

ABSTRACT AND REFERENCES

APPLIED PHYSICS

SOFTWARE SYSTEM DEVELOPMENT TO CALCULATE ELECTRO-OPTICAL CHARACTERISTICS OF ORGANIC LIGHT-EMITTING STRUCTURES (p. 4–7)

**Zenon Hotra, Khrystyna Ivaniuk, Marian Chapran,
Ores Bilas, Orestes Malanchuk**

The current state of development of organic electronics was analyzed in the paper. The problem of elaborating low-cost express measurements of chromatic and luminance characteristics as an alternative to costly, located in specialized laboratories was considered.

Methodology for determining the chromatic characteristics of organic light-emitting diodes (OLED), adapted to planar light-emitting structures was developed. The software to calculate the basic electro-optical characteristics of OLED, namely chromatic, luminance and current-voltage characteristics of organic light-emitting diodes according to the previously developed calculation methodology was designed.

The developed software solves the problem of cumbersome calculations of basic electro-optical characteristics of OLED, it is adapted to a modern operating system, provides calculation correctness and accuracy, easy interface to effectively solve the computational problem for the platform.

Keywords: chromaticity, luminance, OLED, light-emitting diodes.

References

- Bulovic, V., Gu, G., Burrows, P. E., Forrest, S. R., Thompson, M. E. (1996). Transparent light-emitting devices. *Nature*, 380 (6569), 29–29. doi: 10.1038/380029a0
- Organic and Printed Electronics. Available at: <http://www.oe-a.org/roadmap>
- Fyfe, D. (2009). LED Technology: Organic displays come of age. *Nature Photon*, 3 (8), 453–455. doi: 10.1038/nphoton.2009.132
- Sorokin, V. et al. (2009) Organic light-emitting structures - technologies of the XXI century. *Technology and designing in the electronic equipment*, 1, 3–9.
- Cherpak, V., Stakhira, P., Minaev, B., Baryshnikov, G., Stromylo, E., Helzhynskyy, I. et al. (2014). Efficient “Warm-White” OLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. *The Journal of Physical Chemistry C*, 118 (21), 11271–11278. doi: 10.1021/jp503437b
- Gotra, Z., Cherpak, V., Stakhira, P., Ivanyuk, H., Barilo, G., Helzhynskyy, I. (2013). Schematic development solutions automatic brightness control oleds glow. *Eastern-European Journal of Enterprise Technologies*, 6/12 (66), 99–103. Available at: <http://journals.uran.ua/eejet/article/view/19688/17580>
- Schubert, E. F., Miller, J. N.; Webster, J. G. (Ed.) (1999). Light-emitting diodes – An introduction. *Encyclopedia of Electrical Engineering*. John Wiley and Sons, New York, 326.
- Wójcik, V., Gotra, Z. Yu., Gotra, O., Grigoriev, V., Kalita, V., Miller, O., Potentski, E., Cherpak, V.; Gotra, Z. Yu. (Ed.) (2007). *Microelectronic Physical sensors: Scientific and educational publications*. Lviv: League-Press, 250.
- CSharp (programming language). Available at: [http://en.wikipedia.org/wiki/C_Sharp_\(programming_language\)](http://en.wikipedia.org/wiki/C_Sharp_(programming_language))
- MSDN, WindowsForms. Available at: <http://www.codenet.ru/progr/cpp/WinForms.php>
- MSDN, Oledb. Available at: <http://msdn.microsoft.com/ru-RU/library/system.dataoledb.oledbconnection.aspx>

METHODS FOR RECOVERING THE DISLOCATIONS CONTOUR LINE OF GALLIUM ARSENIDE WAFER OF DIGITAL IMAGE (p. 8–16)

Andrey Samoilov, Igor Shevchenko

The production volume growth of high-speed semiconductor devices based on gallium arsenide determines the necessity of semiconductor wafers dislocations control effectiveness increase.

In the article the methods of etching pits contour dislocation of gallium arsenide wafers recover have been suggested. Pretreatment performs binarization of the plate surface images highlighting the contours of the present parts of the image. The improved method of the width of the contour line determination defines the width of the line bounds of etch pits in suspected dislocation taking into consideration the variability of their reflection in the binarized image. The current width of the contour line is compared to the standard line width of dislocation contour.

The recovering method of contour line determines the suggested bounds of dislocations monitoring changes in the direction of the dislocation contour line in the plane of the plate image based on the value of the dislocation contour line width. The recovering method of contour line branching takes into account various options of adjacency line and determines the direction of further recovering of etch pits dislocation contour lines. It has been given a stepwise description of the methods.

Keywords: dislocation, etching pits, contour line recovering, gallium arsenide, digital image.

References

- Samoilov, A. N. (2013). Metody poluchenija konturov na cifrovyh rastrovyh izobrazhenijah s nechjotkim otobrazheniem dislokacij v plastinah GaAs. *Kompiuterno-integrovani tehnologii: osvita, nauka, vironictvo*, 63–69.
- Samoilov, A. N. (2014). Issledovanie mediannoj filtracii binarizovannyh konturov dislokacij plastiny GaAs na rastrovyh cifrovyh izobrazhenijah. *Materialy I Vseukrains'koi naukovo-praktichnoi konferencii «IT-Perspektiva», 10–11*
- Samoilov, A. N. (2012). Sravnenie effektivnosti globalnyh metodov binarizacii rastrovyh cvetnyh izobrazhenij. *Vestnik KrNU imeni Mihaila Ostrogradskogo*, 4 (75), 49–54.
- Samoilov, A. N., Shevchenko, I. V. (2013). Metod obnaruzhenija linij konturov v jarkostnyh perepadah predpolagaemyh granej binarizovanogo izobrazhenija sledov dislokacij na plastinah GaAs. *Avtomatizirovannye sistemy upravlenija i pribory avtomatiki*, 165, 22–27.
- Smith, S. M., Brady, J. M. (1997). SUSAN – A new approach to low level image processing. *International Journal of Computer Vision*, 34, 45–78.
- Rosten, E., Drummond, T. (2006). Machine learning for high-speed corner detection. *Proceedings of the European Conference on Computer Vision*, 430–443. doi: 10.1007/11744023_34
- Harris, C., Stephens, M. (1988). A combined corner and edge detector. *Alvey Vision Conference*, 147–151. doi: 10.5244/c.2.23
- Schmid, C., Mohr, R., Bauckhage, C. (1998). Comparing and evaluating interest points. *Proceedings of the International Conference on Computer Vision*, 230–235. doi: 10.1109/iccv.1998.710723
- Schmid, C., Mohr, R., Bauckhage, C. (2000). Evaluation of interest point detectors. *International Journal of Computer Vision*, 2, 151–172.
- Lowe, D. G. (2004). Distinctive Image Features from Scale-Invariant Keypoints. *International Journal of Computer Vision*, 60 (2), 91–110. doi: 10.1023/b.visi.0000029664.99615.94
- Bay, H., Tuytelaars, T., Van Gool, L. (2006). SURF: Speeded up robust features H. Bay. *Proceedings of the European Conference on Computer Vision*, 404–417. doi: 10.1007/11744023_32
- Ablamejko, S. V., Lagunovskij, D. M. (2000). *Obrabotka izobrazhenij: tehnologija, metody, primenie*. Minsk: Amalfeja, 304.
- Duda, R., Hart, H. (1973). Pattern classification and scene analysis. New York: John Wiley & Sons, 507.
- Freeman, H., Davis, L. S. (1977). A corner finding algorithm for chain coded curves. *IEEE Transactions on Computers*, 26 (3), 297–303. doi: 10.1109/tc.1977.1674825

