ISSN 2224-087X. Електроніка та інформаційні технології. 2022. Випуск 19. С. 26–37
Electronics and information technologies. 2022. Issue 19. P. 26–37

UDC 526:669 DOI: https://doi.org/10.30970/eli.19.2

SIMULATION OF THE TUNNELING CONDUCTIVITY IN REFRACTORY NANOTUBE/DIELECTRIC COMPOSITE SYSTEMS

I. Zhydenko[1,2], H. Klym[2,3]

[1]*Lviv State University of Life Safety*
35 Kleparivska St. UA-79007, Lviv, Ukraine
zhidenkoillya@gmail.com, illia.v.zhydenko@lpnu.ua

[2]*Specialized Computer Systems Department,*
Lviv Polytechnic National University,
12 Bandery St., UA-79013, Lviv, Ukraine
halyna.i.klym@lpnu.ua, klymha@yahoo.com

[3]*Radielectronic and Computer Systems Department,*
Ivan Franko National University of Lviv,
50 Drahomanova St., UA–79005 Lviv, Ukraine
halyna.klym@lnu.edu.ua

An approach to calculating the integral conductivity of a model refractory nanotube/dielectric composite system is considered. The conductivity of a random network of nanotubes formed in a dielectric medium was simulated taking into account the tunneling conductivity between individual nanotubes located in close proximity and taking into account the internal conductivity of the nanotubes. It is established that the "solid core" model can be effectively used to predict the parameters of the manufactured composite, which is an important step towards creating a material with the desired properties. It is shown that the conductivity in the composite system deteriorates at using nanotubes with a larger diameter. This is due to the reduction of the percolation effect for such nanotubes.

Key words: nanocomposite, nanotube, tunneling conductivity, computer simulation.

Introduction. Systems characterized by a network of randomly arranged carbon nanotubes (CNTs) formed in the volume of the matrix are promising refractory materials for modern electronics [1-3]. However, the creation of CNT-based devices for real applications is a complex multi-step process that requires not only complex experimental procedures, but also thoughtful planning [4-6]. Therefore, it is advisable to start the design of a nanocomposite device with numerical calculations. This allows to establish the main characteristics of the system and the influence of the most important parameters of the model (technological parameters of the device under development) on these characteristics.

At forming a network of nanotubes inside a non-conducting matrix, an important phenomenon is percolation (percolation threshold) [7,8], characteristic of this type of stochastic systems [9]. In the theory of percolation, the connection of a very large number of elements is considered, provided that the connection between neighboring elements is completely random. Such systems are crystalline semiconductors with impurities, composites consisting of two materials - a conductor and a dielectric, for example, an insulating polymer and CNT fillers.

The phenomena described by the theory of percolation are classified as critical phenomena characterized by a critical point, after which the properties of the system change radically. The physics of critical phenomena is peculiar and has common features, the most important of which is that near the critical point. The system breaks up into blocks with different properties, while the size of these blocks grows steadily.

Percolation is influenced by a number of different factors, for example, the arrangement of elements [10] or specific features of the base matrix [11]. An issue to be addressed is that the conductivity of the nanotube network within the composite varies with nanotube concentration, alignment and geometric factor. Taking this into account, numerical modeling also allows to evaluate the possibilities of using such structures in sensor devices [4,5,12].

There are different approaches to modeling composite structures with formed networks of nanotubes. These include the use of analytical models to predict the macroscopic properties of nanocomposite [13] and the use of neural networks to simulate the effect of nanotubes on the properties of the base material [14]. Computer experiments showing the effect of CNT agglomeration on the conductivity of composite-based polymer were described in [15,16].

New applications and corresponding numerical models require powerful computing resources. Therefore, one should always look for ways to optimize rough calculations and use high-performance computing systems for computer experiments [17].

Although, as shown above, many works are devoted to simulation of nanocomposites, there are practically no systematic studies that use three-dimensional statistical modeling taking into account the various physical processes of conduction in the junctions of adjacent nanotubes. In this work we present peculiarities of tunneling effect affects the integral conductivity of a nanocomposite system defined as a dielectric matrix randomly filled with CNTs.

