

Influence of the Elastic Field of Quantum Dots on the Electronic Band Structure of III-Nitride Wire Semiconductors

Nguyen Van Tuyen^{1,2}, A.L. Kolesnikova^{1,3} , A.E. Romanov¹ 

¹ ITMO University, 49 Kronverksky pr., St. Petersburg, 197101, Russia

² Sao Do University, No 24, Thai Hoc 2, Sao Do Ward, Chi Linh City, Hai Duong, Vietnam

³ Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences, 61 Bolshoj pr., V.O., St. Petersburg, 199178, Russia

Received: June 02, 2025

Corresponding author: [Nguyen Van Tuyen](mailto:nguyenvan.tuyen@itmo.ru)

Abstract. In this work, we investigate the effect of the strains induced by axially symmetric quantum dots of cylindrical, hemispherical and conical shapes in a III-nitride semiconductor nanowire on the band structure of the nanowire material. To study the elastic properties of quantum dots, a model of an elastic inclusion with eigenstrain has been used. To consider the influence of the free surface of the wire on the elastic fields of quantum dots, the corresponding boundary value problems have been solved analytically. The $\mathbf{k}\cdot\mathbf{p}$ perturbation method has been applied to analyze the strain induced effect on the energy band structure of the material. The results obtained demonstrate that the band gap width clearly depends on the shape of the embedded quantum dot. The effect of quantum dot strains on the electropolarization of the material possessing ferroelectric properties, was investigated. It was shown that the largest jump in electric charge density is achieved near the apex of the conical inclusion.

Acknowledgements. This work was supported by the Ministry of Science and Higher Education of the Russian Federation, project no. FSER-2025-0005.

Citation: Rev. Adv. Mater. Technol., 2025, vol. 7, no. 2, pp. 124–140

View online: <https://doi.org/10.17586/2687-0568-2025-7-2-124-140>

View Table of Contents: <https://reviewsamt.com/issues>

REFERENCES

- [1] R.A. Ferreyra, C. Zhu, A. Teke, H. Morkoç, Group III Nitrides, in: S. Kasap, P. Capper (Eds.), *Springer Handbook of Electronic and Photonic Materials*, Springer, Cham, 2017.
- [2] J.I. Pankove, E.A. Miller, J.E. Berkeyheiser, GaN blue light-emitting diodes, *Journal of Luminescence*, 1972, vol. 5, no. 1, pp. 84–86.
- [3] M.S. Shur, GaN based transistors for high power applications, *Solid-State Electronics*, 1998, vol. 42, no. 12, pp. 2131–2138.
- [4] C. Zhao, Y.H. Chen, B. Xu, C.G. Tang, Z.G. Wang, F. Ding, Study of the wetting layer of InAs/GaAs nanorings grown by droplet epitaxy, *Applied Physics Letters*, 2008, vol. 92, no. 6, art. no. 063122.
- [5] J. Yan, J. Wang, P. Cong, L. Sun, N. Liu, Z. Liu, C. Zhao, J. Li, Improved performance of UV-LED by p-AlGaIn with graded composition, *Physica Status Solidi C*, 2011, vol. 8, no. 2, pp. 461–463.
- [6] J. Yan, J. Wang, Y. Zhang, P. Cong, L. Sun, Y. Tian, C. Zhao, J. Li, AlGaIn-based deep-ultraviolet light-emitting diodes grown on high-quality AlN template using MOVPE, *Journal of Crystal Growth*, 2015, vol. 414, pp. 254–257.
- [7] F. Bernardini, V. Fiorentini, D. Vanderbilt, Spontaneous polarization and piezoelectric constants of III-V nitrides, *Physical Review B*, 1997, vol. 56, no. 16, pp. R10024–R10027.
- [8] F. Bernardini, V. Fiorentini, Spontaneous versus Piezoelectric Polarization in III-V Nitrides: Conceptual Aspects and Practical Consequences, *Physica Status Solidi B*, 1999, vol. 216, no. 1, pp. 391–398.
- [9] F. Bernardini, V. Fiorentini, Nonlinear macroscopic polarization in III-V nitride alloys, *Physical Review B*, 2001, vol. 64, no. 8, art. no. 085207.
- [10] G.L. Bir, G.E. Pikus, P. Shelnitz, D. Louvish, *Symmetry and strain-induced effects in semiconductors*, Wiley, New York, 1974.
- [11] C.P. Kuo, S.K. Vong, R.M. Cohen, G.B. Stringfellow, Effect of mismatch strain on band gap in III-V semiconductors, *Journal of Applied Physics*, 1985, vol. 57, no. 12, pp. 5428–5432.
- [12] T. Manku, A. Nathan, Valence energy-band structure for strained group-IV semiconductors, *Journal of Applied Physics*, 1993, vol. 73, no. 3, pp. 1205–1213.
- [13] M.V. Fischetti, S.E. Laux, Band structure, deformation potentials, and carrier mobility in strained Si, Ge, and SiGe alloys, *Journal of Applied Physics*, 1996, vol. 80, no. 4, pp. 2234–2252.
- [14] Y. Sun, S.E. Thompson, T. Nishida, *Strain Effect in Semiconductors*, Springer, New York, NY, 2010.
- [15] M. Hetzl, M. Kraut, J. Winnerl, L. Francaviglia, M. Döblinger, S. Matich, A. Fontcuberta i Morral, M. Stutzmann, Strain-Induced Band Gap Engineering in Selectively Grown GaIn–(Al,Ga)N Core–Shell Nanowire Heterostructures, *Nano Letters*, 2016, vol. 16, no. 11, pp. 7098–7106.
- [16] M. Benaissa, W. Sigle, H. Zaari, M. Tadout, P.A. van Aken, Strain and size combined effects on the GaN band structure: VEELS and DFT study, *Physical Chemistry Chemical Physics*, 2017, vol. 19, no. 7, pp. 5430–5434.
- [17] M. Sopanen, H. Lipsanen, J. Tulkki, J. Ahopelto, Strain-induced quantum dot superlattice, *Physica E: Low-dimensional Systems and Nanostructures*, 1998, vol. 2, no. 1–4, pp. 19–22.
- [18] A.E. Romanov, G.E. Beltz, W.T. Fischer, P.M. Petroff, J.S. Speck, Elastic fields of quantum dots in subsurface layers, *Journal of Applied Physics*, 2001, vol. 89, no. 8, pp. 4523–4531.
- [19] E. Melezhik, O. Korotchenkov, Elastic fields of quantum dots in semi-infinite matrices: Green’s function analytical analysis, *Journal of Applied Physics*, 2009, vol. 105, no. 2, art. no. 023505.
- [20] N.A. Bert, A.L. Kolesnikova, I.K. Korolev, A.E. Romanov, A.B. Freidin, V.V. Chaldyshev, E.C. Aifantis, Elastic fields and physical properties of surface quantum dots, *Physics of the Solid State*, 2011, vol. 53, no. 10, pp. 2091–2102.
- [21] T. Mura, *Micromechanics of defects in solids*, Springer, Dordrecht, 1987.
- [22] J.D. Eshelby, The determination of the elastic field of an ellipsoidal inclusion, and related problems, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 1957, vol. 241, no. 1226, pp. 376–396.

