ABSTRACT

Diploma work: 75 pages, 15 figures, 5 tables,38 literare sources.

MODELING CARBON NANOTUBES, DEFECTS STONY WELLS, MEASUREMENT OF YOUNG'S MODULUS.

Carbon nanotubes due to its unique properties (CNT) attract the attention of researchers in various research fields and practical developments. Variety of applications invented for nanotubes impress. For example, that's the use of nanotubes as solid microscopic cores and threads. As the results of experiments, the Young's modulus of single-layer nanotube reaches the order of 1 TPA ÷ 5 TPA, which is much greater than the Young's modulus of steel. Cable for space elevator is another example of use, as the nanotubes theoretically may hold more than one ton... but only in theory. Because pretty long carbon tubes with a thickness of wall up to one atom was not possible to get until now.

Several applications of nanotubes in the computer industry have already been developed. For example, created and tested prototypes of thin flat displays operate on a matrix of nanotubes. But the mechanical properties of nanotubes have a significant influence on the defects of the structure, which are formed in the process of their production.

It is for studying the physical properties of nanotubes of different structures, finding new fields of application of BNT and testing under given conditions, and computer simulation is required.

The purpose of this work is to study the peculiarities of the influence of structural defects on the mechanical properties of carbon nanotubes by means of computer simulation.

In accordance with the aim of the work, the following research tasks are set:

1) To study literature, to familiarize with methods of computer simulation of nanostructures and to prepare an overview of modern literary sources;

2) Master modern mathematical and computer methods and acquire skills to use the ATK-VNL QuantumWise software.

3) Modulate nanostructures with defects.

4) To study the mechanical properties of the models obtained;

5) Analyze the results and form conclusions.

The QuantumWise Atomistix ToolKit software package was chosen as the simulation environment because it has the advantages of visualizing the data received, compatibility with other software for further research of materials, owning the base of empirical potentials, the ability to determine the functionality of the received elements and display the results in a two-dimensional environment, Free Academic License.

A computer simulation of NW with a defect-free structure and a Stone-Wales defect was performed.

The dependence of mechanical properties on the presence of a defect is obtained.

Thus, the resulting result - the Young's module of a carbon nanotube with a Stone-Wells defect and a defect-free nanotube proves that defects strengthen carbon nanotubes. Based on the conducted simulation, more complex calculations can be made for several defects or defects of another type. The proposed models can be used To investigate the destruction of nanotubes in various situations.