Nanocomposite conductivity simulation method. A composite based on CNTs can be represented as a three-dimensional 3D parallelepiped filled with randomly placed conductive nanotubes (Fig. 1).

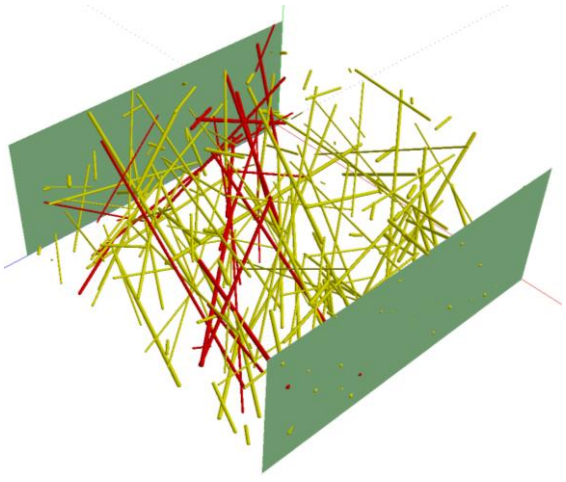

Fig. 1. General view of the modeled system with conductive path between two opposite planes of the parallelepiped.

Such a three-dimensional sample of the composite is connected to the model electric circuit with the help of two electrodes located on its opposite palnes.

Nanotubes can touch each other connecting to each other. Taking into account that the position of these tubes is random, the presence or absence of connection between two particular nanotubes are also random events. The peculiarity of such system is that it is impossible to predict the connections between its individual elements, but for a large collection of such objects. It is possible to calculate the parameters of the system with fairly high accuracy, which directly depend on the presence of connections between nanotubes - the percolation threshold of the system.

The model of the system does not allow the intersection of nanotube volumes and the electrical contact between them exists due to the tunneling effect, which plays an important role in electrical interactions between nanoscale objects.

A nanotube is described as a hollow cylinder with hemispheres at the ends. The geometric axis of such tube starts at point *A* with (x_1, y_1, z_1) coordinates and ends at point *B*(x_2, y_2, z_2). The process of generating and placing nanotubes in space consists of several phases. First, the coordinates of the starting point are defined as [18]:

$$x_1 = rand \times L_x , \tag{1}$$

$$y_1 = rand \times L_y , \tag{2}$$

$$z_1 = rand \times L_z , \tag{3}$$

where *rand* is a random number from the interval [0,1], L_x,L_y,L_z are the dimensions of the parallelepiped. The direction from point *A* is randomly set, which is described by two angles α and β:

$$\alpha = 2\pi \times rand_1 , \tag{4}$$

$$\beta = 2\pi \times rand_2 . \tag{5}$$

Using this direction and the coordinates of the starting point of nanotube, the coordinates of the end point are calculated as:

$$x_2 = x_1 + length \times \cos(\alpha)\cos(\beta) , \tag{6}$$

$$y_2 = y_1 + length \times \sin(\alpha) cos(\beta) , \tag{7}$$

$$z_2 = z_1 + length \times \sin(\beta) . \tag{8}$$

If point A is outside the parallelepiped, then the protruding part of the nanotube is cut-off by one of the planes of parallelepiped. This procedure is performed so that all the tubes fall completely inside the parallelepiped.

Although such model distribution of the filling elements in simulated volume is quite sufficient to satisfactorily describe the experimentally observed percolation threshold. It is important to take into account physically reasonable dispersion and intersection criteria for nanotubes in the simulation volume. The physical contact of any two nanotubes actually means that they are still separated from each other by a small distance dictated by the van der Waals interaction. Therefore, the direct overlapping of tubes or their parts is not implemented in practice, except in the case when the ratio of the length of the tubes to their diameter is sufficiently large. The generally accepted approach in this direction involves the application of the “hardcore” model concept, which prohibits the overlap of the volumes of nanotubes and,

accordingly, should take into account the effect of electron tunneling [18]. Thus, when modeling the behavior of a CNT network in an insulating matrix, it is necessary to take quantum effects into account.

