, but the Young modulus is so large and it is placed in the range of some teraPascals. Thus, the Fresnel losses can be decreased, the transparency can be increased, and the mechanical parameters can be improved.

It should be noticed that in order to study the structuration process influence on the physical and the chemical characteristics of the ZnSe and ZnS materials, the substrates with the polished surfaces have been used. The photos of the ZnSe and the ZnS samples studied are presented in Figure 2. It is worth noting that the ring is visible on the ZnS sample in Figure 2b, which was obtained when testing this sample for an abrasion to determine the mechanical strength, which will be discussed later.



**Figure 2.** Photos of the ZnSe (a) and ZnS (b) samples studied in the current research.

Some change of the spectral characteristics of the ZnSe and the ZnS substrate in the range of 1,4 microns to 2,4 microns is shown in Figure 3. The image shows the influence of the CNTs structuration on the spectral parameters. Figure 3a (curve 1) presents the transmission of the pure ZnSe substrate on the wavelength range indicated above. Figure 3a (curve 2 and curve 3) shows the spectral characteristics after the treatment of the ZnSe surface from one side (Figure 3a; curve 2) and from both sides (Figure 3a; curve 3), respectively. The change of the spectral parameters for the pure ZnS and for the ZnS with one side treated by the CNTs is presented in Figure 3b. The green curve (lower one) shows the transmittance for the pure substrate; the blue curve (upper one) presents the transmittance for the ZnS covered with the CNTs. It is important that the surface treatment of samples with the CNTs can increase the transparency of both materials. It can be coincided with the fact that the CNTs refractive index is close to 1.1 [21,22], which is less than the refractive index of the ZnSe or ZnS materials; thus, the Fresnel losses can be decreased dramatically, which can predict the increase in the transparency.



**Figure 3.** The ZnSe (a) and ZnS (b) transmittance in the near-IR-range.

The mechanical properties of the studied materials were investigated by two methods. Experiments were carried out to establish the microhardness of the nanostructured samples as well as to measure the comparative abrasion strength.

The microhardness improvement can be shown in the data presented in Table 1 for the ZnSe and ZnS structures. It was found that an implantation could increase the microhardness of the material up to 5% and 6.7%, respectively. Thus, the same tendency of the microhardness increasing via the CNTs covering by the LOD technique has been obtained for the ZnS and ZnSe substrates.

**Table 1.** The comparative data of the ZnSe and ZnS microhardness change, when an indenter was 20 g.

Material Studied	Middle Value of the Microhardness, Pa $\times 10^9$
Pure ZnSe	0.1118
ZnSe structured with CNTs	0.1175
Pure ZnS	0.8589
ZnS structured with CNTs	0.91675

Moreover, the surface mechanical hardness (abrasive strength) for the ZnS and ZnSe materials has been established. The data are shown in Table 2. It should be noticed that the abrasion strength was compared with the abrasion of the glass K8 (crown glass), on which, with an indenter of 100 g, 3000 revolutions can be reached until a distinct ring appears. That is, with such a standard, namely crown glass K8, zero strength of the glass is achieved. Analyzing the data from Table 2, one can testify that the tendency to increase not only the microhardness but also the surface strength can be found for the ZnS and ZnSe materials with good advantage.

**Table 2.** The comparative data of the ZnS and ZnSe surface hardness when an indenter was 100 g.

Material Studied	The Number of Revolutions on the Abrasion Surface before the Appearance of a Distinct Ring
Pure ZnS	100–120
ZnS structured with CNTs	200–220
Pure ZnSe	420
ZnSe structured with CNTs	600