15. Bribeasca, E., Guzman, A. (1978). Shape description and shape similarity for two dimensional regions. Paper presented at the 41h International Conference on Pattern Recognition, Kyoto, Japan.
16. Gonzalez, R., Woods, R. (2002). Digital image processing. Prentice Hall: Pearson Education, 616.
17. Epshtain, B. (2009). Detecting Text in Natural Scenes with Stroke Width Transform. Microsoft Corporation. Available at: <http://research.microsoft.com/pubs/149305/1509.pdf> (Last accessed: 23.12.12).
18. Pratt, W. (1978). Digital Image Processing. New York: John Wiley & Sons, 781.

THE STUDY OF INERTIAL BROWNIAN MOTOR WITH FLUCTUATING POTENTIAL ENERGY SIGN (p. 17–20)

Natalia Shkoda, Taisiya Korochkova, Viktor Rozenbaum,
Irina Shapochkina

The model of a Brownian motor with potential profile fluctuating in the sign, which is described by piecewise-linear periodic function, not belonging to the classes of symmetric and antisymmetric functions was presented. The model with the potential of this type shows unidirectional motion just in the case when inertialess motion is prohibited. The simplicity of the potential profile makes the problem analytically solvable and greatly simplifies the symmetry analysis. In approximations of the adiabatic mode of fluctuations and low inertia amendments, an analytical expression for the average velocity of the Brownian motor, which is different from zero only at a non-zero mass of the particle, i. e., motor effect is purely inertial was obtained. The resulting expression depends on the mass of the particle, parameters of the nonantisymmetric potential profile, the friction coefficient of the particle and temperature. It is shown that by changing the values of the parameter characterizing the profile shape deviation from antisymmetric allows to control the motion direction, and the dependence of the average velocity on this parameter is non-monotonic.

Keywords: nanomachines, nanomechanisms, Brownian motors, molecular pumps, subsurface diffusion, nonequilibrium fluctuations.

References

1. Smoluchowski, M. (1915). Brownsche Molecularbewegung unter Einwirkung äußerer Kräfte und deren Zusammenhang mit der verallgemeinerten Diffusionsgleichung. Ann. Phys., 48, 1103–1112.
2. Reimann, P. (2002). Brownian motors: noisy transport far from equilibrium. Physics Reports, 361 (2–4), 57–265. doi: 10.1016/s0370-1573(01)00081-3
3. Hänggi, P., Marchesoni, F. (2009). Artificial Brownian motors: Controlling transport on the nanoscale. Reviews of Modern Physics, 81 (1), 387–442. doi: 10.1103/revmodphys.81.387
4. Bressloff, P. C., Newby, J. M. (2013). Stochastic models of intracellular transport. Reviews of Modern Physics, 85 (1), 135–196. doi: 10.1103/revmodphys.85.135
5. Magnasco, M. O. (1993). Forced thermal ratchets. Physical Review Letters, 71 (10), 1477–1481. doi: 10.1103/physrevlett.71.1477
6. Klein, O. (1922). Zur statistischen Theorie der Suspensionen und Lösungen. Ark. för Mat. (German): Astron. och Fys., 16 (5), 51.
7. Kramers, H. A. (1940). Brownian motion in a field of force and the diffusion model of chemical reactions. Physica, 7 (4), 284–304. doi: 10.1016/s0031-8914(40)90098-2
8. Rozenbaum, V. M., Makhnovskii, Y. A., Shapochkina, I. V., Sheu, S.-Y., Yang, D.-Y., Lin, S. H. (2014). Inertial effects in adiabatically driven flashing ratchets. Physical Review E, 89 (5), 052131-1–052131-9. doi: 10.1103/physreve.89.052131
9. Ghosh, P. K., Hänggi, P., Marchesoni, F., Nori, F., Schmid, G. (2012). Brownian transport in corrugated channels with inertia. Physical Review E, 86 (2), 021112. doi: 10.1103/physreve.86.021112

10. Rozenbaum, V. M., Shapochkina, I. V. (2010). Neadiabaticheskie po-pravki k skorosti brounovskogo motora so slozhnym potencial'nym rel'efom. Pis'ma v ZhJeTF, 92 (2), 124–129.

IMPLEMENTATION PLASMA CHEMICAL ETCHING IN SUBMICRON TECHNOLOGY WSI STRUCTURE (p. 21–24)

Stepan Novosyadlyy, Liubomyr Melnyk Svyatoslav Novosyadlyy

With the development of a range of sub-micron devices elements inthralnyh large schemes, a number of problems, which either did not exist in the development of technology of integrated circuits with minimum dimensions of elements, or they did not identify significant. Thus reducing the geometric dimensions topology structures LSI, accompanied by a decrease in the thickness of the functional layers of multilayer structures used to represent a theoretical requirements for selectivity and anisotropy etching layers introduced defects and radiation damage to the surface of the processed wafers of silicon or gallium arsenide structures of integrated circuits. To determine the optimal technological regimes digestion ranged basic operating parameters of the process – the composition and working gas pressure, bias voltage and holder, holder distance to the source plasma. This article reveals the same perspective and alternative use of submicron technology of plasma chemical etching.

Keywords: plasma chemical etching, deposition, boron phosphorus silicate glass, photoresist, reactor.