In th mentioned model of solid-state tubes ("hard core" model), it is necessary to ensure that the tubes do not cross each other. For this, immediately after generating the coordinates of a new tube, the minimum distances between the central axes of the newly generated nanotube and the tubes already contained in the system are checked. If this distance is smaller than the diameter of the nanotubes in the system, it means that the tubes intersect. In this case, the newly generated tube is discarded and will not be added to the system. The process of adding new tubes continues until the desired volume concentration of tubes in the system is reached.

Electrical contact between any two nanotubes is said to exist if the shortest distance between them is less than the threshold distance of the tunneling effect. A Union Find algorithm with path weighting and compression was used to find a conducting (percolation) cluster extending between opposite electrodes [19].

To calculate the equivalent electrical conductivity of the nanotube system, we used the model of a random network of resistors. In order to convert a set of interconnected nanotubes, which form the conducting cluster of the system, into a random network of resistors, it is necessary to determine the coordinates of all contact points between the tubes.

To describe the contact between the tubes [20], the concept is shown in Fig. 2. Each point of contact between two connected tubes is represented as a pair of "intersection points": one of them is located on the central axis of the first tube and the other on the axis of the second tube, respectively. At the same time, a pair of "crossing points" placed on the same tube delimits a segment of the nanotube with length l_s through which the current passes between the places of the tube junctions.

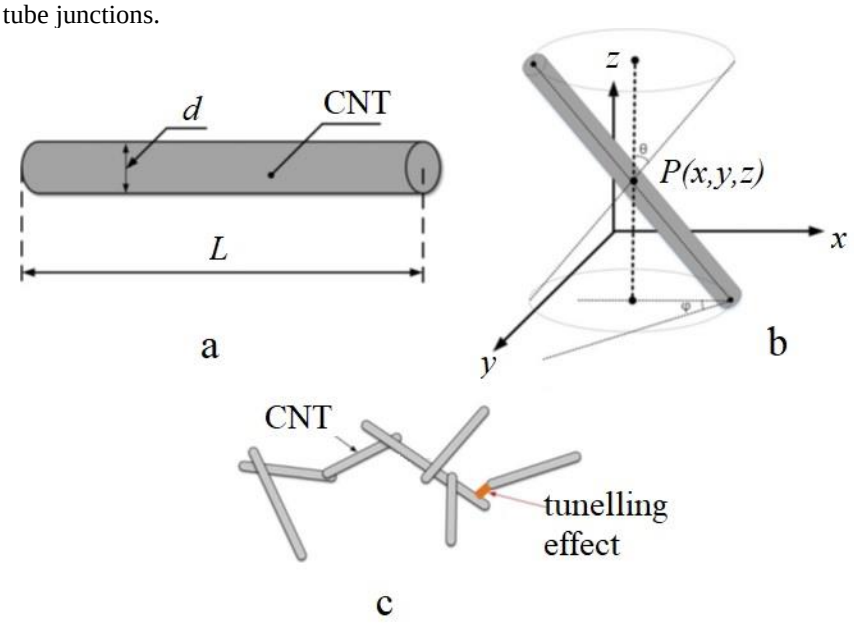

Fig. 2. Main 3D parameters of CNT (a), definition of location and orientation of a CNT (b) and possible contact between CNTs and tunneling effect (c).

Let's describe a process that will allow us to find the shortest distance between CNTs and the actual coordinates of these "joining" points. The coordinates of point on the CNT axis can be described by the following expression:

$$p + \alpha \cdot \vec{d}, \tag{9}$$

where p is the point of the start of the CNT, $\vec{d}$ is the directional vector of the CNT and α is a variable coefficient ($\alpha \in [0,1]$), whose concrete values define the points located on the CNT axis.

Let $p_1 + \alpha \cdot \vec{d}_1$ and $p_2 + \beta \cdot \vec{d}_2$ are arbitrary points on the first and second CNTs, respectively, and the distance between these segments must be found. Then $(p_1 + \alpha \cdot \vec{d}_1) - (p_2 + \beta \cdot \vec{d}_2)$ is the vector that connects these two points. The minimum distance between CNTs can be obtained as the norm of this aforementioned vector:

$$D = \| (p_1 + \alpha \cdot \vec{d}_1) - (p_2 + \beta \cdot \vec{d}_2) \|^2 . \tag{10}$$

Taking into account the property of the scalar product $(\vec{a}, \vec{a}) = \| \vec{a} \|^2$, we can conclude that in order to find the values of the coefficients, it is necessary to find the values that provide the minimum scalar product of the vector by itself. So, after some transformations, we get the following expressions for finding the coefficients α and β.

