

The Hamburg score of Professor Yuri Shunin

Arnold Kiv¹, Tamara Lobanova-Shunina², Natalya Burlutskaya³

¹*Ben-Gurion University of the Negev, Beer-Sheva, Israel*

²*Latvian Technical University, Riga, Latvia*

³*ISMA University of Applied Sciences, Riga, Latvia*

*Corresponding author's e-mail: kiv.arnold20@gmail.com

Received 29 March 2019, www.cmmt.lv

Abstract

The Hamburg score is determined by the totality of the scientist's results, which influenced the development of the relevant scientific directions and turned out to be useful for solving related tasks by other scientists. The article gives a brief overview of the scientific results of Professor Yuri Shunin.

Key words

Professor Yuri Shunin, the main scientific results

The scientific activity of Professor Yuri Shunin covered a wide range of areas and at various times affected the problems associated with the latest achievements of world science. There are three main directions in which he obtained significant results that affected progress in the relevant areas: theory of disordered solids, properties and applications of nanostructures, mathematical methods in pedagogy and linguistics.

In the doctoral dissertation of Professor Yuri Shunin the multiple scattering theories and the effective media cluster approach were developed with respect to disordered solids. The electronic structure of different disordered systems was studied. Later these approaches were used to solve many problems of solid-state theory and applied problems of modern electronics.

The developed cluster approach for numerical modelling of disordered solids, based on the multiple scattering theories, cluster conception and effective medium model allowed obtaining important results on the electronic structure of amorphous semiconductors. A number of works were carried out in this direction. The electronic density of states, a phonon density of states, a thermal conductivity and other properties necessary for practical applications were calculated.

The peculiarities of electrical properties of series of novel solid state devices were studied. The mechanism of resistivity was considered as a scattering problem, where the current carriers participate in the transport according to various mechanisms based on the presence of scattering centers (phonons, charge defects, structural defects, etc.). The

developed computational procedure is based on the construction of cluster potentials and the evaluation of the S - and T- matrices for scattering and transfer, respectively. It allowed to realize the full-scale electronic structure calculations for condensed matter ("black box"), where influence means a set of electronic "trial" energy-dependent wave functions that gives sets of scattering amplitudes corresponding to possible scattering channels for any "trial" energy. This allowed "decrypting" the electronic spectra of "black box".

The second direction of an activity of professor Yuri Shunin is devoted to research of nanostructures, in particular nanotubes (CNTs) and graphene nanoribbons (GNR). His research was focused on the junctions of carbon nanotubes (CNTs) and graphene nanoribbons (GNR) with contacting metallic elements of a nanocircuit. Computer simulations on the conductance and resistance of these contacts have been performed using the multiple scattering theory and the effective media cluster approach. It was simulated both single-

wall and multi-wall CNTs as well as single-layered and multi-layered GNRs with different morphology. The model of CNT-Me and GNR-Me nanointerconnects (Fig. 1) has been developed. The electron transport formalism was used which suggests the existence of two regions supporting two different electron transport mechanisms: ballistic (elastic) and collisional (non-elastic). These electron transport processes are simulated using the corresponding boundary conditions in the form of the effective medium. The CNT and GNR chiralities (m, n) are simulated by the corresponding orientation of the chirality vectors within the scattering medium.

Figure 1 represents the contacts of metal substrates with CNTs and GNRs, respectively, as prototype nanodevices. The contact regions (CNT-Me and GNR-Me) are the objects of a microscopic approach responsible for the main contribution to the resistance. The resistances of nanotubes, nanoribbons and the metallic substrate per se are considered as macroscopic parameters.

The electronic structure for CNT-Me

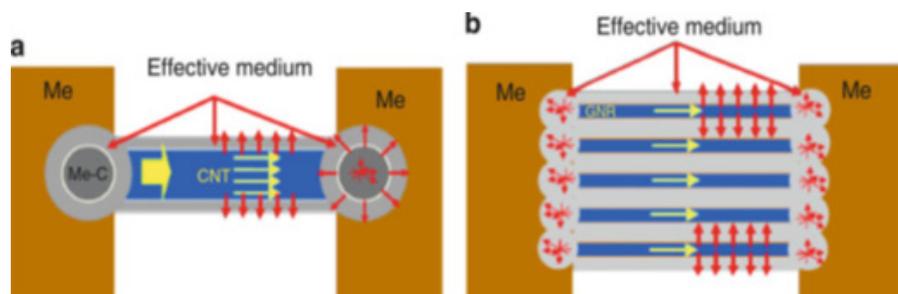


FIGURE 1 Models of C-Me interconnects as a prototypes of novel nanodevices: (a) CNT- Me interconnect; (b) multilayered GNR-Me interconnect

