SCIENTIFIC TREASURY CREATED BY PROFESSOR E.P. POKATILOV

V.M. Fomin [a,b,c]

[a] *Theoretische Fysica van de Vaste Stoffen (TFVS), Departement Natuurkunde, Universiteit Antwerpen, 171, Groenenborgerlaan, B-2020, Antwerpen, Belgium*
[b] *PSN, COBRA, Technische Universiteit Eindhoven, P.O.Box 513, 5600 MB Eindhoven, The Netherlands*
[c] *Physics of Multilayer Structures, Department of Theoretical Physics, State University of Moldova, 60, A. Mateevici, MD-2009, Chisinau, Republic of Moldova*
(Received 17 April 2007)

The brilliant creative activity of Professor Evgenii Petrovich Pokatilov, Associate member of the Academy of Sciences of Moldova, member of the Academy of Natural Sciences of Russia, winner of the State Prize of Moldova, over more than 55 years provided an outstanding contribution to the field of solid-state physics, which has been recognized by the physical community worldwide. In the present paper, I briefly overview the key directions of his scientific research, which represent Prof. E.P. Pokatilov as a visionary with a powerful and penetrating mind.

1. Early years

From 1950 to 1961, Prof. E.P. Pokatilov was engaged in investigations of thermoelectricity and of transport phenomena occurring in semiconductors with a 'loop of extrema' in the conduction band, for example, in CdSe structures. His first published paper was devoted to the analysis of the impurity band in ionic semiconductors [1]. The other field of his investigations was drag of electrons by sonic flows with subsequent amplification ping of sound in the presence of an electric field. His papers on the electron resonance in supersonic waves and the resonance absorption of supersonic energy by electrons in magnetic field were published in *ZhETF* [2, 3]. In 1961, he defended his PhD thesis *Some Problems of the Interaction of Electron with Acoustical Vibrations and Impurities in Semiconductors* at the Institute of Physics of Ukrainian Academy of Sciences in Kiev.

In 1963 through 1975, Prof. E.P. Pokatilov performed pioneering investigations of polaron states in piezoelectric crystals. He calculated the ground state energy and the effective mass for the aforementioned crystals and developed the theory of cyclotron absorption [4-6]. Calculations performed for CdS and InSb crystals revealed a close agreement between theoretical and experimental data. Magnetically affected hydrogen-like systems were another subject of his investigations, see review [7]. In paper [8], a very useful variational scheme was proposed together with M.M. Rusanov for calculation of the energy levels of the hydrogen-like systems in magnetic field, which was extensively cited. Prof. E.P. Pokatilov and his coworkers performed variational studies of the energy spectra of impurity states with the electron-phonon interaction taken into account (together with K.S. Kabisov) and of the electron states in crystals in the impurity and magnetic fields (together with M.M. Rusanov) (see review [9]), trapping of charge carries by shallow impurities and thermoionization of shallow impurities [10].

In 1971, Prof. E.P. Pokatilov was awarded a title of Doctor of the Physical & Mathematical Sciences [equivalent to Doctor rerum naturam habilitat] by the Institute of Semiconductors of Ukrainian Academy of Sciences (Kiev) for the thesis: *Polaronic and Dissipative-Relaxational Processes Due to Lattice Imperfections.*

Since 1975 Prof. E.P. Pokatilov has been heading applied research aimed at a development of space-time light modulators operating in real-time mode. The theory of potential for multi-layered systems was developed to analyze the distribution of electric potentials across the layers as a function of the values of dielectric constant and layer thickness. This theory was used to obtain the optimum sensito-resolvometric parameters for the multilayer structures. Liquid crystal-semiconductor samples on the basis of GaAs and CdTe structures were produced and demonstrated a good photosensitivity and resolution performance. Prof. E.P. Pokatilov patented a number of inventions in this field.

2. Path integrals

A path-integral derivation of the tensor of the electron conductivity in a magnetic field was performed for all main mechanisms of the electron-phonon interaction and extended to the electron scattering on impurities by Prof. E.P. Pokatilov together with A.A. Klyukanov; those results were published in *ZhETF* [11, 12].