Auxiliary designations:

$$\begin{aligned}
&A_1 = (\vec{d}_1, \vec{d}_1), \;\; A_2 = (\vec{d}_1, \vec{d}_2), \\
&B_1 = (\vec{d}_2, \vec{d}_1), \;\; B_2 = (\vec{d}_2, \vec{d}_2), \\
&C_1 = (\overrightarrow{p_2 - p_1}, \vec{d}_1), \\
&C_1 = (\overrightarrow{p_2 - p_1}, \vec{d}_2), \\
&D = (A_1 \cdot B_2 - B_1 \cdot A_2).
\end{aligned} \tag{10}$$

The values of the coefficients:

$$\begin{aligned}
\alpha &= \frac{(C_1 \cdot B_2 - B_1 \cdot C_2)}{D}, \\
\beta &= \frac{(C_2 \cdot A_1 - C_1 \cdot A_2)}{D}.
\end{aligned} \tag{11}$$

If the values of the found coefficients α and β do not belong to the interval [0,1], then their values should be reduced to the nearest values from this interval. Only then will these coefficients represent points located within the nanotube.

In the proposed model two types of conductivity are considered in the model: conductivity between CNTs at the points of their contact and intrinsic conductivity of nanotubes. The conductivity of the connection between the tubes is based on the tunnel effect. Two CNTs are treated as the connected ones, when the shortest distance between them is shorter than some preset value of the cut-off distance d_{cutoff}.

Let's define a part of the CNT by a pair of points located on its axis. Suppose the length of this segment is equal to l_s (see Fig. 2). Then the intrinsic resistance of this part of CNT can be calculated by the equation [18]:

$$R_{intrinsic} = \frac{4l_s}{\pi\sigma_{CNT}d^2}, \tag{12}$$

where σ_{CNT} is the intrinsic electrical conductivity of the CNT, and d is the diameter of the CNT.

The contact resistance between pair of nanotubes is caused by the tunneling effect at the "junction" points. Assume that the shortest distance between a pair of nanotubes is equal to d_{kp}, where d_{kp} is less than d_{cutoff}. Then the contact resistance can be estimated using the Landauer-Büttiker formalism [21-24]:

$$R_{contact} = \frac{h}{2e^2}\frac{1}{NP}, \tag{13}$$

$$P = \begin{cases} \exp(-\frac{d_{vdw}}{d_{tunnel}}) \quad for\ 0 \le d_{kp} \le d + d_{vdw}, \\ \exp(-\frac{d_{kp} - d}{d_{tunnel}}) \quad for\ d + d_{vdw} \le d_{kp} \le d + d_{cutoff}, \end{cases} \tag{14}$$

$$d_{tunnel} = \frac{h}{2\pi}\frac{1}{\sqrt{2m_e\Delta E}}, \tag{15}$$

where h is Planck's constant; P is the probability of electron transfer to tunneling between CNTs; N is the number of conduction channels, (a dimensionless quantity related to the diameter of the CNT [22]); e is electron charge; d_{vdw} is van der Waals distance [25,26], which limits the minimum distance between a pair of CNTs; d_{tunnel} is characteristic length of tunneling; m_e is electron mass; ΔE is the height of the energy barrier [27].

At modeling, a network of random resistors is represented by a matrix of conductivity between all "joint" points. After applying Kirchhoff's law, a system of linear equations is created. Since the "joint" point has only a few connections with other points, the resulting matrix is sparse. Therefore, a special sparse solver is used to achieve good simulation performance. The SuperLU library [28-30] was used to solve the system of linear algebraic equations and obtain the electric potential values at all *"*joints*"*. After that, the equivalent conductance of the random resistance network is calculated.

Simulation of electrical conductivity of nanocomposite system within the framework of the percolation model. Software was developed to simulate the conductivity of the nanotube-dielectric composite using the "hard core" model. The simulation was to investigate the influence of the tunneling effect on the overall conductivity of the nanocomposite described by the "hard core" model for CNTs. For comparison, the "soft core" model was also implemented.

