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Nanostructured lithium fluoride in X-ray spectroscopy

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Abstract: Due to the importance of conducting materials science research according to Critical Technologies of the Russian Federation and taking into account the demand for lithium fluoride-based matrices for UV and IR spectroscopy, laser technology and biomedicine, the paper highlights the advantages and prospects for the process of structuring the surface of the LiF matrix material with nanoobjects. Spectral characteristics (changes in transmission and reflection), mechanical parameters (microhardness), as well as the wetting angle of the lithium fluoride LiF surface modified with carbon nanotubes are considered; in comparison with those data for pure LiF crystals. The innovative laser-oriented deposition (LOD) technique and additional electric field varied in the range of 100–600 V·cm^{-1} are applied to structure the surface of the materials and deposit nanotubes in the vertical position. An extensive package of experimental results obtained is quite well confirmed by quantum chemical modeling.

Keywords: lithium fluoride; carbon nanotubes; modified surfaces; coatings; laser-oriented deposition technique; spectra; microhardness; wetting angle.

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Наноструктурированный фтористый литий в рентгеновской спектроскопии

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Аннотация: В силу важности проведения материаловедческих исследований по критическим технологиям РФ, учитывая большой спрос в матрицах на основе фторида лития для УФ- и ИК-спектроскопии, лазерной техники и биомедицины, выделен аспект на преимущества и перспективы процесса структурирования поверхности матричного материала LiF нанообъектами. Рассмотрены спектральные характеристики (изменение пропускания и отражения), механические параметры (микротвердость), а также угол смачивания поверхности фторида лития, модифицированной углеродными нанотрубками, в сравнении с таковыми данными для чистых кристаллов LiF. Для структурирования поверхности материалов применяется инновационный метод лазерного ориентированного осаждения (Laser Oriented Deposition – LOD) и дополнительное электрическое поле, варьируемое в диапазоне напряженностей 100…600 В·см$^{-1}$, что позволяет осаждать нанотрубки вертикально к поверхности изучаемого материала. Обширный пакет экспериментальных полученных результатов подтверждается квантово-химическим моделированием.

Ключевые слова: фторид лития; углеродные нанотрубки; модифицированные поверхности; покрытия; метод лазерно-ориентированного осаждения; спектры; микротвердость; угол смачивания.

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1. Introduction

Using known physical principles and approaches to create nanoparticles and nanostructures with laser technologies [1], options for changing the morphology and forming the structure of structured LiF, which is characterized by an array of periodic parameters, are shown. Lithium fluoride (LiF) is a widely used matrix for X-ray spectroscopy materials and laser technology. These materials are widely used in laboratory research and in industry. Therefore, modeling of lithium fluoride properties under different methods of external action, both on its volume and on the surface, is relevant and in demand. The considered crystals of lithium fluoride from fluorides of alkali and alkaline earth materials have the highest transparency in the UV region of the spectrum, starting from wavelengths of ~110 nm. It is assumed that this is due to the inclusion of the lightest of the alkali and halide elements in its composition [2–4]. LiF is a widely used material both for UV and IR spectroscopy and laser technology, as well as for X-ray spectroscopy [5–9]. If lithium fluoride is considered as a material for laser technology (a matrix for a passive laser shutter), it is necessary to ensure its high mechanical and laser strength. In X-ray spectroscopy, the angular position of a crystal is specified depending on the wavelength to be extracted from the spectrum. In X-ray spectrometers, mainly focusing monochromators with bent analyzer crystals are used, each adjusted by the manufacturer to a certain wavelength and thereby tuned to a certain element. Spectral decomposition schemes are used. Two main requirements are imposed on the analyzer crystal: it must have a high luminosity and good resolution. These qualities largely depend on the wavelength region in which the crystal is used. Crystals are composed of periodically arranged atoms (molecules) that make up the crystal lattice. In this arrangement of particles, there are many planes of different directions through which the nodes of the crystal lattice (atoms, molecules) pass. These planes are called lattice planes. They are equidistant from each other at a certain distance, called the interplanar distance *d*. For the long-wave region (K_α are lines of elements from chlorine to oxygen), crystals with a large interplanar distance *d* are used, and for the short-wave region – with a small distance *d*. The resolution is the higher, the smaller *d*. Ideal analyzers are LiF single crystals with a unit lattice parameter of ~0.40279 nm.

