Phonon Scattering and Excitons in Carbon Nanotubes.¹
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Due to their low dimensionality, carbon nanotubes (CNTs) have striking properties, quite different from those of traditional semiconductors, with important implications for technology. The performance of electronic devices relies on carrier mobility, which is extraordinary high in CNTs at low fields. However, at high fields the mobility is dramatically reduced due to inelastic optical phonon scattering. Optical properties of CNTs, essential for electro-optical devices, are dominated by excitons with binding energies and oscillator strengths orders of magnitude larger than those in conventional semiconductors. We calculate the electron-phonon scattering and binding in CNTs, within a tight binding model [1]. We derive the mobility as a function of temperature, electric field, and nanotube chirality using a multi-band Boltzmann treatment. We find the drift velocity saturates at approximately half the graphene Fermi velocity. Polaronic binding give a band-gap renormalization of 70 meV, an order of magnitude larger than previously suggested. We calculate the properties of excitons in CNTs embedded in a dielectric, for a wide range of tube radii and dielectric environments, by solving the Bethe-Salpeter Equation in a tight binding basis. We find that simple scaling relationships give a good description of the binding energy, exciton size, and oscillator strength as a function the tube radius, the dielectric constant of the embedding material, and the chirality [2]. In addition we calculate optical absorption including the exciton-phonon interaction. We find a phonon sideband at 200 meV above the zero phonon line, due to the creation of exciton plus one optical phonon [3]. [1] V. Perebeinos, J. Tersoff, and Ph. Avouris, cond-mat/0411021. [2] V. Perebeinos, J. Tersoff, and Ph. Avouris, Phys. Rev. Lett. 92, 257402 (2004). [3] V. Perebeinos, J. Tersoff, and Ph. Avouris, cond-mat/0411618.

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