The very first task we face is, obviously, the comparison of our computer simulation results with experimental measurements, which are available, for example, in [18]. To achieve this goal, the parameters of the simulated system were set as shown in Table 1.

As can be seen from Fig. 3, the conductivity of CNTs increases with an increase in the content of the volume fraction, both for the case of "hard core" and for the case of "soft core". The data shown in Fig. 3 for the "main" part coincide with the experimental results [18] both qualitatively and quantitatively. Difference in the actual values of the simulation results can be seen between the "soft core" and "hard core" models, but the behavior of both models evolves in the same way as the volume fraction changes.

Table 1. Parameters of simulation for CNTs

Parameter name	**Value**
RVE size	1000 nm 1000 nm 100 nm
CNT diameter (d_{CNT})	2 nm
CNT length	200 nm
CNT aspect ratio	100
CNT intrinsic conductivity	10^4 S/m
Tunnel cut-off distance	1.9 nm

The results of the simulations for various CNTs volume fractions are shown on Fig 3.

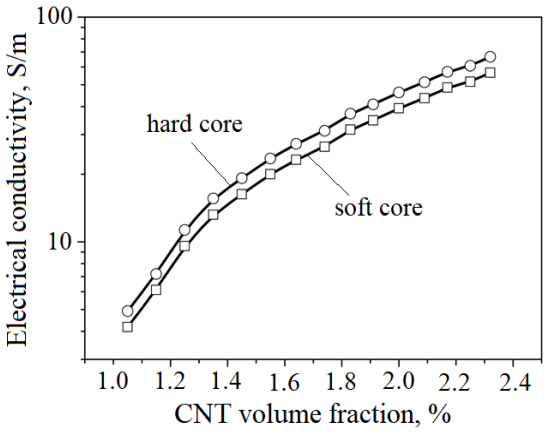

Fig. 3. Composite conductivity both "soft core" and "hard core" models.

Dependency of composite conductivity on tunneling cut-of distance of 1.5 nm, 2 nm, 2.5 nm and 3 nm is shown in Fig. 4. Composites with a tunneling distance of 1.5 nm are characterized by the lowest electrical conductivity at the same values of the volume fraction of CNTs. It is logical that with larger values of the tunneling distance, the electrical conductivity also increases. In this case, the CNT diameter was 2 mn. So, from the histograms in Fig. 4, we can conclude that the change in the maximum distance at which there is a tunnel effect does not change the nature of the electrical conductivity of the system, it depends on the concentration of nanotubes. In turn, this distance significantly affects the value of the total electrical conductivity of the CNTs.

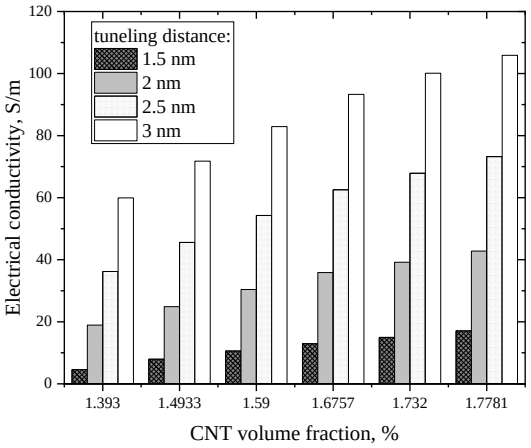

Fig. 4. Dependency of composite conductivity on tunneling cut-of distance.

Dependence of composite conductivity on volume fraction at different CNT diameter (1, 2, 3, 4 and 5 nm) is shown in Fig. 5. The best electrical conductivity at a small CNT volume fraction is characterized by the use of nanotubes with a minimum size of 1 nm. In the case of CNT diameter of 2 nm, a decrease in conductivity is observed, while a larger number of nanotubes is required to achieve the percolation effect. The results of modeling when using nanotubes with a diameter of 3.4 and 5 nm demonstrate a further decrease in electrical conductivity and the need to increase the content of CNTs to achieve percolation. However, when using CNTs with a size of 5 nm, it is difficult to achieve percolation, the electrical conductivity is close to zero.