The resolution and luminosity of X-ray wave spectrometers are determined, first of all, by X-ray optical parameters of monochromator crystals used in them. That is why, due to the high reflectivity in the X-ray range, lithium fluorides (LiF) are used as single crystals [10–12]. Moreover, lithium fluoride can be chosen as a good model matrix for performing analytical and quantum chemical calculations during surface modification, which is useful both for laboratory research and for industry. Recently, carbon nanotubes (CNTs) with a high Young’s modulus and a low refractive index at the level of 1.1 have become such nanostructures deposited on the surface of materials and significantly changing properties of the matrices [13–19].

There are works devoted to atomic modeling at the interface between carbon nanostructures and LiF. For example, in publications [20–22], the interaction of lithium with fullerene was rather actively modeled by quantum chemical methods. In [20], a lithium atom was placed strictly above one of the six-membered rings in fullerene. In calculations, as a result of partial charge transfer from Li atoms to fullerene C_{60}, a fulleride anion was formed. The interaction energy between fullerene and lithium, calculated by the B3LYP method, is rather high (1.52 eV). The energy value shows that the formation of a bond between lithium and fullerene is much more favorable than the formation of lithium clusters around C_{60}. In this case, the distance from Li to C_{60} is ~2.3 Å, which is comparable with the distances between fullerene molecules in fullerite (6.5–10,0 Å) and with the sizes of tetrahedral and octahedral cavities (2.210 and 4.210 Å, respectively). This allows us to hope for the possibility of lithium fulleride formation.

The interaction of lithium with chair-shaped nanoribbons and two-dimensional graphene is much lower energetically (1.70 and 1.55 eV, respectively, in the LSDA calculation and 1.04 and 1.20 eV in the PBE calculation) than with zigzag nanoribbons (binding energy at the edges of nanotubes is 2.27 – LSDA and 1.70 eV – PBE). When the adsorption position is shifted from the edges to the center of the zigzag nanoribbon, the binding energy decreases. It is assumed that narrow graphene nanoribbons will be an ideal option for achieving the adsorption of lithium ions with a high concentration [23].

X-ray devices need to test the interaction of lithium with single-walled carbon nanotubes, which are suitable for coating medical X-ray equipment. Single-walled carbon nanotubes (SWNTs) belong to a class of carbon containing materials with excellent physicochemical, thermomechanical and electrochemical properties: a single-walled carbon nanotube with chirality (7,6), carbon base ≥ 90 % and directly pure carbon nanotubes ≥ 77 % is a suitable material for surface structuring of optoelectronic materials. This material can be used in various areas of sustainable energy such as solar cells, photocatalysis, thin film conductors, field-effect transistors (FETs), biosensors, gas sensors, supercapacitors and nanomechanical resonators.

All of the above indicates the possibility of creating composite materials based on structuring using carbon nanotubes with a higher transmission and microhardness of modified lithium fluoride than in existing analyzer crystals in X-ray spectrometers. In this work, the search for ways to improve the main properties of the LiF + CNT composite is continued: experimental studies and quantum chemical modeling are carried out in order to develop new approaches to modifying the properties of the LiF + CNT composite.

2. Materials and Methods

To change the optoelectronic properties of materials, lithium fluoride substrates (Alkor Technologies, St. Petersburg) 5 mm thick and 35 mm in diameter and CNT #704121 with a diameter in the range from 0.7 to 1.1 nm, purchased from the company “Aldrich Co”, are used. Particular emphasis is placed on changing the basic properties of the LiF material during structuring of its surface. To change the properties of the selected material by depositing CNTs, a CO_2 laser was used at a wavelength of 10.6 micrometers with a power of 30 W. Additionally, for orientational deposition (vertically deposited CNTs) by the laser oriented deposition (LOD) method, an electrical circuit was used that allows varying the electric field strength in the range of 100–600 $V \cdot cm^{-1}$. The block diagram and built-in electrical circuit for surface modification of optoelectronic materials of various compositions, including lithium fluoride, are partially shown in publications [24–27].