References

1. Novosyadlyy, S. P. (2010). Sub-nanomykron technology structures LSI. Ivano-Frankivsk: City NV, 456.
2. Novosyadlyy, S. P. (2003). Physical and technological bases submicron VLSI. Ivano-Frankivsk: Simyk, 52–54.
3. Simon, V. V. Kornilov, L. (1988). Equipment of ion implantation. Moscow: Radio and Communications, 354.
4. Ryssel, H., Ruge, I. (1983). Ion implantation. Moscow: Science, 360.
5. Boltaks, B. I., Kolotov, M. N., Skoretyna, E. A. (1983). Deep centers in gallium arsenide tied up with their own structural defects. Physics, 10.
6. Afanasiev, V. A., Duhvskyy, M., Krasov, G. A. (1984). Equipment for impulse heat treatment of semiconductor materials. Microwave Electronics, 56–58.
7. Okamoto, T. (1985). Devices of ion implantation. Saymitsu Kikai, 1322–1325.
8. Cherylov, A. V. (1984). Investigation of electro-physical characteristics of ion-doped layers . Electronic equipment, 8–12.
9. Di Lorenzo, A. V., Kandeluola, D. D. (1988). Field-effect transistors on gallium arsenide. M: Radio and Communications, 489.
10. Watanabe, N., Asada, K., Kani, K., Otsuki, T. (1988). VLSI Design. Moscow: Mir, 304.

THE CURRENT DISTRIBUTION IN THE ELECTRODES OF ELECTROSURGICAL INSTRUMENTS DURING WELDING OF BIOLOGICAL TISSUES (p. 24–28)

Volodymyr Sydorets, Andrey Dubko

The analysis of the current density distribution in the electrodes of electrosurgical instruments during welding of soft biological tissues was performed. For that, the solution algorithm was developed, and the elliptic problem that simulates the skin effect in the compact section conductors was solved. Verification of the mathematical model of the current density distribution in a monopolar electrode by comparing with the experimental data during surgical operation of welding the retina to the choroid was carried out. The mathematical model shows that high-frequency current hardly flows in a round electrode and this explains the formation of coagulation

rings in practical studies of contact retia welding. This model is a one-dimensional elliptic problem for modeling the skin effect in conductors. By changing the current frequency in the electrodes it is possible to influence the width of the coagulation ring and solve the problem of its optimization since too great width of the ring leads to a more traumatic course of the operation, and too small - does not provide the quality and strength of the weld.

Keywords: welding of soft biological tissues, electrosurgical instruments, electrodes, high-frequency current, skin effect.

References

1. Drabkin, R. L. (1976). Apparat dlya visokochastotnoy elektrokhirurgii EN-57-M. Medisinskaya tekhnika, 1, 47–49.
2. Dolesikiy, S. Y., Drabkin, R. L., Lenyushkin, A. I. (1980). Visokochastotnaya elektrokhirurgiya. Moscow: Meditsina, 198.
3. Paton, B. E. (2004). Elektricheskaya svarka myagkikh tkanej v khirurgii. Avtomaticheskaya svarka, 9, 7–11.
4. Lebedev, A. V., Dubko, A. G. (2012). Osobennosti primeneniya teorii kontaktnoy svarki metallov k svarke zhivih tkanej. Tehnichna elektrodinamika, 2, 187–192.
5. Paton, B. E., Lebedev, V. K., Lebedev, A. V., Vasilchenko, V. A., Makarov, A. V., Myasnikov, D. V., Trunov, A. E. (2008). Patent 29797 Ukraina. Instrument dlya bipolyannoyi visokochastotnoy koagilyasiy zhivih tkanin tvarin I lyudini. Prior. 10.10.2007. Opubl. 25.01.2008.
6. Paton, B. E., Lebedev, V. K., Furmanov, Yu. A. et al. (2007) Patent 0276363 A1. Instrument and metod for the end-to-end reconnection of intestinal tissues. Publ. Date: Nov.29, 2007.
7. Podpryatov, S. S. (2008). Patent 36225 Ukraina. Sposob khirurgichnogo likuvannya gemoroyu cherez slizovo. Opubl. 27.10.2008. Byul. № 20.
8. Bozhko, N. V. (2008). Tehnologiya elektrozvaryuvannya pri vikonanni funktsii rezeksii gortani. Ukr. nauk.-med. volod. zhurnal, 3, 465.
9. Gluhenyk, A. I., Mihals, A. A. (2010) Raschetnaya otseinka sostavlyayushih impedansya tsilindricheskogo provodnika pri ih izmerenii na peremennom toke. Tehnichna elektrodinamika, 1, 15–22.
10. Suarez, A. G., Hornero, F., Berjano, E. J. (2010) Mathematical modeling of epicardial RF ablation of atrial tissue with overlying epicardial fat. The Open Biomedical Engineering Journal, 4 (1), 47–55. doi: 10.2174/1874120701004010047
11. Umanets, N. N., Naumenko, V. A., Dumbrova, N. E., Molchanyuk, N. I., Nazaretyan, R. E. (2014). Ultrastruktururnye izmeneniya sosudistoy obolochki i setchatki glaza krolika neposredstvenno posle vozdeystviya razlichnih rezhimov visokochastotnoy elektrosvarki biologicheskikh tkanej. Zhurnal NAMN Ukrainskogo, 20 (3), 359–364.
12. Popovic, Z., Popovic, B. D. (1999). Introductory Engineering Electromagnetics. Prentice Hall, 548.

SENSITIVITY OF ACOUSTIC EMISSION AMPLITUDE-ENERGY PARAMETERS TO CHANGE IN PROPERTIES OF TREATED COMPOSITE (p. 28–31)

Sergii Filonenko

Control and monitoring of composite machining is an important task in ensuring the quality of manufactured products. One of the ways to solve the problem is using the acoustic emission method. Modeling of the change in the energy of acoustic emission signals in the composite machining, depending on the parameter that is determined by its properties was considered. Data processing showed that the increase in the influencing parameter leads to a drop in acoustic emission energy parameters. Herewith, the dispersion with an average energy level of the generated signal has the largest drop. Comparison of changes in the acoustic emission energy-amplitude parameters showed that with the increasing influencing factor, percent drop of dispersion of the average energy level outstrips the percent drop of its average level and standard deviation, as well as all the amplitude parameters of acoustic emission signals. The results show that the dispersion of the average energy level of acoustic emission signals can be used to develop methods for control, diagnosing and

monitoring of the unevenness of the surface properties of manufactured products in the composite machining process.

Keywords: acoustic emission, composite, signal, amplitude, machining, material properties.

