

Elastic Moduli of Carbon Nanotubes Computed with Tight-Binding Methods¹

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Carbon nanotubes (CNTs) have novel properties that are of great interest in various areas of nanotechnology. In particular, they are known for their exceptionally high tensile strengths and elastic moduli. Since CNTs are relatively simple covalently bonded systems, molecular modeling techniques have yielded elastic moduli that are in good agreement with experimental results. Using the Slater-Koster method, I will demonstrate the dependence of the elastic modulus on the tube diameter and compare it to other models in the literature¹. Tubes of various sizes will be generated using the nanotube coordinate generator designed by Shigeo Maruyama². In addition, I aim to investigate the effects of chirality the elastic modulus.

¹ Chang, T., Gao, H., Size-dependent elastic properties of a single-walled carbon nanotube via a molecular mechanics model, *Journal of the Mechanics and Physics of Solids*, 51, pp. 1059-74, 2003.

² <http://www.photon.t.u-tokyo.ac.jp/~maruyama/wrapping3/wrapping.html>