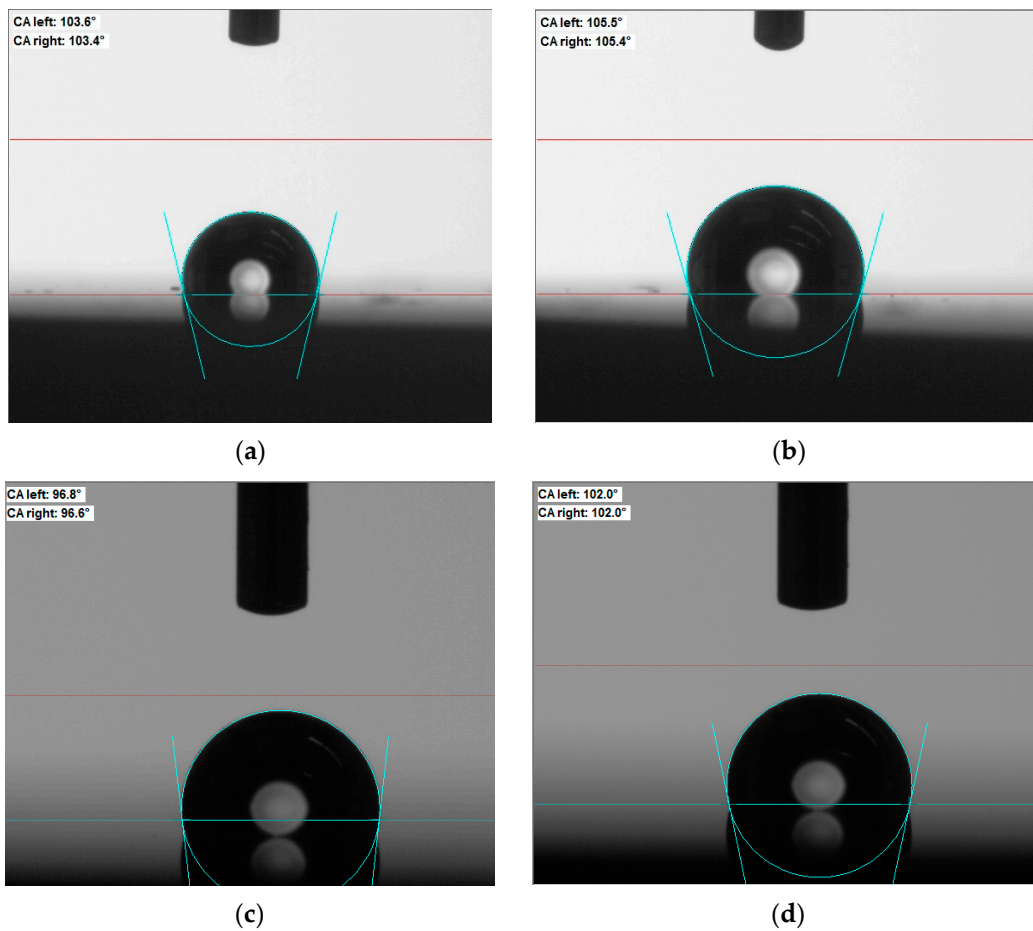
It is worth paying attention to the fact that different methods for determining the mechanical strength for the semiconductor materials based on the ZnS and ZnSe systems are not always the same for both. Different methods are more preferable for each of the materials. However, the general tendency of the mechanical strength increasing is maintained always and consistently.

Furthermore, for the ZnS and ZnSe materials, the wetting angle before and after the CNTs deposition has been established. The data of the wetting angle change are shown in Figure 4. When evaluating the averaging by the wetting angle, a sample was taken from the measurements of a batch of samples in the amount of 10 pieces.