and GNR-Me interconnects was evaluated through the electronic density of states (DOS) for carbon-metal contact considered as a "disordered alloy", where clusters containing both C and Me atoms behave as scattering centers. The computational procedure that was developed for these calculations is also based on the construction of cluster potentials and the evaluation of both scattering and transfer matrices. The general model of multiple scattering using the effective media approximation (EMA) combined with the coherent potential approach (CPA) for condensed matter was developed. When using the CPA as EMA approximation, the resistance of the interconnect was evaluated through Kubo-Greenwood formalism, or in the simplest cases, through Ziman formalism. So far, the

cluster formalism has been successfully applied for Cu metal, as well as for semiconductors. Special attention was paid for the latter, since the concept of statistical weighing has been applied for the binary components in solid solutions. Structural models for CNT-Me and GNR-Me junctions were developed, based on their precise atomistic structures, which take into account the CNT chirality effect and its influence on the interconnect resistance.

The most problematic areas for simulation of CNT-Me and GNR-Me were the necessity to account that there is the atomic structural disorder and the conductivity mechanism changing. The influence of chirality on resistance in the vicinity of interconnect depends on the number of statistically realized bonds between the CNT (GNR) and the metal

contact (e.g., Ni, Cu, Au, Ag, Pd, Pt). For the case of side type contact for GNR-Me interconnects the model of effective bonds was developed and it was shown that the number of effective bonds per contact square is essential.

It was accounted in the calculations of interconnects that here a probabilistic process occurs when only more-or-less equilibrium bonds ('effective bonds') are formed at inter-atomic distances corresponding to the minimum total energies. The evaluation of a number of "effective bonds" is principal for determination of the number of 'conducting channels', since the conductance is proportional to the number of appeared "effective bonds" within the CNT-Me interconnect. The features of contacts were studied in detail.

It was established that the radial conductance per CNT length depends on the morphology (chirality) of the nearest nanotubes, when the number of shortest effective barriers is varied in a probabilistic way. This also means that current-voltage parameters of contacts can be less stable. It has been found that inter-shell interactions, such as inter-shell tunneling of electrons and Coulomb interactions cause a reduction of the total conductance in considered contacts.

A large cycle of works was performed by Professor Yuri Shunin in the field of research and creation of fundamentally new biosensors based on previously studied nanostructures. These results are connected with applications

of CNTs and GNRs based interfaces with other materials. When creating biosensors, the well known electron devices, field-effect transistors (FET-transistors) (Fig. 2) were used which are very sensitive to various external influences of different nature such as mechanical, chemical, electrical, magnetic etc. A FET is of nano in size, whose on/off threshold voltage depends on the tube dimensions, shape and temperature, amongst others. A local deformation of CNT (GNR) creates a change in the on/off threshold voltage of the transistor. The electrical properties of carbon based interconnects are changed under the influence of different external factors. The advantage of CNTs and GNRs over other structures occurs due to their small size, great strength, high electrical and thermal conductivity, and high specific area. Unique physical properties of CNTs and GNRs and their various interconnects allow considering them as sensing nanomaterials in various kinds of sensors – pressure, flow, thermal, gas, optical, mass, position, stress, strain, chemical, and biological sensors. Taking into account specific physical properties of CNTs and GNRs metal interconnects which are explained by the presence of "dangling" chemical bonds, it was pointed out the expressed sensitivity of electric properties of interconnect space to chemical, electric and magnetic factors' influence. Thus it was shown that interconnects in the mentioned devices are important elements for a perspective group of nanosensors.