For spectral measurements, an SF-26 visible spectrophotometer, an FSM-1202 IR Fourier spectrometer, a Lambda 1050 spectrophotometer (Perkin Elmer), with a 150 mm analytical module InGaAs Int. Sphere – integrating sphere, were used. To study the surface roughness, a Solver Next atomic force microscope (Zelenograd, Moscow region) was used. The wetting angle was determined using an OSA 15 EC device (LabTech Co., Saint-Petersburg-Moscow, Russia) using the sessile drop method. Microhardness was measured on a PMT-3M device (JSC LOMO, St. Petersburg).

Quantum-chemical calculations were carried out using the Gaussian program by the DFT method in the 6-31G(d,p) basis [28, 29].

3. Results and Discussion

The main experimental results obtained are shown in Figs. 1–3.

Due to the fact that the refractive index of CNTs is close to 1.1, and a similar refractive parameter of lithium fluoride is: $n = 1.77$ (at a wavelength of 112.7 nm); 1.3978 (at 420 nm); 1.3915 (at 620 nm); 1.2912 (at 6200 nm), it is quite logical to establish an increase in transmission associated with a decrease in Fresnel reflection loss. Fig. 2 shows atomic force analysis data for the original and modified lithium fluoride surfaces.

It can be seen that structuring of the lithium fluoride surface occurs (the relief changes, a “forest of nanotubes” is visible), and the height of the protrusions varies. Measurements were made on a batch of samples in the amount of 10 pieces, which made it possible to find such changes.

Fig. 3 shows the wetting angle data for the surface of unstructured and structured lithium fluoride.

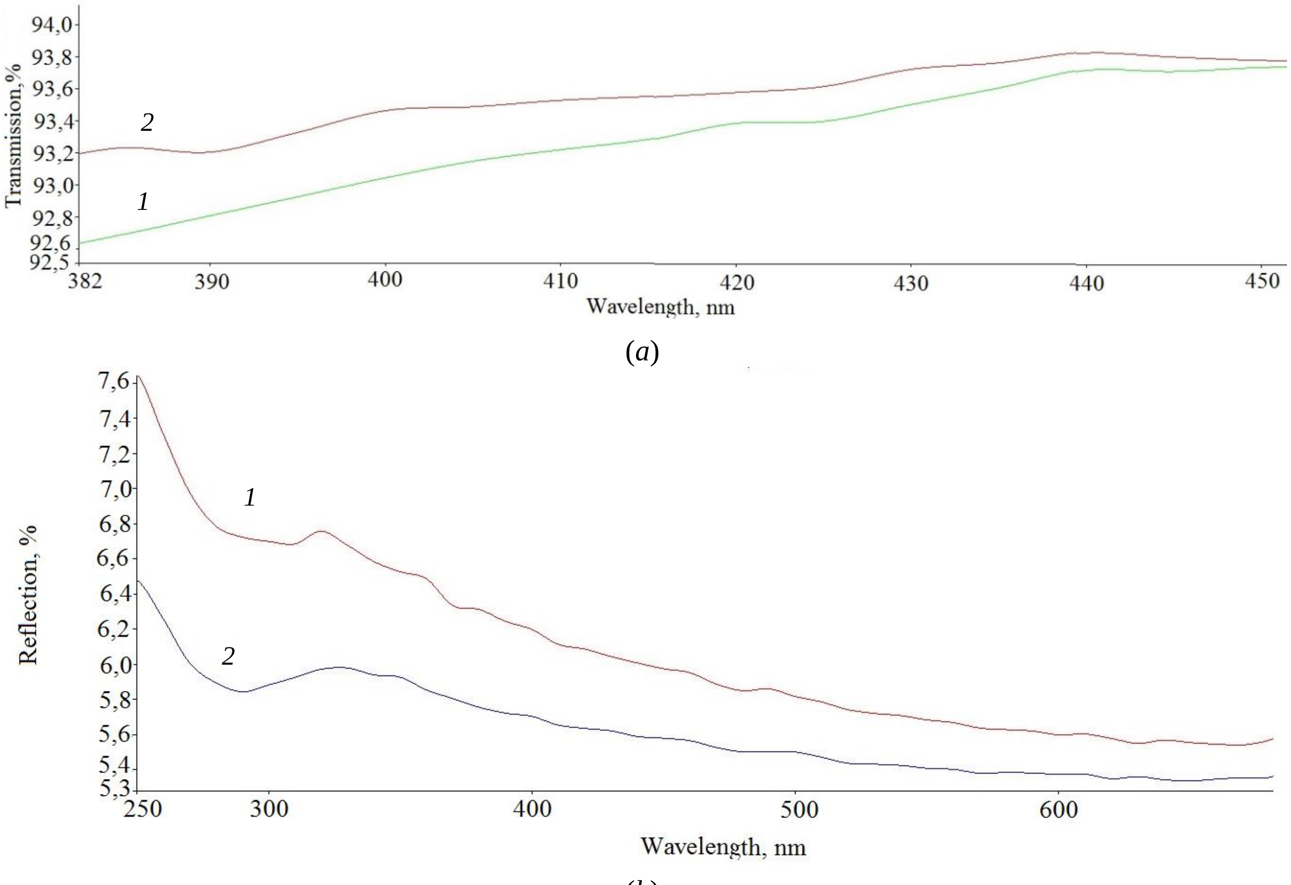
It has been established that the wetting angle increases from 97.5–97.8 to 107.3–107.5 degrees, i.e. by almost 10 degrees, according to the method given in the publication [30].