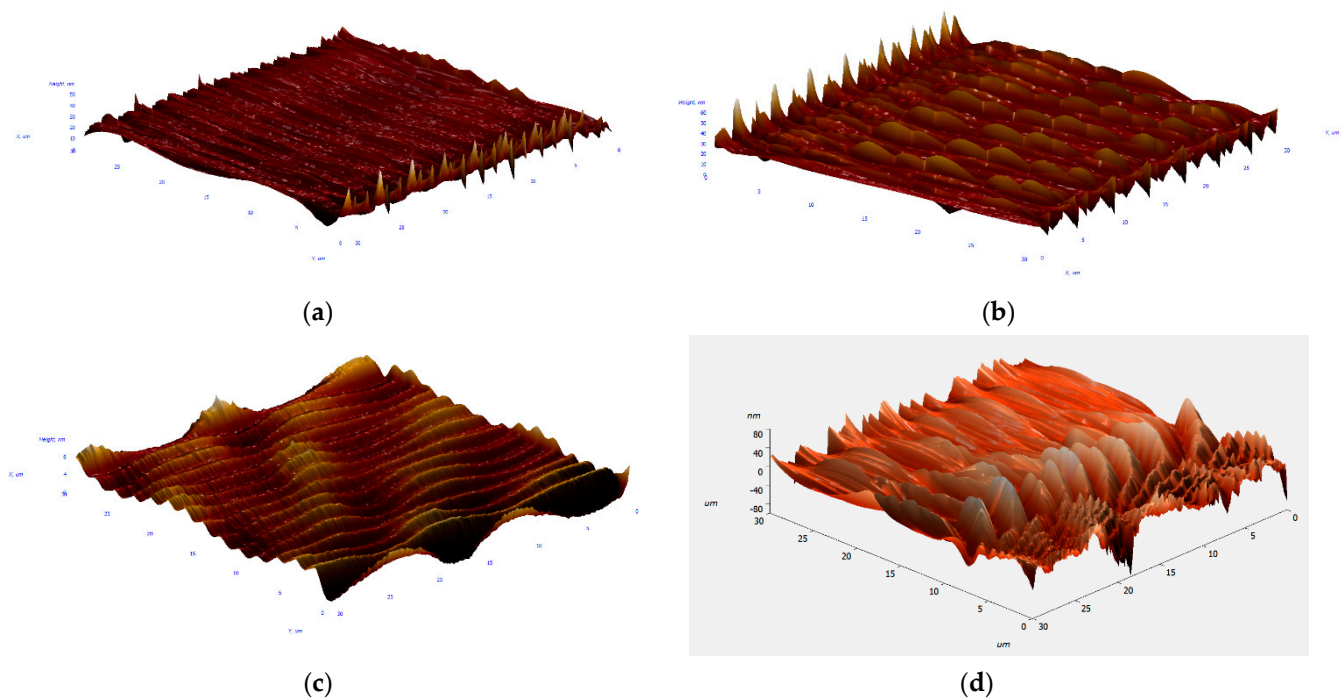
One can see the slight change of the wetting angle for the ZnS (Figure 4a,b) and a better increase in the wetting angle for the ZnSe structure after its structuration by the CNTs (Figure 4c,d).

In addition, in order to support the matrix ZnS and ZnSe materials' relief, modification of the AFM images have been made. The data are shown in Figure 5. One can see that the surface relief shown for the pure ZnS and ZnSe materials (Figure 5a,c) is absolutely different from the one that presented for the nanostructured surfaces (Figure 5b,d). Moreover, since the CNTs can be considered as donor–acceptor systems, the formation of the globules at the structured surfaces can be found.



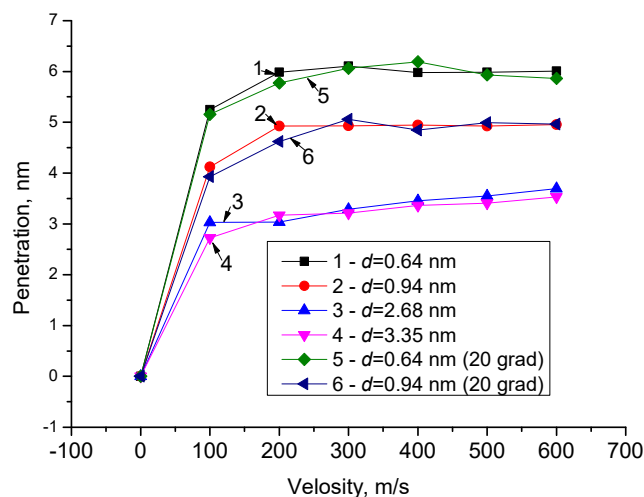


**Figure 4.** The wetting angle for the ZnS surface, pure (a) and with CNTs treatment (b). The wetting angle for the ZnSe surface, pure (c) and with CNTs treatment (d).