References

1. Dongre, P. R., Chidderwar, S. S., Deshpande, V. S. (2013). Tool Condition Monitoring in various machining operations and use of acoustic signature analysis. International Journal on Mechanical Engineering and Robotics, 1 (1), 34–38.
2. Ali, Y. H., Abd Rahman, R., Raja Hamzah, R. I. (2014). Acoustic Emission Signal Analysis and Artificial Intelligence Techniques in Machine Condition Monitoring and Fault Diagnosis: A Review. Jurnal Teknologi, 69 (2), 121–126. doi: 10.11113/jt.v69.3121
3. Mandal, S. (2014). Applicability of Tool Condition Monitoring Methods Used for Conventional Milling in Micromilling: A Comparative Review. Journal of Industrial Engineering, 2014, 1–8. doi: 10.1155/2014/837390
4. Mukhopadhyay, C. K., Jayakumar, T., Raj, B., Venugopal, S. (2012). Statistical analysis of acoustic emission signals generated during turning of a metal matrix composite. Journal of the Brazilian Society of Mechanical Sciences and Engineering, 34 (2), 145–154. doi: 10.1590/s1678-58782012000200006
5. Lu, P. (2013). An investigation into interface behavior and delamination wear for diamond-coated cutting tools. A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the department of mechanical engineering in the Graduate School of the University of Alabama, 155.
6. Qin, F., Hu, J., Chou, Y. K., Thompson, R. G. (2009). Delamination wear of nano-diamond coated cutting tools in composite machining. Wear, 267 (5–8), 991–995. doi: 10.1016/j.wear.2008.12.065
7. Thepsonthi, T. (2014). Modeling and optimization of micro-end milling process for micro-micromanufacturing. A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the Graduate School-New Brunswick Rutgers, The State University of New Jersey, 246.
8. Giriraj, B. (2012). Prediction of progressive tool wear using acoustic emission technique and artificial neural network. Journal of Civil Engineering Science: An International Journal, 1 (1–2), 43–46.
9. Fadare, D. A., Sales, W. F., Bonney, J., Ezugwu, E. O. (2012). Influence of Cutting Parameters and Tool Wear on Acoustic Emission Signal in High-speed Turning of Ti-6Al-4V Alloy. Journal of Emerging Trends in Engineering and Applied Sciences, 3 (3), 547–555.
10. Filonenko, S. F. (2015). Influencing processed composite material properties on acoustic emission. Eastern-European Journal of Enterprise Technologies, 2/5(74), 60–64. doi: 10.15587/1729-4061.2015.40191
11. Ren, Q., Balazinski, M., Baron, L. (2012). High-order interval type-2 Takagi-Sugeno-Kang fuzzy logic system and its application in acoustic emission signal modeling in turning process. The International Journal of Advanced Manufacturing Technology, 63 (9–12), 1057–1063. doi: 10.1007/s00170-012-3956-z

NANOREFRIGERANTS APPLICATION POSSIBILITIES STUDY TO INCREASE THE EQUIPMENT ECOLOGICAL-ENERGY EFFICIENCY (p. 32–40)

Mykola Lukianov, Olga Khliyeva, Vitaly Zhelezny, Yury Semenyuk

The results of experimental and theoretical studies of the TiO_2 and Al_2O_3 nanoparticle additives in the working fluid R600a/mineral oil on the eco-energy efficiency of the compressor system have been considered. The experimental setup (refrigeration compressor system) and the experimental methodology have been described.

Following working fluids have been selected for compressor refrigeration system: R600a/compressor oil; R600a/compressor oil/nanoparticle TiO_2 (1,0 and 0,48 wt. %.) and R600a/compressor oil/nanoparticles Al_2O_3 (0,52 and 0,08 wt. %.). The results of experimental studies of cooling capacity, compressor power and coefficient of

performance at the different values of working fluid flow rate in the compressor refrigeration system have been reported. It was shown that the nanoparticle additives may lead to increase in energy consumption of the compressor system up to 23 % at flow rate of the working fluid equal to 0.00025 kg/s at the evaporator temperature 258 K.

The method of eco-energy analysis has been proposed to science-based evaluation of an expediency of nanoparticle additives to the refrigeration equipment working fluids. This method is based on assessment of total equivalent greenhouse gases emissions on the equipment life cycle (TEGHGE).

Expressions to assessment the value of TEGHGE and the specific eco-indicator have been proposed. The values of TEGHGE and eco-indicator on the life cycle of the compressor system based on experimental data obtained for the cooling capacity and compressor power for different working fluids have been analyzed. It was shown that Al_2O_3 nanoparticle additives with 0.52 % mass concentration provide the best eco-energy effect.

Keywords: nanoparticles, nanofluids, compressor system, cooling capacity, coefficient of performance, ecological-and-energy analysis.

