

Misfit Stress in Radial Core-Shell Nanowires with Diffuse Interface Boundaries

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Abstract. The elastic models of radial core-shell nanowires with diffuse interphase boundaries are suggested. The concept of eigenstrain is employed to consider a misfit stress distribution induced by diffusive interfaces with different range of distinctness. The eigenstrain profile described by the misfit parameter is approximated by piecewise-linear, error and arctangent functions. For these approximations the elastic stresses in core-shell nanowires are analytically derived, illustrated with plots and discussed in detail.

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REFERENCES

- [1] M.S. Gudiksen, L.J. Lauhon, J. Wang, D.C. Smith, C.M. Lieber, *Growth of nanowire superlattice structures for nanoscale photonics and electronics*, Nature, 2002, vol. 415, no. 6872, pp. 617–620.

- [2] G. Priante, F. Glas, G. Patriarche, K. Pantzas, F. Oehler, J.-C. Harmand, *Sharpening the interfaces of axial heterostructures in self-catalyzed AlGaAs nanowires: experiment and theory*, Nano Lett., 2016, vol. 16, no. 3, pp. 1917–1924.
- [3] V. Zannier, F. Rossi, V.G. Dubrovskii, D. Ercolani, S. Battiato, L. Sorba, *Nanoparticle stability in axial InAs–InP nanowire heterostructures with atomically sharp interfaces*, Nano Lett., 2018, vol. 18, no. 1, pp. 167–174.
- [4] D.V. Beznasyuk, P. Stepanov, J.L. Rouvière, F. Glas, M. Verheijen, J. Claudon, M. Hocevar, *Full characterization and modeling of graded interfaces in a high lattice-mismatch axial nanowire heterostructure*, Phys. Rev. Mater., 2020, vol. 4, no. 7, art. no. 074607.
- [5] V.G. Dubrovskii, A.A. Koryakin, N.V. Sibirev, *Understanding the composition of ternary III-V nanowires and axial nanowire heterostructures in nucleation-limited regime*, Mater. Des., 2017, vol. 132, pp. 400–408.
- [6] A.E. Romanov, A.L. Kolesnikova, M.Yu. Gutkin, V.G. Dubrovskii, *Elasticity of axial nanowire heterostructures with sharp and diffuse interfaces*, Scr. Mater., 2020, vol. 176, pp. 42–46.
- [7] A.E. Romanov, A.L. Kolesnikova, M.Yu. Gutkin, *Elasticity of a cylinder with axially varying dilatational eigenstrain*, Int. J. Solids Struct., 2021, vol. 213, pp. 121–134.
- [8] A.L. Kolesnikova, M.Yu. Gutkin, A.E. Romanov, V.E. Bougov, *Strain energy in hybrid nanowire structures with axially varying eigenstrain*, Int. J. Solids Struct., 2022, vol. 254–255, art. no. 111819.
- [9] V.G. Dubrovskii, *Understanding the vapor-liquid-solid growth and composition of ternary III-V nanowires and nanowire heterostructures*, J. Phys. D: Appl. Phys., 2017, vol. 50, no. 45, art. no. 453001.
- [10] A.M. Smirnov, S.A. Krasnitckii, S.S. Rochas, M.Yu. Gutkin, *Critical conditions of dislocation generation in core-shell nanowires: A review*, Rev. Adv. Mater. Technol., 2020, vol. 2, no. 3, pp. 19–43.
- [11] S.A. Krasnitckii, A.M. Smirnov, M.Yu. Gutkin, *Axial misfit stress relaxation in core-shell nanowires with polyhedral cores through the nucleation of misfit prismatic dislocation loops*, J. Mater. Sci., 2020, vol. 55, no. 22, pp. 9198–9210.