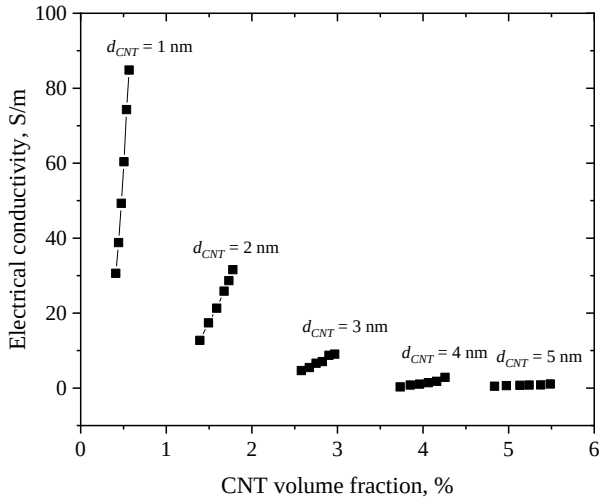

Fig. 5. Dependence of composite conductivity on volume fraction at different CNT diameter.

Conclusion. The influence of the tunneling distance parameter on the conductivity of the CNTs system was investigated. The simulation results agree with experimental data obtained by other researchers, and also indicate a difference for the cases of overlapping nanotubes ("soft core" model) and non-overlapping nanotubes ("hard core" model). Comparison with the measured results shows that the "solid core" model can be effectively used to predict the parameters of the fabricated composite, which is an important step towards creating a material with the desired properties.

Acknowledgement. This work was supported by Ministry of Education and Science of Ukraine.

References

[1] *Qiu S.* Solution-processing of high-purity semiconducting single-walled carbon nanotubes for electronics devices / S. Qiu, K. Wu, D. Gao, L. Li, H. Jin, Q. Li // Advanced Materials. – 2019. – Vol. 31(9). – P. 1800750.

[2] *Xia F.* High-performance carbon nanotube-based transient complementary electronics / F. Xia, T. Xia, L. Xiang, F. Liu, W. Jia, X. Liang, Y. Hu // ACS Applied Materials & Interfaces. – 2022. – Vol. 14(10). – P. 12515-12522.

[3] *Zhang S.* Emerging Internet of Things driven carbon nanotubes-based devices / S. Zhang, J. Pang, Y. Li, F. Yang, T. Gemming, K. Wang, ...M.H. Rümmeli // Nano Research. – 2022. – P. 1-25.

[4] *Jain N.* Plethora of Carbon nanotubes applications in various fields–A state-of-the-art-review / N. Jain, E. Gupta, N.J. Kanu // Smart Science. – 2022. – Vol. 10(1). – P. 1-24.

[5] *Boschetto G.* Graphene and carbon nanotubes for electronics nanopackaging / G. Boschetto, S. Carapezzi, A. Todri-Sanial // IEEE Open Journal of Nanotechnology. – 2021. – Vol. 2. – P. 120-128.

[6] *Pang J.* Applications of carbon nanotubes in the internet of things era / J. Pang, A. Bachmatiuk, F. Yang, H. Liu, W. Zhou, M.H. Rümmeli, G. Cuniberti // Nano-Micro Letters. – 2021. – Vol. 13(1). – P. 1-15.

[7] *Bauhofer W.* A review and analysis of electrical percolation in carbon nanotube polymer composites / W. Bauhofer, J.Z. Kovacs // Composites science and technology. – 2009. – Vol. 69(10). – P. 1486-1498.

[8] *Zare Y.* Simulation of percolation threshold, tunneling distance, and conductivity for carbon nanotube (CNT)-reinforced nanocomposites assuming effective CNT concentration / Y. Zare, K. Y. Rhee // Polymers. – 2020. – Vol. 12(1). – P. 114.

[9] *Tarlton T.* A stochastic approach towards a predictive model on charge transport properties in carbon nanotube composites / T. Tarlton, J. Brown, B. Beach, P.A. Derosa // Composites Part B: Engineering. – 2016. – Vol. 100. – P. 56-67.

[10] *Molotnikov A.* Percolation mechanism of failure of a planar assembly of interlocked osteomorphic elements / A. Molotnikov, Y. Estrin, A.V. Dyskin, E. Pasternak, A.J. Kanel-Belov // Engineering fracture mechanics. – 2007. – Vol. 74(8). – P. 1222-1232.