References

- UNEP 2014. Report of the Refrigeration, air Conditioning and Heat Pumps Technical Options Committee (2014). Assessment. Available at: http://www.montreal-protocol.org/Assessment_Panels/TEAP/Reports/RTOC/RTOC-Assessment-Report-2014.pdf
- Zhelezny, V. P. (2014). An application of nanotechnologies in refrigeration – perspectives and challenges. Proc. 11th IIR Gustav Lorentzen Conference on Natural Refrigerants, IIR Hangzhou, China.
- Fisher, S. K., Fairchild, P. P., Hughes, P. S. (1990). Global warming implications of replacing CFC. ASHRAE Journal, 34 (4), 14–19.
- McCulloch, A. (1994). Life Cycle Analysis to Minimise Global Warming Impact. Renewable energy, 5 (5–8), 1262–1269. doi: 10.1016/0960-1481(94)90160-0
- ISO 14040:2006 (2006). Environmental management – Life cycle assessment – Principles and framework.
- Zhelezny, V., Hlieva, O., Artemenko, S. (2004). Assessment of Total Equivalent of Greenhouse Gases Emission in the Industry CD Proceedings of the 3rd Europeans Congress "Economics and Management of Energy in Industry". Lisboa, Portugal.
- Zhelezny, V. P., Bykovets, N. P., Khliyeva, O. Ya, Stepanova, V. P., Sukhodol'skaya, A. B. (2004). Method of calculating the total equivalent greenhouse gases emissions in the industry Ekotekhnologhyy y resursoberezhnye [Energy thechnologies & resource saving], 6, 34–43. [in Russian]
- UNEP (1987). Montreal Protocol on Substances that Deplete the Ozone Layer. Final Act, 6.
- Kyoto Protocol to the United Nations Frame work Convention on Climate Change (1998). United Nations.
- Celen, A., Çebi, A., Aktas, M., Mahian, O., Dalkilic, A. S., Wongwises, S. (2014) A review of nanorefrigerants: Flow characteristics and Applications. International Journal of Refrigeration, 44, 125–140. doi: 10.1016/j.ijrefrig.2014.05.009
- Efstathios, E. (Stathis) Michaelides (2014). Nanofluidics Thermodynamic and Transport Properties Springer International Publishing Switzerland, 335. doi:10.1007/978-3-319-05621-0
- Nikitin, D., Zhelezny, V., Grushko, V., Ivchenko, D. (2012). Surface tension, viscosity, and thermal conductivity of nanolubricants and vapor pressure of refrigerant/nanolubricant mixtures. Eastern-European Journal of Enterprise Technologies, 5/5 (59), 12–17. Available at: <http://journals.uran.ua/ejet/article/view/4566/4230>
- Zhelezny, V. P., Semenyuk, Yu. V. (2012). Working medium of vapor compression refrigerator: properties, analysis, applications. Odesa: Feniks, 420. [in Russian]
- Bi, S., Shi, L., Zhang, L. (2008). Application of nanoparticles in domestic refrigerators. Applied Thermal Engineering, 28, 1834–1843. doi: 10.1016/j.applthermaleng.2007.11.018
- Bi, S., Guo, K., Liu, Z., Wu J. (2011). Performance of a domestic refrigerator using TiO_2 -R600a nano-refrigerant as working fluid. Energy Conversion and Management, 52 (1), 733–737. doi: 10.1016/j.enconman.2010.07.052
- Bi, S., Shi, L. (2007). Experimental investigation of a refrigerator with a nano-refrigerant. Journal of Tsinghua University, 47, 1999–2002.
- Padmanabhan, V. M. V., Palanisamy, S. (2012). The use of TiO_2 nanoparticles to reduce refrigerator ir-reversibility. Energy Conversion and Management, 59, 122–132. doi: 10.1016/j.enconman.2012.03.002
- Subramani, N., Prakash, M. J. (2011). Experimental studies on a vapour compression system using nanorefrigerant. International Journal of Engineering, Science and Technology, 3 (9), 95–102. doi: 10.4314/ijest.v3i9.8
- Wang, R., Wu, Q., Wu, Y. (2010). Use of nanoparticles to make mineral oil lubricants feasible for use in a residential air conditioner employing hydro-fluorocarbons refrigerants. Energy and Buildings, 42 (11), 2111–2117. doi: 10.1016/j.enbuild.2010.06.023
- Jwo, C. S., Jeng, L. Y., Teng, T. P., Chang, H. (2009). Effects of nanolubricant on performance of hydrocarbon refrigerant system. Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures, 27 (3), 1473–1477. doi: 10.1116/1.3089373
- Kumar, D. S., Elansezhan, R. D. (2012). Experimental Study on Al_2O_3 -R134a Nanorefrigerant in Refrigeration System. International Journal of Modern Engineering Research, 2 (5), 3927–3929.
- Sabareesh, R. K., Gobinath, N., Sajith, V., Das, S., Sobhan, C. B. (2012). Application of TiO_2 nanoparticles as a lubricant-additive for vapor compression refrigeration systems – An experimental investigation. International Journal Refrigeration, 35 (7), 1989–1996. doi: 10.1016/j.ijrefrig.2012.07.002
- Sajumon, K. T., Jubin, V. J., Sreejith, S., Aghil, V. M., Seeraj Kurup, P. N., Sarath, S. (2013). Performance analysis of nanofluid based lubricant. Proc. of International Conference on Energy and Environment – 2013 (ICEE 2013), 832–838.
- Kuleshov, D. K. (2014). Influence of TiO_2 nanoparticles on the energy efficiency of the refrigeration machines operating on isobutane. Eastern-European Journal of Enterprise Technologies, 5/8 (71), 47–52. doi: 10.15587/1729-4061.2014.28038
- Kuleshov, D. K., Krasnovskiy, I. N. (2014). Experimental Study of the Characteristics of Domestic Refrigerator Using Nanoflyuid R600A/ TiO_2 . Refrigeration Engineering and Technologies, 5 (151), 12–16. doi: 10.15673/0453-8307.5/2014.28690
- Zhelezny, V. P., Chen, G. M., Shestopalov, K. O., Melnyk, A. V. (2014). Experimental and theoretical investigation of heat transfer coefficient for boiling of the isobutene/compressor oil solution flow in the pipe. Proc. 11th IIR Gustav Lorentzen Conference on Natural Refrigerants, IIR, Hangzhou, China.
- Melnyk, V. A., Nikulin, A. G., Zhelezny, V. P. (2014). The Local Heat Transfer Coefficient Variation at the Boiling of the Isobutane/Compressor Oil Solution Flow in the Pipe. Proceedings of CONV-14: Int. Symp. on Convective Heat and Mass Transfer. Turkey.
- Cho, C., Yoo, H. S., Oh, J. M. (2008). Preparation and heat transfer properties of nanoparticle-in-transformer oil dispersions as advanced energy-efficient coolants. Current Applied Physics, 8 (6), 710–712. doi: 10.1016/j.cap.2007.04.060
- Independent Statistics and Analysis. Energy Information Administration. Available at: <http://www.eia.gov/>
- World Statistics. Available at: <http://world-statistics.org/>

METHOD FOR DETERMINING THE BULK TEMPERATURE OF THE ACHESON GRAPHITIZATION FURNACE CORE (p. 41–46)

Yevgen Panov, Anton Karvatskii, Serhii Leleka, Taras Lazarev, Anatoliy Pedchenko, Denis Shvachko

In order to reduce energy consumption in graphitization of electrode products in Acheson furnaces, a method for rapid assessment of the bulk temperature of the furnace core, which is based on the fur-

nace energy balance equation and takes into account active energy loss at the furnace entrance; heat loss from the core surface; heat loss and moisture evaporation; heat loss in the core booster gasification process was developed. The unknown coefficients of the method - the temperature dependences of the effective heat transfer coefficient from the core surface and the proportionality factor, which takes into account active energy loss in the direct core insulation heating, were determined by calculation using the verified numerical model of heat-electro-mechanical state of the Acheson furnace. Analysis of the results showed that the nature of temperature dependence of the proportionality coefficient, which takes into account active energy loss in the direct core insulation heating is similar to the temperature dependence of the specific electrical resistivity of the furnace core (core booster). Verification of the developed method showed good agreement with the numerical simulation results. The developed method was tested in conditions of the electrode manufacturer PJSC "Ukrgrafit", Ukraine and has allowed to reduce specific energy consumption while maintaining the necessary quality level of graphitized products.

Keywords: graphitization, Acheson furnace, gasification, energy loss, temperature, energy balance.