The change in the spectral parameters, the type of AFM images, and the parameters of the wetting angle give a complete picture of the data and do not contradict the established increase in microhardness, which is given in Table 1.

Thus, all experimental dependences obtained in the study of the vertical deposition effect of CNTs on the lithium fluoride surface give an experimentally obtained consistent picture of the change in properties during surface structuring, which makes it possible to suggest the presence of a chemical bond between CNTs and near-surface atoms of the matrix based on lithium fluoride.

To support the experimental data and the model of covalent attachment of CNTs to the lithium fluoride surface (or contradiction to it), quantum chemical modeling was carried out.

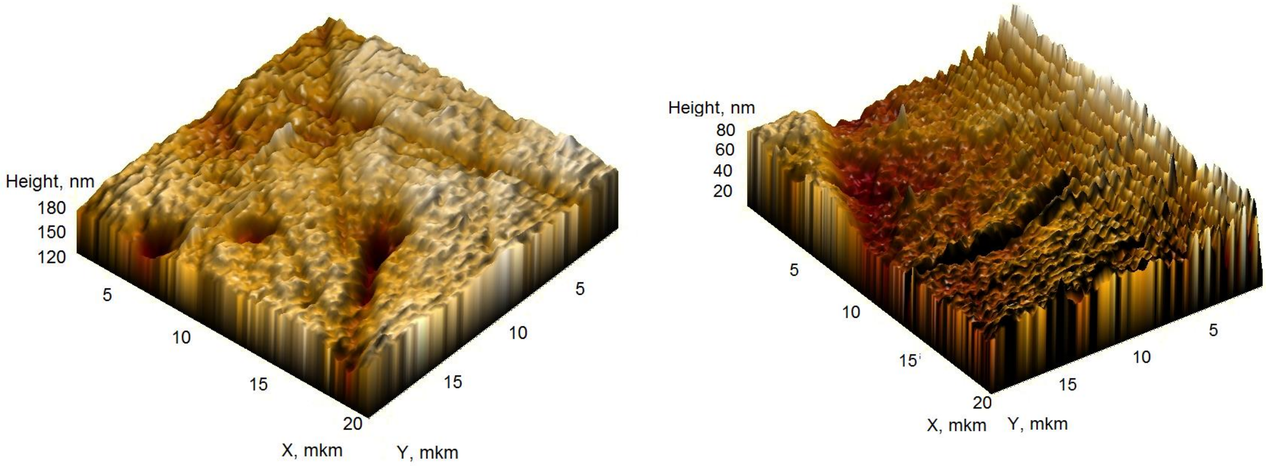
It should be noted that from quantum-chemical modeling the fact of organizing a new system can be evidenced through the connection and formation of new levels [31]. To understand the influence of CNTs on the LiF substrate, an analysis of the electronic structure was carried out, in particular, the analysis of the density of states and redistribution of the electron density at the interface between the substrate (LiF) and CNTs. A 1.2 nm long CNT was used to describe the effect of the tube on the surface properties of the



