Preface

The Fifteenth International Workshop on Nano-Design, Technology and Computer Simulations (NDTCS-2013) took place on 11-15 June 2013 in Minsk, Belarus. The workshop NDTCS-2013 was organized jointly by Belarusian State University of Informatics and Radioelectronics and the St. Petersburg Academy of Sciences on Strength Problems (Russia). All sessions took place in University buildings. Seventy four scientists and graduate students attended the workshop representing Belarus, France, Lithuania, Poland, and Russia.

The Fifteenth Workshop was focused on the synthesis, properties and applications of novel materials, and modern computational methods for their structure and property investigations. New experimental and theoretical results were presented by world leading specialists. Invited tutorial lectures preceded the special sessions. The contributions to the workshop program were organized into three oral/poster sessions:

- Synthesis, Structure and Properties of Nanomaterials (graphene, fullerenes, nanotubes, nanoparticles, composites, etc.)
- Applications of Nanomaterials (electronics, mechanics, biology, etc.)
- Molecular Dynamics and DFT simulations

Workshop NDTCS-2013 is a continuation of the previous workshops, which were held in:

- 1997-2005, St. Petersburg (Russia)
- 2006, Olsztyn (Poland)
- 2007, Bayreuth (Germany)
- 2008, Minsk (Belarus)
- 2009, Vilnius (Lithuania)
- 2011, Espoo (Finland)

The first nine workshops, which took place in Russia, had the name “Nondestructive Testing and Computer Simulations in Science and Engineering.” In due course, the focus of the meetings gradually moved towards Nanoscience and Nanotechnology, so at the Tenth International Workshop (NDTCS-2006) it was decided to conserve the abbreviation, which became a brand, but to change the name. The following workshops (2007-2013) had the new name “International Workshop on New Approaches to High-Tech: Nano-Design, Technology and Computer Simulations” what reflects better their profile.

All the contributions to the Workshops were published in English.

- Proceedings of St. Petersburg Academy of Sciences on Strength Problems (SPAS), vols. 2-11 (1998–2007);
- Proceedings of the International Society for Optical Engineering (SPIE), vols. 3345, 3687, 4064, 4348, 4627, 5127, 5400, 5831, 6253, 6597, 7377 (1998–2008);
- Modelling and Computer Simulation in Materials Science and Engineering, vol. 6, No 4 (1998);
- Reviews on Advanced Materials Science, vol. 20, Nos. 1–2 (2009);

This issue of Materials Physics and Mechanics Journal contains the selected papers presented at the Workshop. All the papers presented here have been peer-reviewed prior to publication. The issue will be of interest to researchers and graduate students in the field of nanotechnology, physics, chemistry, and mechanics.

The scientific discussions continued informally with a series of social events, including the welcome party and visit to National Academic Bolshoi Opera and Ballet Theatre of the Republic of Belarus (Gioachino Rossini “The Barber of Seville”, production conductor Gianluca Marciano, Italy).

Alexander I. Melker, Victor Stempitsky
Vladislav Victorovich NELAEV
(1941-2013)

On 30 October, 2013, Professor of the Micro and Nanoelectronics Department of Belarusian State University of Informatics and Radioelectronics, Doctor of Science, Vladislav Victorovich Nelaev died at the age of 72.

Vladislav Nelaev was born on 12 June 1941, in Omsk region, Siberia, U.S.S.R., but during most of his years lived in Minsk, Belarus. In 1963, he graduated from Belarusian State University with a degree in physics. In 1981, he was awarded the Ph.D. degree in theoretical physics of solids at the Institute of Nuclear Energy of Belarusian Academy of Sciences, and in 2001 he received the Doctor of Science degree in physics and mathematics. Since 2002, he was a professor at the Department of Micro and Nanoelectronics of Belarusian State University of Informatics and Radioelectronics.