References

- Chalyh, E. F. (1990), Oborudovanie elektrodnyh zavodov. Moscow: Metallurgija, 238.
- Fialkov, A. S. (1979). Uglegrafitovyje materialy. Moscow: Jenergija, 320.
- Leleka, S. V., Panov, E. N., Karvaskyy, A. Ja. (2014), Teploelektricheskoe sostojanie pechej grafitirovaniya Achesona. Kiev, NTUU «KPI», 238.
- Znamerovskij, V. Ju. (1994), Matematicheskoe modelirovanie proceessa grafitacii. Moscow: Metallurgija, 64.
- Kuznecov, D. M., Fokin, V. P. (2001). Process grafitacii uglerodnyh materialov. Sovremennye metody issledovanija. Novocherkassk: Ju-RGTU, 132.
- Zhuchenko, A. I., Korzhik, M. V., Kutuzov, S. V. (2013), Keruvannya protsesom hrafatatsiyi pry vyrobnytstvi elektrodnoyi produktsiyi. Kiev, NTUU «KPI», 224.
- Yarymbash, D. S. (2012). Identification of furnace loop electrical parameters of power graphitization furnaces. Elektrotehnika i elektromehanika, 1, 49–54.
- Panov, Ye. M., Karvatskyy, A. Ya., Korzhik, M. V., Shylovych, I. L., Leleka, S. V. (2011). Primenenie modeli Drakera-Pragera dlja issledovanija sostojaniij pechi grafitacii. Visnik NTUU "KPI", Himichna inzhenerija, ekologija ta resursozberezhennja, 1 (7), 37–44.
- Shkulakov, E. E., Kuznecov, D. M. (2000). Osobennosti modelirovaniya temperaturnyh polej v pechah grafitacii prijamogo nagreva. Matematicheskie metody v tehnike i tehnologijah MMTT-2000, 3, 198–199.
- Panov, Ye. M., Kutuzov, S. V., Leleka, S. V., Shilovich, I. L., Bozhenko, M. F. (2007). Raschetno-eksperimental'noe opredelenie temperaturnyh polej kerna v P-obraznyh pechah grafitacii postojannogo toka. Promyshlennaja teplotehnika, 2, 22–28.
- Panov, Ye. M., Kutuzov, S. V., Urazlyna, O. Yu., Leleka, S. V., Shylovych, I. L., Bozhenko, M. F., Korzhik, M. V. (2007), Sposib vyznachennya serednoyi temperatury zahotovok v pechi hrafatatsiyi. UA patent No. 23,422. Kiev.
- Panov, Ye. M., Karvatskyy, A. Ya., Korzhik, M. V., Leleka, S. V., Pulinets, I. V., Lazarev, T. V. (2012). Sposib vypalyuvannya vuhatsevykh vyrobiv v bahatokamerniy kiltseviy pechi. UA patent No. 69,350. Kiev.
- Shulepov, S. V. (1972). Fizika uglegrafitovyh materialov. Moscow, USSR: Metallurgija, 256.
- Borisov, Ju. M., Lipatov, D. N., Zorin, Ju. N. (1985). Elektrotehnika Uchebnik dlja vuзов. 2th edition. Moscow, USSR: Jenergoatomizdat, 552.
- Kalechica, I. V. (Ed.) (1980). Himicheskie veshhestva iz uglja. Moscow, USSR: Himija, 616.
- Bogdanov, N. N. (1947). Polukoksovaniye i gazifikacija koksa. Moscow, USSR: Gosjenergoizdat, 268.

SELECTIVE ETCHING OF DIAMOND SINGLE CRYSTALS OBTAINED BY THERMAL-GRADIENT METHOD (p. 47–50)

Olena Suprun, Sergiy Ivakhnenko

Diamond single crystals were investigated using the selective etching. The crystals obtained by the thermal-gradient method using the Toroid type high-pressure device in the thermodynamic stability region at a pressure of 5.7–6.1 GPa and a temperature of 1420–1450 °C were examined. Diamond samples had a cubooctahedral habit with the size of 2–4 mm; the crystal weight of 0,1–0,26 ct. Studies were carried out on plates prepared by parallel plane grinding (100). Before etching, diamond crystals were purified with a mixture of hydrochloric and nitric acids, then washed with chromic mixture. Etching was carried out using potassium nitride and potassium hydroxide at atmospheric pressure and a temperature of 550±580 °C in a platinum crucible. Experiments were performed in five stages, the total etching time – 85 min. A decrease in weight and changes in the etching patterns of diamond single crystals was observed. It was shown that diamond single crystals have a high perfection degree and low etchability at these temperatures.

Keywords: diamond single crystals, dislocation structure, selective etching, potassium nitride, potassium hydroxide, etch pits.

References

- Novikov, N. V., Nachalna, T. A., Ivakhnenko, S. A., Zanevsky, O. A., Belousov, I. S., Malogolovets, V. G. et al. (2003). Properties of semiconducting diamonds grown by the temperature-gradient method. Diamond and Related Materials, 12 (10-11), 1990–1994. doi: 10.1016/s0925-9635(03)00317-0
- Burns, R., Kessel, S., Sibanda, M., Welbourn, C. et al. (2001). Large synthetic diamonds. The 8th NIRIM International symposium on Advanced materials (ISAM 2001), Tsukuba, Japan, 105–111.
- Kanda, H. (2000). Large diamonds grown at high pressure conditions. Brazilian Journal of Physics, 30 (3), 482–489. doi: 10.1590/s0103-97332000000300003
- Burns, R., Hansen, J., Spits, R., Sibanda, M et al. (1999). Growth of high purity large synthetic diamond crystals. Diamond and Related Materials, 8, 1433–1437
- Novykov, N. V. (Ed.) (2003). Sverkhtverdye materyaly. Poluchenye y prymeneniye. Monohraffya v 6 tomakh. Tom 1: Syntez almaza y podobnuykh materyalov. Kyiv: ISM im. Bakulya, YPTs «Alkon» NANU, 318
- Hryhor'ev, D. P., Shafranovskyy, Y. Y. (1942). Novie opiti po rastvorenyyu almaza. Zapiski Vserossijskogo obshchestva, 1–2 (70).
- Kukharenko, A. A., Tytova, V. M. (1957). Novye dannye po rastvorenyyu krystallov almaza. Uchenie zapiski LHU, 215.
- Tytova, V. M. (1962). Novye dannye po rastvorennyyu almaza. Zapiski Vses. Myn. ob-va, 4 (91).
- Varshav'skyy, A. V. (1968). «Anomal'noe dvulucheperekolmenye y vnutrennyaya morfolohyya almaza». Moscow: Nauka, 92.
- Varshav'skyy, A. V. (1965). Zapiski vsesoyuznogo myneralohychnogo obshchestva, 2 ser. Moscow, Izd-vo AN SSSR, 4 (94), 177–189.
- Bokyy, H. B., Epyshyna, N. Y., Semenova-Tyan-Shanskaya, A. S. (1968). Travlenye oktaedrycheskykh hranej yakut-skykh almazov s tsel'yu podscheta plotnosti dyslokatsyy. Almazy, nauchno-tehnicheskyy referatyvnyy sbornyyk, 4, 3–5.
- Khokhryakov, A. F. (2004). Rastvorennye almaza: eksperimental'noe issledovaniye protsessov y model' krystallomorfologicheskoy evolyutsyy. Ynstytut myneralohyy y petrohrayff RAN, Novosib, 36.
- Pal'yanov, Yu. N., Sokol, A. G., Borzov, Yu. M., Khokhryakov, A. F. (2002). Fluid-bearing alkaline-carbonate melts as the medium for the formation of diamonds in the Earth's mantle: an experimental study Lithos, 60 (3–4), 145–159.