(*a*)

(*b*)

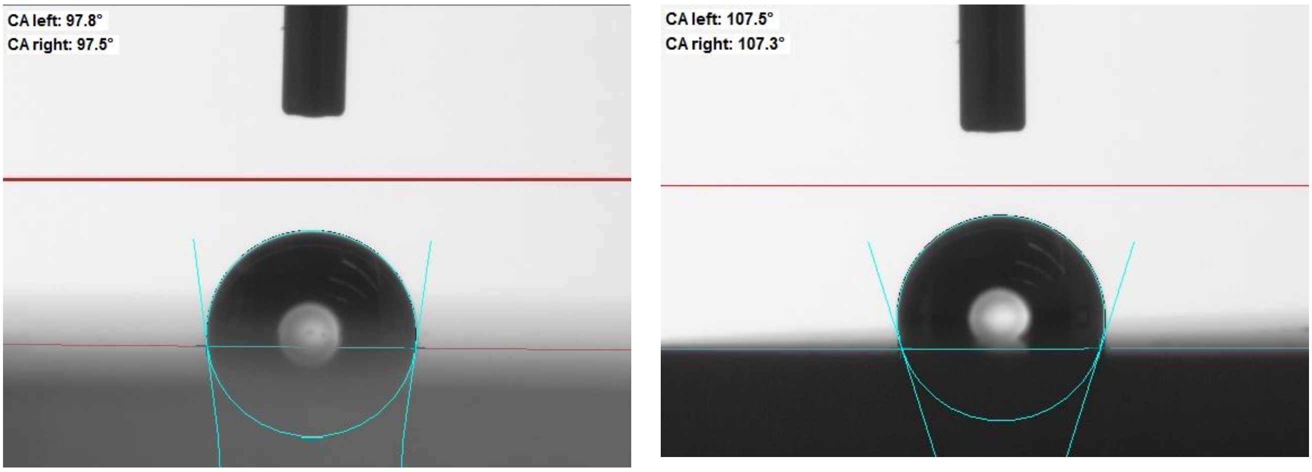
Fig. 1. Transmission spectra in the range of 380–450 (*a*) and reflection spectra in the range of 250–700 nm (*b*) for LiF before the deposition of carbon nanotubes (*1*) and after the deposition of CNTs (*2*)



(*a*)

(*b*)

Fig. 2. AFM image of the surface of unstructured (*a*) and structured (*b*) LiF



(*a*) (*b*)

Fig. 3. Data on the change in the wetting angle of unstructured (*a*) and structured (*b*) LiF surface

Table 1. Data on the change in LiF microhardness during structuring

Material	Microhardness value, Pa × 10^9	Increase in microhardness, %
Non-structurable lithium fluoride	1.304	~10%
LiF + CNT system	1.442	

LiF/CNT system. This length is sufficient to account for these effects, and it is a compromise due to the number of atoms in the unit cell under consideration. The upper end of the nanotube was passivated with hydrogen atoms.