The beginning of Nelaev’s research activity was connected with the investigation of radiation damage of solids by a rather new method at that time, molecular dynamics simulation. As a result, it was found that the zone of spontaneous recombination of point defects in α-iron and silicon depended on hydrostatic pressure and stress state that in its turn influenced on swelling of nuclear fuel materials. This pioneering work allowed formulating the recommendations for reduction of this effect, limiting the reliability of heat-eliminating elements of a nuclear reactor. With the passage of time, his interests moved to the field of micro and nanoelectronics, their foundations and technological applications. The results of these investigations are summarized in the textbook “Introduction to microelectronics CAD. Physical simulation of technology and device”. The last years of his life were devoted to study of new perspective materials for nanoelectronics and spintronics on the basis of ab initio simulations. The materials included graphene, ferromagnetic shape memory alloys, and biological systems (membrane proteins). The methods employed were based on quantum
mechanics (density functional approach) and molecular dynamics with wide use of computers.

During the years of active research, Nelaev and colleagues published more than 250 papers. He took an active part in many international and all-union conferences and symposia. In addition to intensive research activity, teaching was an important part of Nelaev’s life. He lectured a large number of original courses on different parts of physics. Of special note is his role in the development of molecular dynamics investigations in the Soviet Union and after its disintegration in Russia and Belarus.

It should be remembered that molecular dynamics was born in 1956, when two young scientists, B.J. Alder and T.E. Wainwright, applied for a calculation of motion in a liquid a new method. Molecular dynamics draws its name from those first computational experiments. As would be expected, the pioneering study by Alder and Wainwright has not found a wide response because physics of fluids was a rather narrow field of action for scientists. The situation has changed four years later when the work “Dynamics of radiation damage” was done under the direction of G.H. Vineyard. The Djinn appeared from a bottle. “Molecular dynamics is Maxwell demon, who knows everything on the motion of all molecules.” In the middle of seventies the number of molecular-dynamics results became so large that the First International Conference on Computer Simulations Applied to Materials took place in the United States of America in April, 1976.

At that time the number of molecular-dynamics researchers in the Soviet Union did not exceed two dozens. It was connected with lack of computers as well as with lack of understanding from the side of majority of old generation scientists. Nevertheless, In March, 1976, All-Union Seminar on Computer Simulations of Radiation and Other Defects was established on the basis of Leningrad Polytechnic Institute (Department of Metal Physics) and A.F. Ioffe Physico-Technical Institute of Academy of Sciences of the U.S.S.R. (Theoretical Department). Before the Soviet Union disintegration, 31 Seminars and 3 All-Union Schools were hold in different parts of the Soviet Union (Russia, Ukraine, Belarus, Kazakhstan, Uzbekistan, Georgia, Latvia, etc.). Their proceedings were published by A.F. Ioffe Physico-Technical Institute.

Being a young scientist at that time and hence having no prejudices, Vladislav Nelaev took an active part almost in all these actions. He did not only attend the meetings reporting on his own investigations, but organized four seminars in Belarus (Raubichi and Staiki, Olympic centers near Minsk, in 1982; Minsk, 1986; Raubichi, 1991). This activity promoted molecular dynamics investigations in Belarus. Then there came interlunation.

In June, 1997, NDTCS Workshop, a successor of the All-Union Seminar, appeared like a phoenix from ashes. From the very beginning Nelaev participated in all its meetings. Moreover, being the leading specialist on molecular dynamics in Belarus, he organized and conducted two specialized seminars “Frontiers of Nanoelectronics: Nanomeeting” in 2003 (Minsk, Belarus) and in 2004 (Szczecin, Poland). In 2007 Nelaev became a member of Executive Committee of the International NDTCS Society as the representative of Belarus. He was Co-Chairman of Workshop NDTCS-2008 and of Workshop NDTCS-2013. Having incontestable authority in science and engineering, Nelaev succeeded in finding such sponsors as Research and Production Corporation Integral, Motorola, Silvaco Data Systems, Scanwest, LG Electronics, Infopark.

There is no doubt that Nelaev was a splendid, sincere, decent, and noble person with a great sense of responsibility for any problem he dealt with. He was a very hard-working person with high standards for himself as well as for his colleagues. We will hold Vladislav Victorovich Nelaev as an eminent person, scientist, and teacher in our hearts forever.

Colleagues and Friends