In 1975 through 1978 investigations based on Feynman path integration method carried out by Prof. E.P. Pokatilov together with the present author provided a new development to the theory of interaction of strong electromagnetic radiation with free charge carriers in semiconductors. Non-linear optical characteristics of light absorption and refraction, self-focusing, Kerr effect and Faraday rotation effects were calculated. The effect of prevalent scattering mechanism of non-linearity factors versus a radiation energy relationship was theoretically defined. The results of this study were used to account for the laser-induced breakdowns in crystals.

In the further work, the path-integration approach was extended using a method of path integration over Wick symbols of the second quantization operators, see the textbooks by Prof. E.P. Pokatilov and the present author [13-15]. The obtained representation was applied to derive basic relations of quantum statistics and of kinetic theory. Thus, the potentialities of the Feynman method were extended which provided grounds to derive a quantum kinetic equation and to calculate transport coefficients taking into account quantum-mechanical and quantum-statistical degeneracy of electrons. These investigations were represented in a big number of research papers, in a monograph [16] (together with S.N. Klimin and the present author) and in a review published in *Physics Reports* [17].

3. Multi-layer structures

In another series of fundamental research, which has been progressing since 1973, Prof. E.P. Pokatilov focuses on analyses of vibrational excitations of lattice, polarons and excitons in multi-layer structures (MLS) and superlattices (SL). Those studies were conducted with S.I. Beril and further also with the present author. Distributions of electric and magnetic fields for polariton eigenwaves in the layers have been studied. The theory of potential has been developed embracing potentials originating from various kinds of electric field sources in multi-layer structures: bulk and surface charges and polarization of the lattice. The polarization potential was used to evaluate normal modes for polar vibrations and to derive the Hamiltonian for the electron-phonon interaction in MLS and SL. On that basis, a number of polaron theory problems were solved, defined as follows: the interface polaron, the slab polaron, the levitating polaron, the exciton in MLS and SL. The latter cases showed a good agreement with a number of experimental data. Further, a special approach was developed to derive the Hamiltonian of the electron-phonon interaction, taking into account additional boundary conditions. Within that approach, eigenmodes were obtained with symmetry observed in the Raman scattering experiments in GaAs/AlAs superlattices. These studies were reflected in a large number of research papers and in monograph [18] (together with S.I. Beril and the present author). The groundbreaking nature of this scientific direction was recognized by awarding Prof. E.P. Pokatilov, Prof. S.I. Beril and the present author Diploma of a scientific discovery *Phenomenon of the Propagation of Spatially-Extended Interface Phonon Polaritons in Composite Superlattices* by the Academy of Natural Sciences of Russia (Moscow) in 1999.

4. Nanophysics

Prof. E.P. Pokatilov was among the first theorists not only in Moldova but in the whole Soviet Union who had the vision of great potentialities of the emerging new area of nanostructures. A cycle of papers by Prof. E.P. Pokatilov and the present author, published in 1983-1985 [19], laid a methodological basis of the theory of potential due to bulk and interface charge carriers and polarization fields for multi-layered structures with an arbitrary number of layers. The theory was subsequently widely applied for a systematic derivation of phonon modes and the electron-phonon interaction Hamiltonians (within the framework of a dielectric continuum model), the inter-electron interaction and the electron self-interaction potentials for planar (see [18] and references therein), spherical and cylindrical multi-layer nanostructures [20].

Starting from 1994, Prof. E.P. Pokatilov has focused his attention on the principal problems of nanophysics. Since 1995 this direction of studies has become a field of intensive and fruitful collaboration between Prof. E.P. Pokatilov and his laboratory FSMMM at the State University of Moldova and Prof. J.T. Devreese and his laboratory TFVS at the University of Antwerpen. Systems of low dimensions and low dimensionality were profoundly analyzed by Prof. E.P. Pokatilov in a big number of scientific papers and in a recent review [21] (together with J.T. Devreese and the present author).

4.1. Polarons in nanostructures

In a cycle of papers, Prof. E.P. Pokatilov and his co-authors analyzed specific features of energy spectra of charge carriers and phonons due to the size and shape (geometry) of quantum wells, wires and dots. For cylindrical quantum wires and spherical quantum dots, normal modes of polar optical vibrations were obtained and the Hamiltonian of the electron-phonon interaction was derived, taking into account the dispersion of bulk polar optical modes. For planar structures, with special choice of the additional boundary conditions, the hybrid modes were obtained (originating from bulk longitudinal and interface modes) and also the respective Hamiltonian of the electron-phonon interaction was derived. Interaction of free and bound charge carriers with each other and with phonons in nanostructures was a topic of special investigation.

