CALCULATION OF CARBON NANOBELT BAND STRUCTURE

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Abstract

To find the dispersion relation for nanobelt energy, we used the strongly coupled electron method, the one-dimensional subband method for "cutting off" the necessary energy lines and the method of adding subbands. The study shows the results of using the technique for single-layer graphene nanobelts of the "chair" type and "zigzag" type with different initial base vectors.

Keywords

Strongly coupled electron method, dispersion relation for nanobelt energy, carbon nanotube, carbon nanobelt, carbon nanobeltband structure

References

[1] Fujita M., Wakabayashi K., Nakada K., Kusakabe K. Peculiar localized state at zigzag graphite edge. *J. Phys. Soc. Jpn.*, 1996, vol. 65, pp. 1920–1923.

[2] Barone V. Hod O., Scuseria G.E. Electronic structure and stability of semiconducting graphene nanoribbons. *Nano Lett.*, 2006, vol.6, no. 12, pp. 2748–2754.

[3] Ritter K.A., Lyding J.W. The influence of edge structure on the electronic properties of graphene quantum dots and nanoribbons. *Nat. Mater.*, 2009, vol. 8, no. 3, pp. 235–242.

[4] White C.T., Li J., Gunlycke D., Mintmire J.W. Hidden one-electron interactions in carbon nanotubes revealed in graphene nanostrips. *Nano Lett.*, 2007, vol. 7, no. 3, pp. 825–830.

[5] Cai J., Ruffieux R., Jaafar R., Bieri M., Braun T., Blankenburg S., Muoth M., Seitsonen A.P., Saleh M., Feng X., Müllen K., Fasel R. Atomically precise bottom-up fabrication of graphene nanoribbons. *Nature*, 2010, vol. 466, pp. 470–473.

[6] Li W., Tao R. Edge states of monolayer and bilayer graphene nanoribbons. *J. Phys. Soc. Jpn.*, 2012, vol. 81, no. 2, pp. 024704.

[7] Huang Y.C., Chang C.P., Lin M.F. Electric-field induced modification of electronic properties of few-layer graphene nanoribbons. *J. Appl. Phys.*, 2008, vol. 104, pp. 103314.

[8] Topsakal M., Bagci V.M.K., Ciraci S. Current-voltage (I–V) characteristics of armchair graphene nanoribbons under uniaxial strain. *Phys. Rev. B*, 2010, vol. 81, no. 20, pp. 105437.

[9] Jaskolski W., Ayuela A., Pelc M., Santos H., Chico L. Edge states and flat bands in graphene nanoribbons with arbitrary geometries. *Phys. Rev. B*, 2011, vol. 83, no. 23, pp. 235424.

[10] Sorokin P.B., Chernozatonskii L.A. Graphene-based semiconductor nanostructures. *Phys. Usp.,* 2013, vol. 56, no. 2, pp. 105–122.

[11] Wang Z.F., Shia Q.W., Li Q., Wang X., Hou J.G. Z-shaped graphene nanoribbon quantum dot device. *Appl. Phys. Lett.*, 2007, vol.91, no. 5, pp. 053109.

[12] Ezawa M. Peculiar width dependence of the electronic properties of carbon nanoribbons. *Phys. Rev. B*, 2006, vol. 73, no. 4, pp. 45.

[13] Girao E.C., Cruz-Silva E., Meunier V. Electronic transport properties of assembled carbon nanoribbons. *ACS Nano*, 2012, vol. 6, no. 7, pp. 6483–6491.

[14] Barone V., Hod O., Scuseria G.E. Electronic structure and stability of semiconducting graphene nanoribbons. *Nano Lett.,* 2006, vol.6, no. 12, pp. 2748–2754.

[15] De Sousa D.J., de Castro L.V., da Costa D.R., Pereira J.M. Boundary conditions for phosphorene nanoribbons in the continuum approach. *Phys. Rev. B*, 2016, vol. 94, no. 23, pp. 235415.

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