Changes in electronic properties caused by the presence of deposited CNTs were calculated. The electron density distribution was constructed and the density of electronic states was calculated. It has been found that the presence of CNTs on the surface of LiF leads to a charge redistribution directly at the interface, which will undoubtedly lead to a change in the electronic properties. Using the electron density functional theory, a study was made to determine the influence of carbon nanotubes deposited on the surface of lithium fluoride (LiF) on its electronic properties. Fig. 4 shows the atomic structure of the CNT/LiF interface under study. The LiF (110) surface was chosen for consideration due to the fact that both types of atoms (Li and F) were present on this type of surface. Next, CNTs were deposited onto the LiF surface (Fig. 4). Due to the large number of atoms in the unit cell, the CNT model consisted of a small cluster of CNTs, the upper end of which was passivated by hydrogen atoms. As a result, after deposition the main changes in the atomic structure occur directly at the interface, the chosen CNT length is sufficient to qualitatively describe the change in the electronic properties. The system under consideration consisted of 14 lithium atoms, 13 fluorine atoms, as well as 18 carbon and 12 hydrogen atoms that make up the CNT cluster.

The results of the atomic structure optimization showed that the addition of CNTs did not lead to significant structural measurements at the interface. The distance between the lower carbon atoms of the CNT and the LiF surface was about 1.14 Å.

A study of the change in electronic properties was carried out in the Gaussian program, using the example of a change in the density of electronic states (DOS), and the distributions of electron density were built (Fig. 5). Fig. 5 shows a map of the electron density distribution in a LiF crystal structured by a small cluster of CNTs, the upper end of which was passivated by hydrogen atoms in the [110] plane. In the [110] plane, we have a pronounced localization of the electron density between the nearest atoms, which indicates a chemical bond. As can be seen from the map, the shells of the F ions overlap with each other at an electron density value of 0.15 e/Å3. Such overlap is not observed for Li cations. The atomic radii determined from the map were 1.31 Å for F and 0.75 Å for Li, which is in good agreement with the literature data [32–34].

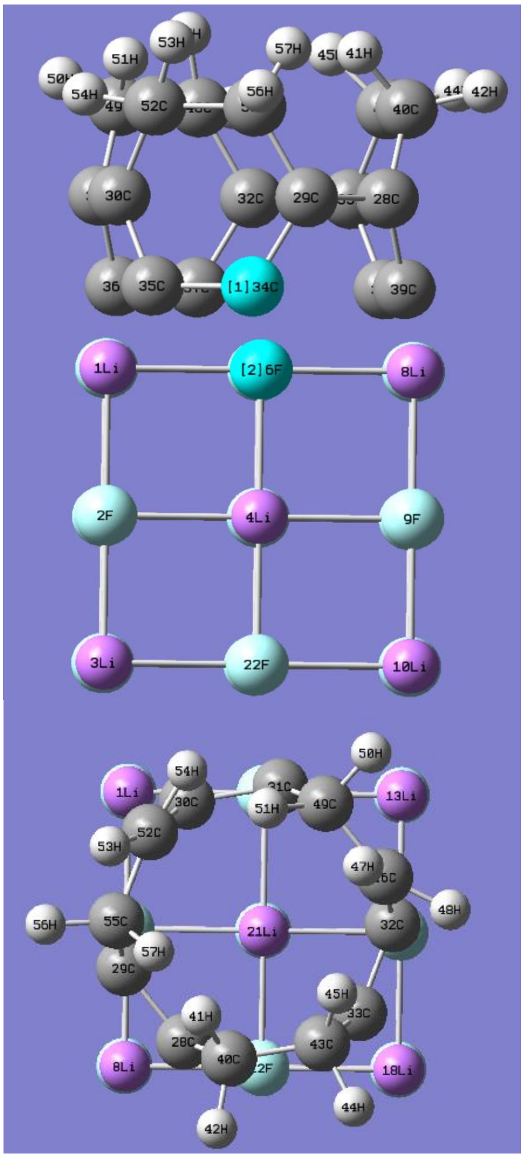


Fig. 4. Atomic structure of the considered interface

Thus, to confirm the experimental data, a study of the change in electronic properties was carried out in the Gaussian program, using the example of the change in the DOS, and patterns of electron density distribution were also built. Changes in electronic properties caused by the presence of deposited CNTs were calculated. The electron density distribution was constructed and the density of electronic states was calculated. It has been found that the presence of CNTs on the surface of LiF leads to a charge redistribution directly at the interface, which will undoubtedly lead to a change in the electronic properties.

