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Wave Propagation in Carbon Nanotubes

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Summary

The wave dispersions of longitudinal and flexural wave propagations in single-walled and multi-walled carbon nanotubes are studied in the frame of continuum mechanics and molecular dynamics simulation. The dispersion relations between the phase velocity, group velocity and the wave number for the flexural and longitudinal waves, described by a beam model and a cylindrical shell model, are established for both single- and multi-walled carbon nanotubes. The effect of micro-structures in carbon nanotubes on the wave dispersion is revealed through the non-local elastic models of beam and cylindrical shell including the second order gradient of strain and a parameter of micro-structure. Compare with molecular dynamics results, it is shown that the micro-structures in the carbon nanotubes play an important role in the dispersion of both longitudinal and flexural waves. In addition, the non-local elastic models predict that the cut-off wave number of the dispersion relation between the group velocity and the wave number is about 10 kilomega 1/m for the longitudinal and flexural wave propagations in both single- and multi-walled carbon nanotubes. This may explain the difficulty that the direct molecular dynamics simulation can not give a proper dispersion relation between the phase velocity and the wave number when the wave number approaches to 10 kilomega 1/m or so, much lower than the cut-off wave number for the dispersion relation between the phase velocity and the wave number predicted by the continuum mechanics.