Energy spectra of a magnetopolaron with infinite and finite potential barriers in cylindrical quantum wires were obtained. In the latter case, a gradual transformation of the polaron in the quantum wire-well into the polaron in the barrier and a change of the polaron contributions (due to the bulk, interface-in, interface-out phonons) were analyzed with decreasing of the cylinder radius. Applying the Feynman variational principle, Prof. E.P. Pokatilov investigated the polaron characteristics (energy shift, mass, number of phonons in the polaron cloud) for a polaron of arbitrary coupling in the ellipsoidal quantum dot [22]. A fundamental conclusion was obtained that, with confinement strengthening, regions of the weak and intermediate coupling shorten, while the strong-coupling region widens. For a "squeezed" polaron state in a quantum dot, when the radius of the confinement potential R is smaller than the polaron radius R_p, the effective electron-phonon coupling constant is scaled as R_p/R.

The problem of existence of stable bipolaron states was investigated for quantum wires and quantum dots. It was established that in case of quantum wires the bipolaron binding energy monotonically increases with decreasing radius of a quantum wire, whereas in quantum dots the binding energy varies in a complicated manner, passing through a minimum within the domain $R < R_p$. Among other fundamental achievements by Prof. E.P. Pokatilov, the analysis of the influence of the valence band degeneracy on the acceptor states of a hole polaron, including resonant excited states, is noteworthy.

4.2. Optical properties of quantum wires and quantum dots

Another field of research performed by Prof. E.P. Pokatilov is related to manifestation of confinement effects on the electron-hole and the electron-phonon interactions in optical spectra of nanostructures.

Changing of the position and the shape of the cyclotron and cyclotron-phonon resonance bands of a magnetopolaron was investigated as a function of the quantum wire radius. Of special importance is a difference of shape found for the cyclotron resonance bands caused by the interaction of an electron with hybrid phonons versus dielectric-continuum-model (DCM) phonons.

In order to interpret the multiphonon photoluminescence and Raman scattering spectra in spherical semiconductor nanocrystals, in particular with structure imperfections, a theory was developed [23, 24] comprising the exciton interaction with both adiabatic and Jahn - Teller phonons and also the external nonadiabacity (pseudo Jahn - Teller effect). The effects of nonadiabacity of the exciton-phonon system are shown to lead to a significant enhancement of the phonon-assisted transition probabilities and multiphonon photoluminescence spectra are considerably different from the Franck - Condon progression. Calculated optical spectra compare well with experimental data in photoluminescence and Raman scattering in various types of quantum dots (e.g., in spherical CdS and PbS quantum dots) [23, 24].

In 2000, a theory of the electron and hole energy spectra for the multilayer CdS/HgS/CdS quantum well-quantum dots was developed on the basis of the eight-band model [25]. Electron states in single rectangular quantum wires, finite and infinite lattices of such wires were investigated. Within the non-adiabatic theory, photoluminescence spectra of tetragonal CdS/HgS/CdS quantum well-quantum dots are calculated in a good agreement with experiment - this work was published in *Physical Review Letters* [26]. A theory of confined polar optical phonons in quantum-dot structures of arbitrary shape has been developed and applied to obtain the interface optical phonon modes in tetragonal CdS/HgS/CdS quantum well-quantum dots [26].

4.3. Quantum transport

A theory considering the influence of the electron-phonon scattering on current voltage characteristics has been developed for cylindrical nanosize silicon-based metal-oxide-semiconductor structures [27]. An important basis for this theory was laid in the studies of the equilibrium state for this system [28].

4.4. Multi-quantum-wells

Photoluminescence spectra of the AIN/GaN/AIN heterostructures have been investigated as a function of the thickness of GaN layers and the magnitude of the built-in electric field. The theory provides a good quantitative interpretation of the experiment without using fitting parameters.