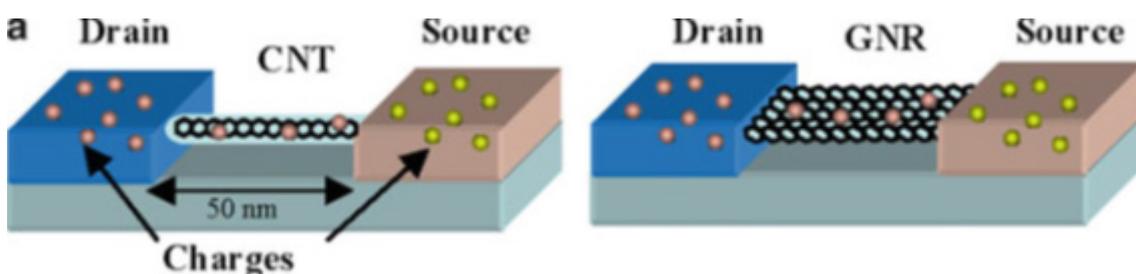


FIGURE 2 The unperturbed field-effect transistors based on a CNT and GNR are given CNT- or GNR- based FET. They are mainly composed of a corresponding semiconducting carbon material suspended over two electrodes

Further, the biological nanosensors based on the use of noble metal nanoparticles were investigated. Mechanism of sensing is connected with an excitation of surface plasmons. The resonant frequency of surface plasmons that are caused by the light irradiation changes when different harmful components are adsorbed on the particles. This technique based on so called localized surface plasmon

resonance (LPSR) is widely used. One of the main constraints of this sensing mechanism is the requirement of an external source of light and a device which is able to measure and compare different resonant frequencies.

In the works of Professor Yuri Shunin various classes of CNT- and GNR-based nanosensors are considered. A wide class of biological nanosensors is investigated for the

application in the biomedical industry, e.g., in cases of diabetes, where regular tests by patients themselves are required. This includes many other diagnostic and therapeutic devices. For example, these are devices such as biosensors for application in eye surgery, hospital beds equipment, patient monitors, inhalers, and kidney dialysis machines, in both invasive and noninvasive blood pressure monitoring. Nanosensors were considered that have a substantial utility in the automotive industry. Their importance is expected to increase while designing the vehicles of the future. In particular, they are used to process information about vehicle parameters such as pressure, vehicle altitudes, flow, temperature, heat, humidity, speed and acceleration, exhaust gas, and engine knock and torque.

In recent years, Professor Yuri Shunin has developed a new direction related to the application of mathematical methods in pedagogy and linguistics. Some new definitions to pedagogical phenomena in the process of language acquisition were proposed on the basis of the general systems theory. A group of learners was considered as a learning system which is reversely charged with a situational managerial system (i.e. mentoring/teaching staff), thus, forming a constituent structural unit of a bigger pedagogical system but keeping at the same time all its main characteristics. Since the learning system experiences a purposeful external pedagogical influence, it is considered a managed system. A model of Intelligent System Management has been worked out. The principles developed are adequate also for other study activities and study courses. The process of imparting educational information by a mentor is distinguished by its qualitative and quantitative indices. It was considered a

process of intellectualization of a study group in connection with the notion of "Homeokinetic Plato", which actually reflects different intellectual levels of tested study group, e.g., in a language acquisition. The proposed System of Intelligence Levels and the Teaching Efficiency Indicator ensure the possibility to estimate the initial level of learner intelligence and the final result and compare these results with a predetermined purposeful goal to see the efficiency of a study course and the progress of student achievement. These techniques can be recommended for use to a variety of educational domains. An empirical study was used to analyze the optimum amount of the language material to be included into the final test on Business English. The empirical results gave grounds to compile effectively the examination paper material amount and to define the time for its fulfilment. Optimization Model of teaching information amount and time distribution has been worked out. The system approach to language teaching and acquisition allows removing the blinders so that it's possible to see the educational world in the light that illuminates the whole – the system – and only then there will be lasting changes for the better.

Conclusion

The results obtained by Professor Yuri Shunin left a significant mark on important fields of science. These results are in many cases obtained with the participation of colleagues and students. Cooperation and the exchange of ideas were the leading principle in the creative work of Professor Yuri Shunin. The ideas embodied in these works will undoubtedly be further developed.