- [23] J.D. Eshelby, The elastic field outside an ellipsoidal inclusion, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 1959, vol. 252, no. 1271, pp. 561–569.
- [24] A.L. Kolesnikova, M.Yu. Gutkin, A.E. Romanov, Elastic models of defects in 3D and 2D crystals, *Reviews on Advanced Materials Science*, 2017, vol. 51, pp. 130–148.
- [25] A.L. Kolesnikova, M.Yu. Gutkin, A.E. Romanov, Analytical elastic models of finite cylindrical and truncated spherical inclusions, *International Journal of Solids and Structures*, 2018, vol. 143, pp. 59–72.
- [26] D. Leonard, K. Pond, P.M. Petroff, Critical layer thickness for self-assembled InAs islands on GaAs, *Physical Review B*, 1994, vol. 50, no. 16, pp. 11687–11692.
- [27] R.J. Warburton, Self-assembled semiconductor quantum dots, *Contemporary Physics*, 2002, vol. 43, no. 5, pp. 351–364.
- [28] P. Waltereit, A.E. Romanov, J.S. Speck, Electronic properties of GaN induced by a subsurface stressor, *Applied Physics Letters*, 2002, vol. 81, no. 25, pp. 4754–4756.
- [29] A.E. Romanov, P. Waltereit, J.S. Speck, Buried stressors in nitride semiconductors: Influence on electronic properties, *Journal of Applied Physics*, 2005, vol. 97, no. 4, art. no. 043708.
- [30] A.E. Romanov, A.L. Kolesnikova, M.Yu. Gutkin, V.G. Dubrovskii, Elasticity of axial nanowire heterostructures with sharp and diffuse interfaces, *Scripta Materialia*, 2020, vol. 176, pp. 42–46.
- [31] A.L. Kolesnikova, R.M. Soroka, A.E. Romanov, Defects in the elastic continuum: classification, fields and physical analogies, *Materials Physics and Mechanics*, 2013, vol. 17, no. 1, pp. 71–91.
- [32] A.L. Kolesnikova, N. Van Tuyen, M.Yu. Gutkin, A.E. Romanov, Dilatational disk and finite cylindrical inclusion in elastic nanowire, *International Journal of Engineering Science*, 2025, vol. 206, art. no. 104169.
- [33] G. Eason, B. Noble, I.N. Sneddon, On certain integrals of Lipschitz-Hankel type involving products of Bessel functions, *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 1955, vol. 247, no. 935, pp. 529–551.
- [34] A.L. Kolesnikova, N. Van Tuyen, M.Yu. Gutkin, A.E. Romanov, General approach to calculating elastic characteristics of axisymmetric quantum dots in whisker-like nanocrystals, *Technical Physics Letters*, 2024, vol. 50, no. 6, pp. 28–32 (in Russian).
- [35] G.B. Dwight, *Tables of integrals and other mathematical formulas*, Fourth edition, The Macmillan Company, New York, 1961.
- [36] K. Pearson, *Tables of Incomplete Beta-Function*, 2nd ed., Cambridge University Press, Cambridge, 1968.
- [37] V.T. Nguyen, A.L. Kolesnikova, A.E. Romanov, Isotropic elasticity of dilatational conical inclusion. An analytical approach, *International Journal of Solids and Structures*, 2024, vol. 294, art. no. 112735.
- [38] B.M. Dwork, *Generalized Hypergeometric Functions*, 1st edition, Clarendon Press, 1990.
- [39] M.H. Sadd, *Elasticity: Theory, Applications, and Numerics*, Elsevier Butterworth–Heinemann, 2005.
- [40] H. Zhu, S. Feng, D. Jiang, Y. Deng, H. Wang, Strain Effect on the Band Structure of InAs/GaAs Quantum Dots, *Japanese Journal of Applied Physics*, 1999, vol. 38, no. 11R, art. no. 6264.
- [41] A.E. Romanov, T.J. Baker, S. Nakamura, J.S. Speck, Strain-induced polarization in wurtzite III-nitride semipolar layers, *Journal of Applied Physics*, 2006, vol. 100, no. 2, art. no. 023522.
- [42] A. Zhang, S. Luo, G. Ouyang, G. Yang, Strain-induced optical absorption properties of semiconductor nanocrystals, *Journal of Chemical Physics*, 2013, vol. 138, no. 24, art. no. 244702.
- [43] J.M. Luttinger, W. Kohn, Motion of Electrons and Holes in Perturbed Periodic Fields, *Physical Review Journals Archive*, 1955, vol. 97, no. 4, pp. 869–883.
- [44] S.L. Chuang, *Physics of Optoelectronic Devices*, John Wiley, New York, USA, 1995.
- [45] S.L. Chuang, C.S. Chang, k-p method for strained wurtzite semiconductors, *Physical Review B*, 1996, vol. 54, no. 4, pp. 2491–2504.
- [46] M. Willatzen, L.C. Lew Yan Voon, *The kp Method*, Springer Berlin, Heidelberg, 2009.
- [47] S. Ghosh, P. Waltereit, O. Brandt, H.T. Grahn, K.H. Ploog, Electronic band structure of wurtzite GaN under biaxial strain in the M plane investigated with photoreflectance spectroscopy, *Physical Review B*, 2002, vol. 65, no. 7, art. no. 075202.
- [48] C. Wood, D. Jena (Eds.), *Polarization Effects in Semiconductors*, Springer New York, NY, 2008.