Prof. E.P. Pokatilov in collaboration with Prof. A.A. Balandin have developed a continuum theory of elastic vibrations for heterostructures possessing hexagonal symmetry. Energy spectra are derived for hetero- or nanostructures coated with acoustically hard and acoustically soft material. It is noteworthy, that in the latter case, the “phonon depletion effect” is revealed: the low-frequency vibrations do not penetrate into an acoustically hard layer [29]. On the basis of those vibrational spectra, a novel theoretical approach to transport phenomena (mobility, thermopower, thermoconductance) is developed for nanoscale heterostructures [30, 31]. Within this approach, a multi-band theory of electronic transitions has been developed that takes into account both acoustical and optical phonons. It is demonstrated that in the structures with a built-in electric field, the mobility can be appreciably increased by compensating the built-in field using an external electric field.

The proposed scheme of a conducting channel with nanogrooves, which isolate the electron wave function from the channel boundaries, allows for a significant increase of the electron mobility. In heterostructures without a built-in field, a novel effect of oscillations of mobility as a function of the width of the conducting channel is revealed. Theoretically predicted by Prof. E.P. Pokatilov new effects provide a significant contribution to the development of the electron-phonon engineering of electronic and optoelectronic devices at nanoscale.

Acknowledgement

It is my great honour and pleasure, to dedicate this paper to the insightful scientist, distinguished educator and charismatic personality - to my precious teacher, academic adviser and friend, Evgenii Petrovich, from fruitful and valuable interactions with whom I have benefited throughout all my life in science.

References

[1] E.P. Pokatilov, Impurity band in ionic semiconductors, Chisinau, Chisinau State University, UZ (Physics), 17, 141, (1955).
[2] E.P. Pokatilov, Electron resonance in supersonic waves, J. Exp. Theor. Physics, 36, 5, 1461, (1959).
[3] E.P. Pokatilov, Resonance absorption supersonic energy by electrons in magnetic field, J. Exp. Theor. Physics, 38, 4, 1153, (1960).
[4] E.P. Pokatilov, The local and polaron states of electron in piezoelectric crystals, Fiz. Tverd. Tela, 6, 9, 2809, (1964).
[5] E.P. Pokatilov, The contribution of the electron-piezoacoustic phonon interaction to the charge carrier ground state energy and effective mass and impurity absorption spectra, Fiz. Tverd. Tela, 7, 8, 2479, (1965).
[6] E.P. Pokatilov, A.A. Klyukanov, The piezopolaron energy and effective mass, Fiz. Tverd. Tela, 11, 766, (1969).
[7] E.P. Pokatilov, K.S. Kabisov and M. M. Rusanov, Impurity and free electron states in