14. Pal'yanov, Yu. N. (1997) Rost krystallov almaza (eksperimental'noe yssledovaniye). Ynstitut myneralohyy y petrohrayf RAN, Novosyb, 37.
15. Hryhor'ev, O. N., Epyfanov, V. Y., Kononenko, V. Y. et. al. (1973). Yzuchenye poverkhnosti almaza metodom yzbyratel'noho travlynyya. Metallofizyka. Kiev: Naukova dumka, 81–89.
16. Zhykhareva, V. P. (1980). Opty po travlenyyu syntetycheskykh almazov. Myneralohchnyy sbornik L'vovskoho hosudarstvennogo unyversyteta, 34 (1), 73–76.
17. Strong, H. M., Wentorf, R. H. (1972). The growth of large diamond crystals. Die Naturwissenschaften, 59 (1), 1–7. doi: 10.1007/bf00594616
18. Vereschagin, L. F., Bakul, V. N., Semerchan, A. A., Prikhna, A. I., Popov, V. V. et. al. (1974). Pat.1360281 Great Britain, MKI 01J 3/00 pparatus For Developing High Pressures And High Temperatures: Pat. GB 1360281.

ESTIMATION OF ATOMIC CHARGES IN BORON NITRIDES (p. 50–57)

Levan Chkhartishvili, Shorena Dekanositze, Nodar Maisuradze,
Manana Beridze, Ramaz Esiava

Boron nitrides (BN) are compounds with bonds of covalent-ionic type. Therefore, binding polarity is an important characteristic affecting their physical properties. Dependencies of measurable parameters on static effective charges of constituent atoms are so complex that, these are virtually undetectable experimentally. As for the theoretically obtained atomic charges in boron nitrides, they are characterized by a significant scatter making them almost unreliable. The general reason for this lies in the impossibility of unambiguous division of the electron density between atoms of elements. It pushes the search for a semiempirical solution of the problem.

We have derived the expression for the effective charge number q in a binary compound (effective charges of B and N atoms should be $+qe$ and $-qe$, respectively) depending on number of molecules N in primitive parallelogram, its sectional area S transverse to the external electric field direction, Young's modulus Y and permittivity ϵ in same direction. Semiempirically estimated values of q (in a- and c-directions) are physically reasonable: hexagonal h-BN – 0.35 and 0.09, cubic c-BN – 0.49, and wurtzite-like w-BN boron nitrides – 0.76 and 0.50.

Also quite natural are qualitative conclusions: in h-BN intralayer bonds polarity is much stronger than that between hexagonal layers; bonds are stronger polarized in denser modifications c-BN and w-BN, which are characterized by higher coordination numbers as well; bonds polarities in c-BN and along c-axis in w-BN are almost indistinguishable; and bonds polarities in a- and c-directions in w-BN are different.

Obtained static charges can be used in the refinement of the BN electron structure calculations.

Keywords: point atomic charges model, semiempirical estimates, boron nitrides.

References

1. Prasad, C., Dubey, J. D. (1984). Electronic Structure and Properties of Cubic Boron Nitride. *Physica Status Solidi B*, 125 (2), 629–638. doi: 10.1002/pssb.2221250223
2. Born, M., Huang, K. (1954). *Dynamical Theory of Crystal Lattices*. Oxford: Oxford University Press, 414.
3. Böttger, H. (1983). *Principles of the Theory of Lattice Dynamics*. Weinheim: Physik–Verlag, 330.
4. Ghosez, P., Michenaud, J.-P., Gonze, X. (1998). Dynamical atomic charges: The case of AB O 3 compounds. *Physical Review B*, 58 (10), 6224–6240. doi: 10.1103/physrevb.58.6224
5. King-Smith, R. D., Vanderbilt, D. (1993). Theory of polarization of crystalline solids. *Physical Review B*, 47 (3), 1651–1654. doi: 10.1103/physrevb.47.1651
6. Resta, R. (1994). Macroscopic polarization in crystalline dielectrics: the geometric phase approach. *Reviews of Modern Physics*, 66 (3), 899–915. doi: 10.1103/revmodphys.66.899
7. Baroni, S., de Gironcoli, S., Dal Corso, A., Giannozzi, P. (2001). Phonons and related crystal properties from density-functional perturbation theory. *Reviews of Modern Physics*, 73 (2), 515–562. doi: 10.1103/revmodphys.73.515
8. García, A., Cohen, M. L. (1993). First-principles ionicity scales. I. Charge asymmetry in the solid state. *Physical Review B*, 47 (8), 4215–4220. doi: 10.1103/physrevb.47.4215
9. García, A., Cohen, M. L. (1993). First-principles ionicity scales. II. Structural coordinates from atomic calculations. *Physical Review B*, 47 (8), 4221–4225. doi: 10.1103/physrevb.47.4221
10. Everage, R. A. (1982). *Quantum-Chemical Methods in Theory of Solids*. Leningrad: Leningrad University Press.
11. Will, G., Kirsch, A., Josten, B. (1986). Charge density and chemical bonding in cubic boron nitride. *Journal of the Less Common Metals*, 117 (1–2), 61–71. doi: 10.1016/0022-5088(86)90012-3
12. Will, G., Kirsch, A. (1986). Electron density distribution studies on cubic BN, TiB₂ and boron carbide B₁₃C₂. *AIP Conference Proceedings*, 140, 87–96.
13. Kawai, J., Muramatsu, Y., Kobayashi, M., Higashi, I., Adachi, H. (1993). Discrete-variational Hartree–Fock–Slater calculations of B36N24 with comparison to C60. *Japanese Journal of Applied Physics*, 10, 72–77.
14. Pokropivny, V. V., Skorokhod, V. V., Oleinik, G. S., Kurdyumov, A. V., Bartnitskaya, T. S., Pokropivny, A. V., Sisonyuk, A. G., Sheichenko, D. M. (2000). Boron Nitride Analogs of Fullerenes (the Fulbornenes), Nanotubes, and Fullerites (the Fulborenes). *Journal of Solid State Chemistry*, 154 (1), 214–222. doi: 10.1006/jssc.2000.8838
15. Vandebosch, R. (2003). Gas-phase anions containing B and N. *Physical Review A*, 67 (1). doi: 10.1103/physreva.67.013203
16. Silver, A. H., Bray, P. J. (1960). NMR Study of Bonding in Some Solid Boron Compounds. *The Journal of Chemical Physics*, 32 (1), 288–292. doi: 10.1063/1.1700918
17. Bray, P. J. (1986). NMR studies of borates and borides. *AIP Conference Proceedings*, 140, 142–167.
18. Khushidman, M. B., Neshpor, V. S. (1970). Investigation of hexagonal and cubic boron nitrides by electron paramagnetic resonance. *Powder Metallurgy*, 8, 72–73.
19. Zunger, A. (1974). A molecular calculation of electronic properties of layered crystals. II. Periodic small cluster calculation for graphite and boron nitride. *Journal of Physics C: Solid State Physics*, 7 (1), 96–106. doi: 10.1088/0022-3719/7/1/017
20. Joyner, D. J., Hercules, D. M. (1980). Chemical bonding and electronic structure of B₂O₃, H₃BO₃, and BN: An ESCA, Auger, SIMS, and SXS study. *The Journal of Chemical Physics*, 72 (2), 1095. doi: 10.1063/1.439251
21. Xu, Y.-N., Ching, W. Y. (1991). Calculation of ground-state and optical properties of boron nitrides in the hexagonal, cubic, and wurtzite structures. *Physical Review B*, 44 (15), 7787–7798. doi: 10.1103/physrevb.44.7787
22. Lawniczak-Jablonska, K., Suski, T., Gorczyca, I., Christensen, N. E., Attenuator, K. E., Perera, R. C. C. et. al. (2000). Electronic states in valence and conduction bands of group-III nitrides: Experiment and theory. *Physical Review B*, 61 (24), 16623–16632. doi: 10.1103/physrevb.61.16623
23. Levin, A. A., Syrkin, Ya. K., Deyatkin, M. E. (1966). Selection of parameters for semi-empirical description of electronic structure of tetrahedral crystals. *Journal of Structural Chemistry*, 7, 583–588.
24. van Vechten, J. A. (1969). Semiempirical band calculations. *Physical Review*, 187, 1007–1016.
25. Samsonov, G. V. (1969). *Non-Metallic Nitrides*. Moscow: Metallurgy, 264.
26. Neshpor, V. S., Khushidman, M. B. (1969). On electronic structure of boron nitride. *Inorganic Materials*, 5, 600–601.
27. Zunger, A., Freeman, A. J. (1978). Ab initio self-consistent study of the electronic structure and properties of cubic boron nitride. *Physical Review B*, 17 (4), 2030–2042. doi: 10.1103/physrevb.17.2030
28. Harrison, W. A. (1980). *Electronic Structure and the Properties of Solids – The Physics of the Chemical Bond*. San Francisco: W. H. Freeman & Co, 61.
29. Dovesi, R., Pisani, C., Roetti, C., Dellarole, P. (1981). Exact-exchange Hartree-Fock calculations for periodic systems. IV. Ground-

