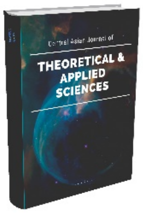

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THEORETICAL METHOD FOR THE ANALYSIS OF MICRO AND NANOSTRUCTURES OF THIN-FILM COATINGS USING THE PRINCIPLES OF QUANTUM MECHANICS

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Abstract. *The purpose of this theoretical study is to reduce the number of experiments and thereby reduce the development time for thin-layer (thin-film) and planar technologies by simulating the processes occurring at the micro and nanoscale under the influence of radiation.*

Keywords. *thin-layer coatings, thin-film coatings, interaction of radiation with matter*

Introduction. It is difficult to imagine the modern world without thin-layer and planar technologies. These technologies are found almost everywhere - antireflection optics, which are used in most optical devices, ranging from household devices such as mobile phones (lenses), binoculars and ending with professional equipment (for example, devices for professional photography and video shooting, gas sensors, etc.) [one]. On the basis of thin-layer (thin-film) technologies, modern technology for the production of microcircuits is based. Since the technology is in great demand, all over the world they pay great attention to the development of new and improvement of existing technologies in the field of thin-film technologies [2]. Thin-film technologies are referred to as nanotechnologies [3].

Thin films

Thin films are layers of different materials with a thickness from fractions of a nanometer to several micrometers. As an illustrative example from everyday life, we can cite rainbow-colored stains of gasoline or oil stains on the surface of the water.

A characteristic feature of thin layers of a substance is that they can have properties that are very different from the properties of the same substance in an object of greater thickness. The reason for this is the emergence of quantum effects.

Artificially created thin layers are used in electronics, mechanics and optics.

Thin ceramic layers are widely used in mechanical products. The high hardness and inertness of thin-layer ceramic coatings provide protection against corrosion, oxidation and wear.

In the form of thin films, materials have useful properties that can be used in practice - as a single layer or as part of a thin-layer structure.

In hard drives, a series of thin layers of non-metallic subcoats are applied to an aluminum or glass plate to help ensure the correct crystallographic orientation and grain size of the last, magnetic layer that stores the bits of information. In addition, a thin protective layer of carbon and a very thin layer of polymer are deposited on the magnetic layer.

In electronics, thin layers of semiconductors, insulators and metals are the basis for planar technology and, in particular, for the manufacture of integrated circuits.

In the production of solar panels, thin layers are also used. A p-n junction with a thickness of several microns is created, on polycrystalline silicon substrates with a thickness of 0.25–0.30 mm, and anti-reflective coatings of nanoscale thickness are applied, which increase the amount of absorbed light.

In optics, thin layers are used in the form of optical and light coatings for the manufacture of optical elements with certain properties - filters, mirrors, beam splitters. The most common in everyday life are anti-reflective (anti-reflective, anti-reflective) coatings on the lenses of glasses, thanks to which stray light reflection can be reduced to almost zero [4], In general, thin layers can be classified according to their purpose: for use in electronics and optics, for coatings that provide chemical and mechanical resistance. Another type of classification can be made according to the type of material that makes up the thin layer - organic and inorganic. Most technologies for applying thin layers are vacuum or so-called "wet" methods [5, 6].

Nanotechnology and quantum objects

Nanotechnology - technologies that use the properties of materials less than 1 micrometer in size in one, two or three spatial coordinates (1 μm = 10–6 meters; 1 nm = 10–9 meters). The nanoscale of an object in itself can cause the appearance of new properties that are very different from the properties of the same substance in an object of greater thickness.

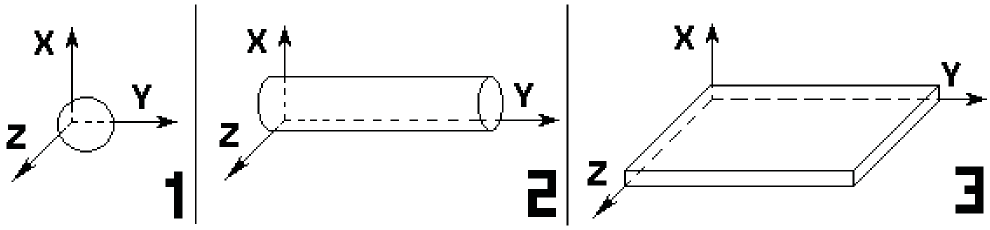

Fig. 1: 1 - quantum dot model; 2 - model of a quantum thread; 3 - model of the quantum plane (picture by the author)

For example, a cubic nanometer of silicon has properties different from a 100x100x100mm silicon cube. The difference in the properties of nanoscale and macroscopic objects is explained by the presence of so-called quantum effects. Quantum effects appear if the dimensions of an object are commensurate (quantum dimensions) with the wavelength (de Broglie) or the size of particles (electrons, photons, etc.) that move inside the object or interact with it. Thus, the nanoscale of objects imposes additional restrictions on the motion of particles, which is the reason for the appearance of new properties.