magnetic field, Chisinau, Chisinau State University, UZ (Physics), 90, 27, (1967).
[8] E.P. Pokatilov, M.M. Rusanov, Variational calculation of the energy levels of the hydrogenlike systems in magnetic field, Fiz. Tverd. Tela, 10, 10, 3117, (1968).
[9] Yu.E. Perlin, E.P. Pokatilov, K.S. Kabisov, Sh.N. Gifeisman, B.S. Tshukerblat, M.M. Rusanov, Local electron states in crystals, Chisinau, Chisinau State University, UZ (Physics), 80, 3, (1965).
[10] E.P. Pokatilov, A.G. Cheban and M.M. Rusanov, The thermoionization of shallow impurities in cubic piezoelectric crystals, Fiz. Tverd. Tela, 7, 7, 2227, (1965).
[11] E.P. Pokatilov, A.A. Klyukanov, Tensor of the electron conductivity in the magnetic field (I), J. Exp. Theor. Physics, 60, 1, 313, (1971).
[12] E.P. Pokatilov, A.A. Klyukanov, Tensor of the electron conductivity in the magnetic field (II), J. Exp. Theor. Physics, 60, 5, 1878, (1971).
[13] E.P. Pokatilov, V.M. Fomin, Investigations of thermodynamic and kinetic properties of semiconductors by the path integration methods, Part 1: Fundamental of the path integration in phase and co-ordinate space, Chisinau, Chisinau State University, 1988.
[14] E.P. Pokatilov, V.M. Fomin, Investigations of thermodynamic and kinetic properties of semiconductors by the path integration methods, Part 2: Fundamental of the path integration over the Wick symbols, Chisinau, Chisinau State University, 1989.
[15] E.P. Pokatilov, V.M. Fomin, Investigations of thermodynamic and kinetic properties of semiconductors by the path integration methods, Part 3: Kinetic theory of semiconductors, Chisinau, State University of Moldova, 1991.
[16] E.P. Pokatilov, V.M. Fomin and S.N. Klimin, Transport and optical properties of semiconductors in strong fields, Chisinau, Shtiintsa, 1986.
[17] V.M. Fomin, E.P. Pokatilov, Non-equilibrium properties of charge carriers with arbitrary coupling to the lattice in semiconductors, Physics Reports, 158, 4-5, 205, (1988).
[18] E.P. Pokatilov, V.M. Fomin and S.I. Beril, Vibrational excitations, polarons and excitons in multi-layer structures and superlattices, Chisinau, Shtiintsa, 1990.
[19] E.P. Pokatilov, V.M. Fomin, Deposited paper No. 366M-05.84, Chisinau, MoldNIINTI, 1983; No. 388M-07.84, Ibid., 1984; No. 500M-05.85, Ibid., 1984; No.508-05.85, Ibid., 1984; No. 564M-01.86, Ibid., 1984.
[20] S.N. Klimin, E.P. Pokatilov and V.M. Fomin, Bulk and interface polarons in quantum wires and dots, Phys. Stat. Solidi (b), 184, 373, (1994).
[21] J.T. Devreese, V.M. Fomin and E.P. Pokatilov, Polarons and Bipolarons in Nanostructures. Part II. Polaron Effects in Nanostructures, in Handbook of Semiconductor Nanostructures and Nanodevices, Edited by A.A. Balandin and K.L. Wang. - American Scientific Publishers, Los Angeles, 4, 339, (2006).
[22] E.P. Pokatilov, V.M. Fomin, J.T. Devreese, S.N. Balaban and S.N. Klimin, Polarons in anellipsoidal potential well, Physica E, 4, 2, 156, (1999).
[23] V.M. Fomin, V.N. Gladilin, J.T. Devreese, E.P. Pokatilov, S.N. Balaban and S.N. Klimin, Photoluminescence of spherical quantum dots, Phys. Rev. B, 57, 2415, (1998).
[24] E.P. Pokatilov, S.N. Klimin, V.M. Fomin, J.T. Devreese and F.W. Wise, Multiphonon Raman scattering in semiconductor nanocrystals: Importance of nonadiabatic transitions, Phys. Rev. B, 65, 075316, 1, (2002).
[25] E.P. Pokatilov, V.A. Fonoberov, V.M. Fomin and J.T. Devreese, Development of an eight-band theory for quantum-dot heterostructures, Phys. Rev. B, 64, 245328, 1, (2001).
[26] V.A. Fonoberov, E.P. Pokatilov, V.M. Fomin and J.T. Devreese, Photoluminescence of tetra-hedral quantum dot quantum wells, Phys. Rev. Lett., 92, 127402, 1, (2004).

[27] S.N. Balaban, E.P. Pokatilov, V.M. Fomin, V.N. Gladilin, J.T. Devreese, W. Magnus, W. Schoenmaker, M. Van Rossum and B. Soree, Quantum transport in a cylindrical sub-0.1 μm silicon-based MOSFET, Solid-State Electronics, 46, 435, (2002).

[28] E.P. Pokatilov, V.M. Fomin, S.N. Balaban, V.N. Gladilin, S.N. Klimin, J.T. Devreese, W. Magnus, W. Schoenmaker, N. Collaert, M. Van Rossum and K. De Meyer, Distribution of fields and charge carriers in cylindrical nanosize silicon-based metal-oxide-semiconductor structures, J. Appl. Phys., 85, 6625, (1999).

[29] E.P. Pokatilov, D.L. Nika and A.A. Balandin, A phonon depletion effect in ultrathin heterostructures with acoustically mismatched layers, Appl. Phys. Lett., 85, 5, 825, (2004).

[30] E.P. Pokatilov, D.L. Nika and A.A. Balandin, Built-in field effect on the electron mobility in AIN/GaN/AIN quantum wells, Applied Physics Letters, 89, 113508, 1, (2006).

[31] E.P. Pokatilov, D.L. Nika and A.A. Balandin, Electron mobility enhancement in AIN/GaN/AIN heterostructures with InGaN nanogrooves, Applied Physics Letters, 89, 112110, 1, (2006).