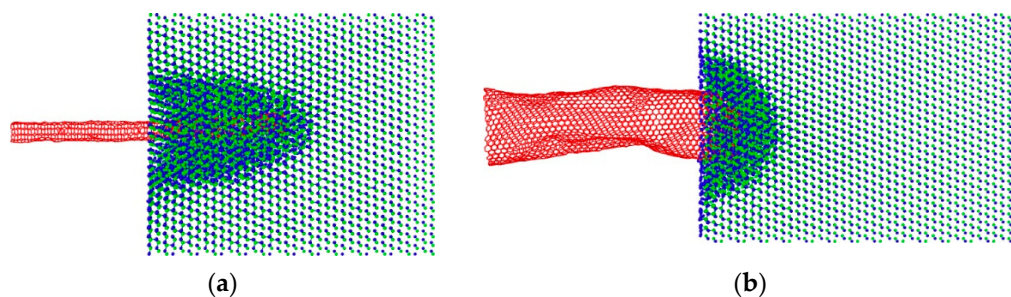
**Figure 5.** The AFM images of the pure (a) and the structured (b) ZnS surfaces; the AFM images of the pure (c) and structured (d) ZnSe surfaces.

Figure 6 shows the results of the MD simulations carried out. We calculated the dependence of the penetration depth of the CNT into the ZnS surface on the CNT diameter and its velocity and an inclination angle. The nanotube diameter was varied from 0.64 to 3.35 nm.



**Figure 6.** The dependence of the penetration depth of CNTs into ZnS surface on the CNT velocity and its diameter.

It can be seen that the CNT speed and their diameter as well as the angle of inclination on the substrate affects the final values of the penetration depth of the nanoobject into the ZnS surface. The qualitative representation of the process of the penetration of the CNTs with diameters of 0.64 nm (Figure 7a) and 2.68 nm (Figure 7b) into the ZnS surface layers with an initial velocity of 100 m/s is shown. It was found that the CNT with the smaller diameter penetrates more deeply than the CNTs with the wider diameter at the same initial velocity, which reflects its higher stiffness [37]. Figure 6 shows the process at the CNTs speed of 100 m/s.



**Figure 7.** The qualitative representation of the CNT penetration with the diameter of 0.64 nm (a) and 2.68 nm (b) into the ZnS surface.

We can plan to make the analogous simulation for the ZnSe materials and will show the results in the future publications.

Thus, the experimental results partially can be added by this simulation; it supports the fact of the effective application of the LOD technique in order to improve the basic properties of such materials with good advantage.

#### 4. Conclusions

Analyzing the obtained and discussed data, the following conclusions should be drawn.

We have compared the properties of pure ZnS and ZnSe materials with those obtained after the modification procedure by the LOD method.

Structuration of the inorganic semiconducting surfaces (based on ZnS and ZnSe) by the CNTs shows the promising way of the surface modification with the aim of their transparency increase. The stronger increasing was observed in the case of treating both sides of the ZnS and ZnSe surfaces. This is due to the low refractive index of the CNTs, which allows reducing the loss of the reflection along the Fresnel law. The structuration of the ZnS and ZnSe surfaces shows the slight increase in the microhardness and the wetting angle. It can be connected with the large value of the Young's module of the CNTs. The formation of the possible link between the carbon atoms and the surface materials permits increasing the hardness of the matrix materials as well. The laser-oriented deposition method can be applied with good advantage in order to improve the properties of the semiconductor materials. The obtained experimental results are partially supported by the molecular dynamic simulations.

It should be noted that all results are repeatedly checked with a multiplicity of the checks once a month. The error is plus or minus 0.5% and less. Moreover, all results of the modified ZnS and ZnSe have testified better data than shown, for example, in the classical books [38,39] for the pure materials.

Established data can show the promising route of the modification of the semiconductors surface with the purpose to form the structured materials with the desired optical properties which make them suitable for the applications as elements of optoelectronics, solar energy, gas storage systems, information technology, displays, and biomedicine. The knowledge accumulated can be used in the education process and for the practices as well.

For the future study, it will be useful to obtain and present the electronic microscopy images; it will be considered for the ZnS and ZnSe structures as well as other semiconducting materials.

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**Institutional Review Board Statement:** This work was carried out as an initiative. Consequently, it did not require any approval and conclusion from the Institute.

**Informed Consent Statement:** Consent to work; of course, it was obtained from all participants in this study.

**Data Availability Statement:** Using these primary materials of the article, as well as taking into account earlier developments on other materials, a patent will be created, as well as a message will be published in the media, for example, at LETI University, since the results are useful for teaching students.

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