Acoustic and Optical Phonons in Nanotubes

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The elastic continuum model is applied for single wall nanotubes (SWNTs) and multiple wall nanotube (MWNTs) with the nanotube approximated as an elastic cylindrical membrane of finite thickness. Donnell's equations of motion for a cylindrical membrane are solved using the Rayleigh-Ritz method to give the acoustic vibrational modes of SWNTs. The displacement modes are used to calculate the deformation potential and the dispersion relations are compared for various diameter nanotubes.

The quantized normalization amplitudes for the optical modes are solved analytically and the dispersion relations are calculated. Figure 1 and Figure 2 give the dispersion relation and the deformation potential for a 2.8-nm-radius (10,10) nanotube clamped at the ends. In this case, the deformation potential is influenced by the boundary conditions corresponding to clamping the nanotube at both ends. The deformation potential can be used to calculate the carrier interactions in nanotubes.

These results indicate that the frequencies of the axial, circumferential, and radial modes deviate form their expected values at wavevectors in close proximity to each other. Moreover, these calculations provide the full set of phonon modes for the SWNTs; this is in contrast to most calculations that consider a subset of these modes. Finally, these results indicate that phonon-bottleneck effects should be important for the short nanotubes being considered for nanotube-based devices exhibiting quasi-ballistic transport. The authors gratefully acknowledge the support and guidance of Dr. Todd Steiner of AFOSR and Dr. Dwight Woolard of ARO.

A full journal publication of this work will be published in the Journal of Computational Electronics.

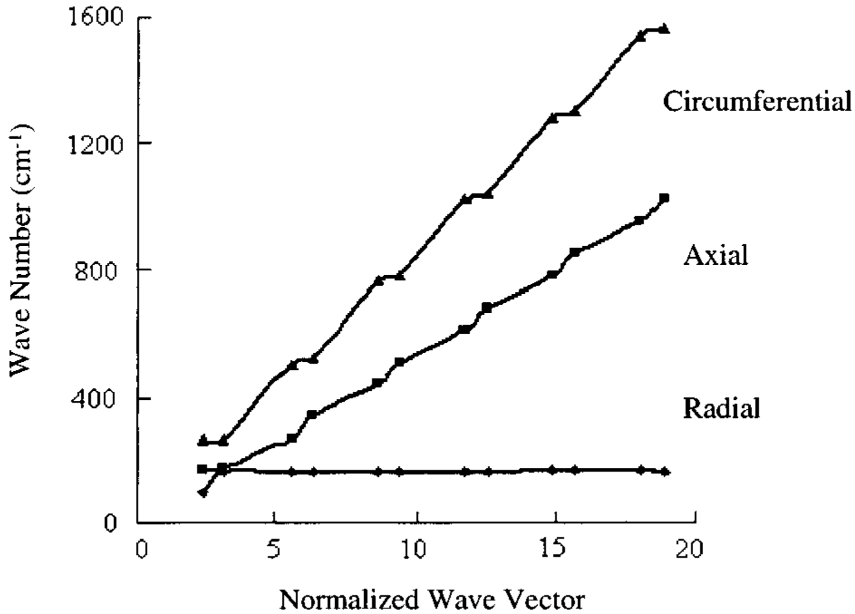

Figure 1: Dispersion curve for (10,10) nanotube with a length of 28 Angstroms.

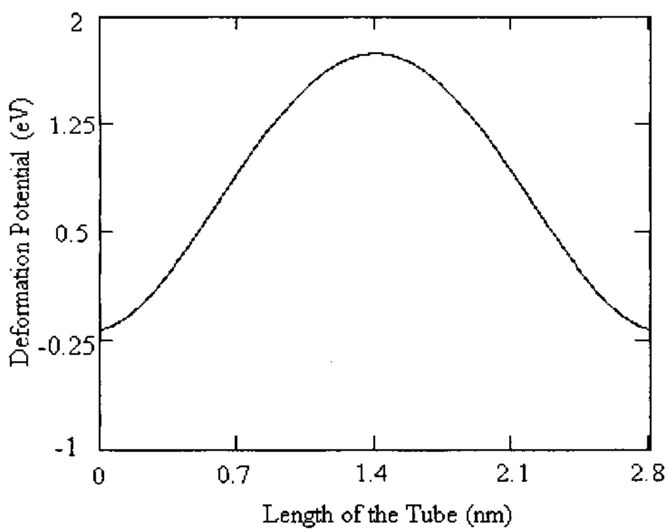

Figure 2: Deformation potential for the lowest-order axial mode (10,10) nanotube with a length of 28 Angstroms.

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