- [12] A.M. Smirnov, S.A. Krasnitckii, M.Yu. Gutkin, *Generation of misfit dislocations in a core-shell nanowire near the edge of prismatic core*, Acta Mater., 2020, vol. 186, pp. 494–510.
- [13] S.A. Krasnitckii, A.M. Smirnov, K.D. Mynbaev, L.V. Zhigilei, M.Yu. Gutkin, *Axial misfit stress relaxation in core-shell nanowires with hexagonal core via nucleation of rectangular prismatic dislocation loops*, Mater. Phys. Mech., 2019, vol. 42, no. 6, pp. 776–783.
- [14] S.A. Krasnitckii, D.R. Kolomoetc, A.M. Smirnov, M.Yu. Gutkin, *Misfit stress relaxation in composite core-shell nanowires with parallelepiped cores using rectangular prismatic dislocation loops*, J. Phys. Conf. Ser., 2018, vol. 993, no. 1, art. no. 012021.
- [15] S.A. Krasnitckii, D.R. Kolomoetc, A.M. Smirnov, M.Yu. Gutkin, *Misfit stresses in a composite core-shell nanowire with an eccentric parallelepipedal core subjected to one-dimensional cross dilatation eigenstrain*, J. Phys. Conf. Ser., 2017, vol. 816, no. 1, art. no. 012043.
- [16] M.Yu. Gutkin, A.M. Smirnov, *Initial stages of misfit stress relaxation through the formation of prismatic dislocation loops in GaN–Ga₂O₃ composite nanostructures*, Phys. Solid State, 2016, vol. 58, no. 8, pp. 1611–1621.
- [17] M.Yu. Gutkin, S.A. Krasnitckii, A.M. Smirnov, A.L. Kolesnikova, A.E. Romanov, *Dislocation loops in solid and hollow semiconductor and metal nanoheterostructures*, Phys. Solid State, 2015, vol. 57, no. 6, pp. 1177–1182.
- [18] M.Yu. Gutkin, A.M. Smirnov, *Initial stages of misfit stress relaxation by rectangular prismatic dislocation loops in composite nanostructures*, J. Phys. Conf. Ser., 2014, vol. 541, no. 1, art. no. 012007.
- [19] G. Perillat-Merceroz, R. Thierry, P.-H. Jouneau, P. Ferret, G. Feuillet, *Strain relaxation by dislocation glide in ZnO/ZnMgO core-shell nanowires*, Appl. Phys. Lett., 2012, vol. 100, no. 17, art. no. 173102.
- [20] M.Yu. Gutkin, K.V. Kuzmin, A.G. Sheinerman, *Misfit stresses and relaxation mechanisms in a nanowire containing a coaxial cylindrical inclusion of finite height*, Phys. Status Solidi, 2011, vol. 248, no. 7, pp. 1651–1657.
- [21] J. Colin, *Prismatic dislocation loops in strained core-shell nanowire heterostructures*, Phys. Rev. B, 2010, vol. 82, no. 5, art. no. 054118.

- [22] K.E. Aifantis, A.L. Kolesnikova, A.E. Romanov, *Nucleation of misfit dislocations and plastic deformation in core/shell nanowires*, Philos. Mag., 2007, vol. 87, no. 30, pp. 4731–4757.
- [23] S. Raychaudhuri, E.T. Yu, *Critical dimensions in coherently strained coaxial nanowire heterostructures*, J. Appl. Phys., 2006, vol. 99, no. 11, art. no. 114308.
- [24] I.A. Ovid'ko, A.G. Sheinerman, *Misfit dislocation loops in composite nanowires*, Philos. Mag., 2004, vol. 84, no. 20, pp. 2103–2118.
- [25] A.G. Sheinerman, M.Yu. Gutkin, *Misfit disclinations and dislocation walls in a two-phase cylindrical composite*, Phys. Status Solidi, 2001, vol. 184, no. 2, pp. 485–505.
- [26] M.Yu. Gutkin, I.A. Ovid'ko, A.G. Sheinerman, *Misfit dislocations in wire composite solids*, J. Phys. Condens. Matter., 2000, vol. 12, no. 25, pp. 5391–5401.

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