[11] *Mun S. C.* A new approach to determine rheological percolation of carbon nanotubes in microstructured polymer matrices / S.C. Mun, M. Kim, K. Prakashan, H.J. Jung, Y. Son, O.O. Park // Carbon. – 2014. – Vol. 67. – P. 64-71.

[12] *Karbovnyk I.* Random nanostructured metallic films for environmental monitoring and optical sensing: experimental and computational studies / I. Karbovnyk, J. Collins, I. Bolesta, A. Stelmashchuk, A. Kolkevych, S. Velupillai, H. Klym, O. Fedyshyn, S. Tymoshuk, I. Kolych // Nanoscale Research Letters. – 2015. – Vol. 10. – P. 151.1-151.5.

[13] *Luo D.* Effects of the distribution and geometry of carbon nanotubes on the macroscopic stiffness and microscopic stresses of nanocomposites / D. Luo, W.X. Wang, Y. Takao // Composites Science and Technology. – 2007. – Vol. 67(14). – P. 2947-2958.

[14] *Wang J. F.* Multiscale simulation of mechanical properties and microstructure of CNT-reinforced cement-based composites / J.F. Wang, L.W. Zhang, K. M. Liew // Computer Methods in Applied Mechanics and Engineering. – 2017. – Vol. 319. – P. 393-413.

[15] *Marconnet A. M.* Thermal conduction phenomena in carbon nanotubes and related nanostructured materials / A.M. Marconnet, M.A. Panzer, K.E. Goodson / Reviews of Modern Physics. – 2013. – P. 85(3). – P. 1295.

[16] *Pan J.* Influence of agglomeration parameters on carbon nanotube composites / J. Pan, L. Bian // Acta Mechanica. – 2017. – Vol. 228(6). – P. 2207-2217.

[17] *Matsuda K.* Properties of carbon nanotube complex systems and computer experiments / K. Matsuda, K. Hanami, Y. Maniwa // RIST News. – 2008. P. 3-12.

[18] *Hu N.* The electrical properties of polymer nanocomposites with carbon nanotube fillers / N. Hu, Z. Masuda, C. Yan, G. Yamamoto // Nanotechnology. – 2008. – Vol. 19(21). – P. 215701.

[19] *Grujicic M.* A computational analysis of the percolation threshold and the electrical conductivity of carbon nanotubes filled polymeric materials / M. Grujicic, G. Cao, W.N. Roy // Journal of materials science. – 2004. – Vol. 39(14). – P. 4441-4449.

[20] *Fu X.* Comprehensive analysis on the electrical behavior of highly stretchable carbon nanotubes/polymer composite through numerical simulation / X. Fu, A.M. Al-Jumaily, M. Ramos, Y.F. Chen // Journal of Materials Research. – 2018. – Vol. 33(20). – P. 3398-3407.

[21] *Büttiker M.* Generalized many-channel conductance formula with application to small rings / M. Büttiker, Y. Imry, R. Landauer, S. Pinhas // Phys Rev B. – 1985. – Vol. 31. – P. 6207-6215.

[22] *Tamura R.* Electronic transport in carbon nanotube junctions / R. Tamura, M. Tsukada // Solid State Commun. – 1997. – Vol. 101(8). – P. 601-605.

[23] *Xie S.* Mechanical and physical properties on carbon nanotube / S. Xie, W. Li, Z. Pan, B. Chang, L. Sun // Journal of Physics and Chemistry of solids. – 2000. – Vol. 61(7). – P. 1153-1158.

[24] *Buldum A.* Contact resistance between carbon nanotubes / A. Buldum, J.P. Lu // Phys. Rev. B. - 2001. – Vol. 63. – P. 161403-6.

[25] *Hertel T.* Deformation of carbon nanotubes by surface van der Waals forces / T. Hertel, R.E. Walkup, P. Avouris Phys. Rev. B. – 1998. – Vol. 58. – P. 13870-3.

[26] *Girifalco L.A.* Carbon nanotubes, buckyballs, ropes and a universal graphitic potential / L.A. Girifalco, M. Hodak, R.S. Lee // Phys. Rev. B. – 2000. – Vol. 62. – P. 13104.

