CALCULATION OF CARBON NANOTUBES ZONE STRUCTURE THROUGH DISPERSIVE RELATION FOR GRAPHEN ENERGY

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Abstract

The article describes the implementing techniques for calculating the band structure of single-walled carbon nanotubes of the "chair" and "zigzag" type, as well as numerical calculations and formulas of the simplest analytical calculation. We obtained the dispersion relations of the nanotubes energy and their band structures. Findings of the research can be useful for studying electronic properties of carbon nanotubes of the "chair" and "zigzag" type, determining the conductivity and for the purposes of comparative analysis.

Keywords

Graphene, strongly coupled electron method, dispersion relation for energy, Brillouin zones, band structure, carbon nanotubes of the "chair" type, carbon nanotubes of the "zigzag" type

References

[1] Iijima S. Helical microtubules of graphitic carbon. *Nature*, 1991, vol. 354, pp. 56–58.

[2] Pop E., Dai H. Electrical and thermal transport in metallic single-wall carbon nanotubes on insulating substrates. *Journal of Applied Physics*, 2007, vol. 101, no. 9, pp. 093710.

[3] Morimoto T., Ichida M., Ikemoto Yu., Okazaki T. Temperature dependence of plasmon resonance in single-walled carbon nanotubes. *Physical Review B*, 2016, vol. 93, no. 19, pp. 195409.

[4] Tsuchikawa R., Heligman D., Blue B.T., Zhang Z.Y., Ahmadi A., Mucciolo E.R., Hone J., Ishigami M. Scattering strength of potassium on a carbon nanotube with known chirality. *Physical Review B*, 2016, vol. 94, no. 4, pp. 045408.

[5] Graham A.P., Duesberg G.S., Seidel R., Liebau M., Unger E., Kreupl F. Hönlein W. Towards the integration of carbon nanotubes in microelectronics. *Diamond* & *Related Materials*, 2004, vol. 13, no. 4–8, pp. 1296–1300.

[6] White C.T, Robertson D.H., Mintmire J.W. Helical and rotational symmetries of nanoscale graphitic tubules. *Physical Review B*, 1993, vol. 47, no. 9, pp. 5485–5488.

[7] Spesyvtseva S., Shoji S., Kawata S. Chirality-selective optical scattering force on single-walled carbon nanotubes. *Physical Review Applied*, 2015, vol. 3, no. 4, pp. 044003.

[8] Montes E., Schwingenschlögl U. Nanotubes based on monolayer blue phosphorus. *Physical Review B*, 2016, vol. 94, no. 3, pp. 035412.

[9] Kreupl F., Graham A.P., Duesberg G.S., Steinhögl W., Liebau M., Unger E., Hönlein W. Carbon nanotubes in interconnect applications. *Microelectronic Engineering*, 2002, vol. 64, no. 1–4, pp. 399–408.

[10] Saito R., Dresselhaus G., Dresselhaus M.S. Physical properties of carbon nanotubes. London, Imperial college press. 1998. 272 p.

[11] Datta S. Quantum transport: Atom to transistor. New York, Cambridge University Press, 2013. 417 p.

[12] Ashcroft N.W., Mermin N.D. Solid state physics. Philadelphia, Saunders College Publishing, 1976. 272 p.

[13] Hasegawa M., Nishidate K., Yoshimoto N. Collapsed armchair single-walled carbon nanotubes as an analog of closed-edged bilayer graphene nanoribbons. *Physical Review B*, 2015, vol. 92, no. 24, pp. 245429.
[14] Negi S., Warrier M., Chaturvedi S., Nordlund K. Molecular dynamic simulations of a double-walled carbon nanotube motor subjected to a sinusoidally varying electric field. *Computational Materials Science*, 2009, vol. 44, no. 3, pp. 979–987.
[15] Mylvaganam K., Zhang L.C. Important issues in a molecular dynamics simulation for characterising the mechanical properties of carbon nanotubes. *Carbon*, 2004, vol. 42, no. 10, pp. 2025–2032.

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