- [49] J.F. Nye, *Physical Properties of Crystals: Their Representation by Tensors and Matrices*, Oxford University Press, USA, 1985.
- [50] M.T. Hibberd, V. Frey, B.F. Spencer, P.W. Mitchell, P. Dawson, M.J. Kappers, R.A. Oliver, C.J. Humphreys, D.M. Graham, Dielectric response of wurtzite gallium nitride in the terahertz frequency range, *Solid State Communications*, 2016, vol. 247, pp. 68–71.
- [51] J.G. Gualtieri, J.A. Kosinski, A. Ballato, Piezoelectric materials for acoustic wave applications, *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, 1994, vol. 41, no. 1, pp. 53–59.
- [52] M.E. Levinshtein, S.L. Rumyantsev, M.S. Shur, Properties of advanced semiconductor materials GaN, AlN, InN, BN, SiC, SiGe, John Wiley & Sons, 2001.
- [53] A.R. Denton, N.W. Ashcroft, Vegard's law, *Physical Review A*, 1991, vol. 43, no. 6, pp. 3161–3164.
- [54] L. Vegard, Die Konstitution der Mischkristalle und die Raumfüllung der Atome, *Zeitschrift für Physik*, 1921, vol. 5, no. 1, pp. 17–26.
- [55] K. Kim, W.R.L. Lambrecht, B. Segall, Elastic constants and related properties of tetrahedrally bonded BN, AlN, GaN, and InN, *Physical Review B*, 1996, vol. 53, no. 24, pp. 16310–16326.
- [56] A.L. Kolesnikova, A.E. Romanov, Representations of elastic fields of circular dislocation and disclination loops in terms of spherical harmonics and their application to various problems of the theory of defects, *International Journal of Solids and Structures*, 2010, vol. 47, no. 1, pp. 58–70.