The quantum properties of an object can manifest themselves in three spatial dimensions (X, Y, Z axes). Such objects are called "quantum dots". Quantum dots are, for example, CdSe nanoparticles, which are used in some LED models and in the production of screens (QLED technology). If an object is nanoscale in two spatial dimensions, it is called a "quantum filament." Carbon nanotubes and a polyethylene molecule can be cited as examples of quantum filaments, since a single polyethylene molecule is in the form of a filament. If the object has quantum properties in only one direction, then this is the "quantum plane". A good example illustrating the quantum plane is graphene, since it is a plane composed of carbon atoms one atom thick [7].

Research methods

When developing micro and nanotechnologies, primarily thin-film, several main factors are taken into account. The first factor is the operating conditions. If a thin film is enclosed in a microcircuit case, then it is necessary to bear in mind the temperature modes of operation, since some types of thin films can be sensitive to overheating, for example, organic semiconductors based on phthalocyanine. If thin films are supposed to be used as an outer coating, as, for example, in the case of antireflection optics, then it is necessary to take into account possible mechanical damage, the influence of atmospheric moisture, ultraviolet radiation, etc.

The second factor is the chemical composition of the thin films. The choice of the chemical composition is determined both by the ultimate goal of development, which imposes its own limitations, and by the properties of a specific chemical composition. The third factor to consider is the internal structure of the projected pavement. The internal structure of the coating may depend on the chemical composition of the applied substance, the method of application (for example: vacuum evaporation method; solution application methods), the application rate, the temperature of the applied substance or mixture of the applied substances, the temperature of the substrate on which the coating is applied. All of these factors affect the formation of micro and nanostructures of thin-film coatings.

Method for theoretical determination of the properties of thin-film coatings, micro and nanoobjects

To theoretically determine the properties of thin-film coatings and / or the properties of micro and nanoobjects, it is first of all necessary to understand that such structures have a rather complex internal structure. A thin-film coating can be monocrystalline, amorphous, porous, etc., as well as mono or multicomponent. Thus, it is possible to consider a thin-film coating, micro or nano-object as a set of quantum objects, each of which has certain properties. You should also pay special attention to the fact that the properties of quantum objects differ depending not only on their size and type (types of quantum objects: quantum dot, quantum net, quantum plane), but also on whether they are metals, non-metals or semiconductors.

Example 1

Consider a simplified cell model. To create a model, we assume that we have a regular sphere with a diameter of 100 microns, with a wall thickness of 6 microns. Inside the sphere, we have a smaller sphere depicting the nucleus and having a diameter of 6 μm (6000 nm), as well as a thread two meters long and 0.00034 μm (0.34 nm) in diameter, which plays the role of DNA. In order to understand how such a model interacts with radiation with a wavelength λ, we analyze the cell model according to the following scheme:

1. We accept the entire model as a quantum dot with a diameter of 100 microns and analyze its interaction with radiation with a wavelength λ;
2. We accept the model shell as a quantum plane 6 μm thick and analyze its interaction with radiation with a wavelength λ;
3. We accept a DNA model, namely a thread two meters long and 0.00034 μm in diameter as a quantum thread and analyze its interaction with radiation with a wavelength λ;
4. We accept the model of the nucleus as a quantum wheelbarrow with a diameter of 6 microns and analyze its interaction with radiation with a wavelength λ;

Using such a model, one can explain how certain types of radiation damage the DNA of a living cell and do not damage its membrane.

Example 2

Consider a microdroplet of water 50–100 μm in size (50,000–100,000 nm). Microdroplets of water of this size are present almost everywhere in the air. Analysis method:

1. We accept a microdroplet of water of a certain size as a quantum dot and analyze its interaction with radiation with a wavelength λ;

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2. We accept each H2O molecule as a quantum dot and analyze its interaction with radiation with a wavelength λ; Thus, it is possible to explain the ionization of water under the influence of ultraviolet radiation, as well as the disinfection of water under the influence of ultraviolet radiation (in this case, it is necessary to take into account the parameters of microorganisms).

Example 3

Consider a thin layer of carbon in the form of soot deposited on a glass substrate. The deposited soot is a conglomerate of atoms with a shape close to spherical. These conglomerates, connecting with each other, can form vertical "threads". Analysis method:

1. We accept the entire thin-layer coating as a quantum plane and analyze its interaction with radiation with a wavelength λ;
2. We accept spherical carbon conglomerates as a quantum plane; we analyze its interaction with radiation with a wavelength λ;
3. We take "threads" from spherical conglomerates for a quantum thread and analyze its interaction with radiation with a wavelength λ;

Of course, for each specific analysis, the wavelength is chosen, which is of interest to the researcher.

Conclusion

Based on the analysis shown in example 3, conclusions were made about the possible transparency of the carbon coating outside the visible range. It was also suggested that this type of coating may interact with ultraviolet light. This modeling method has already justified itself: two articles have been published [8, 9] (in both cases, according to the author's idea, which is reflected in the text of the publications themselves), which reveal two properties of carbon coatings that were previously unknown. This theoretical study can be useful for both researchers and developers of new technologies.

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