[27] *Simmons J.G.* Generalized formula for the electric tunnel effect between similar electrodes separated by a thin insulating film / J.G. Simmons // J. Appl. Phys. – 1963. – Vol. 34(6). – P. 1793-1803.

[28] *Li X. S.* An overview of SuperLU: algorithms, implementation, and user interface / X. S. Li // ACM Transactions on Mathematical Software (TOMS) toms. – 2005. – Vol. 31(3). – P. 302-325.

[29] *Li X.S.* SuperLU users` guide / X.S. Li, J.W. Demmel, J.R. Gilbert, L. Grigori, M. Shao, I. Yamazaki // Lawrence Berkeley National Laboratory, 1999.

[30] *Demmel J.W.* A supernodal approach to sparse matrix pivoting / J.W. Demmel, S.C. Eisenstat, J.R. Gilbert, X.S. Li, J.W.H. Liu // SIAM J. Matrix Analysis and Applications. – 1999. – Vol. 20(3). - P. 720-755.

МОДЕЛЮВАННЯ ТУНЕЛЬНОЇ ПРОВІДНОСТІ У ВОГНЕТРИВКИХ КОМПОЗИТНИХ СИСТЕМАХ НАНОТРУБКИ/ДІЕЛЕКТРИК

І. Жиденко[1,2], Г. Клим[2,3]

[1]Львівський державний університет безпеки життєдіяльності,
вул. Клепарівська, 35, 79007, Львів, Україна
zhidenkoillya@gmail.com, illia.v.zhydenko@lpnu.ua

[2]кафедра спеціалізованих комп'ютерних систем,
Національний університет «Львівська політехніка»,
вул. С. Бандери, 12,79013 Львів, Україна
halyna.i.klym@lpnu.ua, klymha@yahoo.com

[3]кафедра радіоелектронних і комп'ютерних систем,
Львівський національний університет імені Івана Франка,
вул. Драгоманова, 50, 79005, Львів, Україна
halyna.klym@lnu.edu.ua

Розглянуто підхід до розрахунку інтегральної провідності модельної вогнетривкої композиційної системи нанотрубка/діелектрик. У запропонованій проаналізовано два типи провідності: провідність між нанотрубками у точках їх контакту та власна провідність нанотрубок. Продемонстровано, що електрична провідність з'єднання між трубками базується на тунельному ефекті.

Розроблено програмне забезпечення для моделювання провідності композиту нанотрубка-діелектрик з використанням моделі «твердого ядра». Моделювання полягало в дослідженні впливу ефекту тунелювання на загальну провідність нанокомпозиту, описаного моделлю «hard core» для нанотрубок. Для порівняння також була реалізована модель «soft core».

Змодельовано провідність випадкової мережі нанотрубок, сформованих у діелектричному середовищі, з урахуванням тунельної провідності між окремими нанотрубками, розташованими в безпосередній близькості, та з урахуванням внутрішньої провідності нанотрубок. Продемонстровано, що провідність нанотрубок зростає при

збільшенні вмісту їх об’ємної частки як при використанні моделі «hard core», так і «soft core». Показано, що модель «hard core» може бути ефективно використана для прогнозування параметрів виготовленого композиту, що є важливим кроком до створення матеріалу з бажаними властивостями для застосування у електроніці.

Досліджено вплив параметра відстані тунелювання на провідність системи нанотрубка-діелектрик. Результати моделювання узгоджуються з експериментальними даними, отриманими іншими дослідниками, а також вказують на різницю для випадків нанотрубок, що перекриваються (модель «soft core») і нанотрубок, що не перекриваються (модель «hard core»). Порівняння з результатами вимірювань показує, що модель «жорсткого ядра» можна ефективно використовувати для прогнозування параметрів виготовленого композиту, що є важливим кроком до створення матеріалу з бажаними властивостями. Показано, що при використанні нанотрубок більшого діаметру погіршується провідність у композитні системі. Це зумовлено зменшенням ефекту перколяції для нанотрубок більшого діаметру.

Ключові слова: нанокомпозит, нанотрубка, тунельна провідність, компютерне моделювання.

Стаття надійшла до редакції 08.11.2022.
Прийнята до друку 11.11.2022.