- state properties of cubic boron nitride. *Physical Review B*, 24 (8), 4170–4176. doi: 10.1103/physrevb.24.4170
30. Nemoshkalenko, V. V., Aleshin, V. G. (1983). Electronic Structure of Crystals. Kiev: Naukova Dumka.
31. Huang, M.-Z., Ching, W. Y. (1985). A minimal basis semi-ab initio approach to the band structures of semiconductors. *Journal of Physics and Chemistry of Solids*, 46 (8), 977–995. doi: 10.1016/0022-3697(85)90101-5
32. Van Camp, P. E., Van Doren, V. E., Devreese, J. T. (1988). Ground State and Electronic Properties of Silicon Carbide and Boron Nitride. *Physica Status Solidi B*, 146 (2), 573–587. doi: 10.1002/pssb.2221460218
33. Ganduglia-Pirovano, M. V., Stollhoff, G. (1991). Electronic correlations of cubic boron nitride. *Physical Review B*, 44 (8), 3526–3536. doi: 10.1103/physrevb.44.3526
34. Christensen, N. E., Gorczyca, I. (1994). Optical and structural properties of III-V nitrides under pressure. *Physical Review B*, 50 (7), 4397–4415. doi: 10.1103/physrevb.50.4397
35. Karch, K., Bechstedt, F. (1997). Ab initio lattice dynamics of BN and AlN: Covalent versus ionic forces. *Physical Review B*, 56 (12), 7404–7415. doi: 10.1103/physrevb.56.7404
36. Shimada, K., Sota, T., Suzuki, K. (1998). First-principles study on electronic and elastic properties of BN, AlN, and GaN. *Journal of Applied Physics*, 84 (9), 4951–4958. doi: 10.1063/1.368739
37. Ferhat, M., Zaoui, A., Certier, M., Aourag, H. (1998). Electronic structure of BN, BP and BAs. *Physica B: Condensed Matter*, 252 (3), 229–236. doi: 10.1016/s0921-4526(98)00149-5
38. Miotti, R., Srivastava, G., Ferraz, A. (1999). First-principles pseudopotential study of GaN and BN (110) surfaces. *Surface Science*, 426 (1), 75–82. doi: 10.1016/s0039-6028(99)00282-4
39. Xu, Y.-N., Ching, W. Y. (1993). Electronic, optical, and structural properties of some wurtzite crystals. *Physical Review B*, 48 (7), 4335–4351. doi: 10.1103/physrevb.48.4335
40. Siklitsky, V. (2015). BN – Boron Nitride. Electronic archive: "New Semiconductor Materials. Characteristics and Properties". Available at: <http://www.ioffe.rssi.ru/SVA/NSM/Semicond/BN/index.html>
41. Shuvalov, L. A., Urusovskaya, A. A., Zheludev, I. S., Zelenskij, A. V., Semiletov, S. A., Grechushnikov, B. N., Chistyakov, I. G., Pinkin, S. A. (1981). Modern Crystallography. Volume 4: Physical Properties of Crystals. Nauka, Moscow.
42. Shackelford, J. F., Alexander, W. (Eds.) (2001). CRC Materials Science and Engineering Handbook. CRC Press LLC, Boca Raton.
43. Chopra, N. G., Zettl, A. (1998). Measurement of the elastic modulus of a multi-wall boron nitride nanotube. *Solid State Communications*, 105 (5), 297–300. doi: 10.1016/s0038-1098(97)10125-9
44. Chkhartishvili, L. (Ed.) (2011). Boron nitride nanosystems. Boron Based Solids. Trivandrum: Research Signpost, 93–145.
45. Chkhartishvili, L., Lezhava, D., Tsagareishvili, O. (2000). Quasiclassical Determination of Electronic Energies and Vibration Frequencies in Boron Compounds. *Journal of Solid State Chemistry*, 154 (1), 148–152. doi: 10.1006/jssc.2000.8826
46. Chkhartishvili, L. S. (2004). Quasi-classical estimates of the lattice constant and band gap of a crystal: Two-dimensional boron nitride. *Physics of the Solid State*, 46 (11), 2126–2133. doi: 10.1134/1.1825560
47. Chkhartishvili, L. (2004). Quasi-classical approach: Electronic structure of cubic boron nitride crystals. *Journal of Solid State Chemistry*, 177 (2), 395–399. doi: 10.1016/j.jssc.2003.03.004
48. Chkhartishvili, L. (2006). Density of electron states in wurtzite-like boron nitride: A quasi-classical calculation. *Materials Science: An Indian Journal*, 2, 18–23.