Selected publications of Professor Yuri Shunin

- [1] Shunin Yu N, Shvarts K K 1986 Calculation of the Electronic Structure in Disordered Semiconductors *Phys. Stat. Sol. (b)* **135** 15-36
- [2] Shunin Yu N, Shvarts K K 1991 Cluster Approach for Disordered Solids *Latv.J.phys.techn.Sci.* **3** 3-29
- [3] Shunin Yu N 1991 *Modeling of atomic and electronic structures of disordered semiconductors* Dr. Sc. Habil, Thesis. Salaspils - Riga
- [4] Shunin Yu, Schwartz K, Trautmann C 1996 *Relaxation of elementary excitations and formation of defects along the path of heavy ions in solids* GSI-Report - 96-03
- [5] Shunin Yu N, Schwartz K K 1997 *Correlation between electronic structure and atomic configurations in disordered solids*, NATO ASI SERIES, *Computer Modelling of Electronic and Atomic Processes in Solids, Space and Electronic Materials* Ed. R.C. Tennyson and A. E. Kiv, Kluwer Publ. 241-57
- [6] Shunin Yu, Danilova N 2000 Random processes and kinetics of point defects in metals *Computer Modelling and New Technologies* **4**(1) 64-8
- [7] Jacobs P W M, Zhukovskii Yu F, Mastrikov Yu, Shunin Yu N 2001 Bulk and surface properties of metallic aluminium: DFT simulations *Computer Modelling and New Technologies* **6**(1) 7-28
- [8] Shunin Yu N, Gopeyenko A V 2005 Phase-shift functions methods for nanoclusters electronic structure calculations in solids *Computer Modelling and New Technologies* **9**(1) 15-31

- [9] Shunin Yu N, Zhukovskii Yu F, Bellucci S 2008 Simulations of properties of carbon nanotubes using the effective media approach *Computer Modelling and New Technologies* **12**(2) 66–77
- [10] Shunin Yu N, Zhukovskii Yu F, Burlutskaya N, Gopeyenko VI, Bellucci S 2010 Theoretical resistance simulations for junctions of SW and MW carbon nanotubes with metal substrates in nanoelectronic devices *Computer Modelling and New Technologies* **14**(2) 7–19
- [11] Shunin Yu N, Zhukovskii Yu F, Burlutskaya N Y, Bellucci S 2011 Resistance simulations for junctions of SW and MW carbon nanotubes with various metal substrates *Cent Euro J Phys* **9**
- [12] Shunin Yu N, Zhukovskii Yu F, Gopeyenko V I, Burlutskaya N, Bellucci S 2011 Ab Initio simulations on electric properties for junctions between carbon nanotubes and metal electrodes *Nanoscience & Nanotechnology Lett* **3** 816–25
- [13] Shunin Yuri N, Zhukovskii Yu F, Burlutskaya N Yu, Gopeyenko V I, Bellucci S 2012 *Simulation of Fundamental Properties of CNT and GNR-Metal Interconnects for Development of New Nanosensors Systems, Nanodevices and Nanomaterials for Ecological Security* Editors: Yu. Shunin and A. Kiv, Series: NATO Science for Peace Series B - Physics and Biophysics (Heidelberg: Springer Verlag) 363 p
- [14] Fink D, Kiv A, Shunin Y, Mykytenko N, Lobanova-Shunina T, Mansharipova A, Koycheva T, Muhamediev R, Gopeyenko V, Burlutskaya N, Zhukovskii Y, Bellucci S 2015 The nature of oscillations of ion currents in the ion track electronics *Computer Modelling and New Technologies* **19**(6) 7-13
- [15] Shunin Yu, Fink D, Kiv A, Alfonta L, Mansharipova A, Muhamediev R, Zhukovskii Yu, Lobanova-Shunina T, Burlutskaya N, Gopeyenko V, Bellucci S 2016 Theory and modelling of physical and bio-nanosensors systems *In: Proceedings of the 5th Intern Workshop Nanocarbon Photonics and Optoelectronics. 1-6 August 2016, Holiday Club Saimaa, Lappeenranta, Finland 2016*, 101
- [16] Shunin Yu, Bellucci S, Gopeyenko V, Lobanova-Shunina T, Kiv A, Fink D, Mansharipova A, Mukhamedyev R, Zhukovskii Yu 2018 *Nanosensors Devices for CBRN-Agents Detection: Theory and Design, Nanostructured Materials for the Detection of CBRN* Editors: Janez Bonca and Sergei Kruchinin, Series: NATO Science for Peace and Security, Series A, Chemistry and Biology, Heidelberg: Springer Verlag 169 p.
- [17] Shunin Yu, Bellucci S, Gruodis A, Lobanova-Shunina 2018 *Nonregular Nanosystems. Theory and Applications* Heidelberg: Springer Verlag