When structuring fluorides with carbon nanotubes, the range of applications for X-ray spectrometers was expanded, with the prospect of varying the interplanar distance *d* in the case of LiF, in X-ray spectroscopy, because single crystals possessed such a perfect [35, 36] crystal structure that it would be possible to use them in the production of X-ray devices in manufacturing firms. The results obtained so far [27] indicate that due to the wide spectral range, availability and ease of use, the nanostructured LiF crystal is improved in terms of spectral transmission compared to the starting material, and atomic modeling at the interface of CNTs and LiF shows changes in electronic properties (red valence band shift) of LiF after CNT deposition, thus confirming the evidence of chemical bond. This bond is confirmed in this paper as well, since we have a pronounced localization of the electron density between the nearest atoms in the [110] plane. Thus, the nanostructured LiF material can be used for an analyzer crystal in X-ray spectral devices.

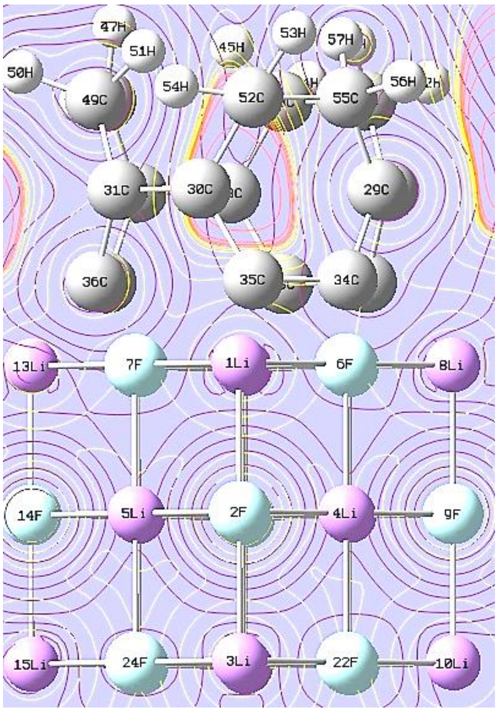


Fig. 5. Map of electron density distribution in a LiF crystal structured by a small cluster of CNTs, the upper end of which was passivated by hydrogen atoms in the [110] plane

4. Conclusions

Analyzing the obtained experimental data, we can say: the transmission is increased, the reflection of structured lithium fluoride is reduced; its microhardness and surface wetting angle are increased. The results of quantum chemical modeling suggest the presence of a weak chemical bond between the carbon atoms from the carbon nanotube and near-surface lithium fluoride atoms.

Thus:

1) LiF materials can be considered as a promising model matrix for obtaining a correlation between changes in the spectral, mechanical, and wetting properties during nanostructuring of their surfaces by laser deposition of nanoobjects.

2) The tendency to form bonds between carbon atoms and near-surface atoms of the model material was confirmed experimentally and theoretically by extended consideration of the LiF matrix using a quantum mechanical approach.

3) Transmission, mechanical and wetting characteristics of LiF-based materials can be improved, which expands the scope of such optical materials in X-ray spectroscopy, as well as in medicine.

4) The presented data make it possible to expand the range of functional materials, the main properties of which can be successfully varied and optimized by structuring their surfaces with carbon nanotubes.

5) The results obtained can be used in the educational process, since the main changes in parameters can be visualized and supported using optoelectronic devices.

The results obtained expand our material science knowledge and can also be practically useful in the development of X-ray spectrometers, passive laser shutters, output windows of UV lamps, etc. In general, structuring of lithium fluoride with carbon nanotubes significantly expands its application in optoelectronics as a whole.

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7. Conflict of interests

The authors declare no conflict of interest.

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