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Simulations of resonant Raman response in bundles of semiconductor carbon nanotubes. OLEKSIY ROSLYAK, ¹Physics and Engineering Physics Department, Fordham University, Bronx, NY 10458, ANDREI PIRYATINSKI, STEPHEN DOORN, ERIK HAROZ, HAGEN TELG, JUAN DUQUE, JARED CROCHET, Los Alamos Natl Lab, J. R. SIMPSON, A. R. HIGHT WALKER, Engineering Physics Division, NIST, Gaithersburg, MD 20886, LANL COLLABORATION, FORDHAM COLLABORATION, NIST COLLABORATION — This work is motivated by an experimental study of resonant Raman spectroscopy under E22 excitation, which shows a new, sharp feature associated with bundling in (6,5) semiconductor carbon nanotubes. In order to provide an insight into the experimental data, we model Raman excitation spectra using our modified discrete dipole approximation (DDA) method. The calculations account for the exciton states polarized along and across the nanotube axis that are characterized by a small energy splitting. Strong polarization of the nanotubes forming the bundle results in the exciton state mixing whose spectroscopic signatures such as peaks positions, line widths, and depolarization ratio are calculated and compared to the experiment. Furthermore, the effects of the energy and structural disorder, as well as structural defects within the bundle are also examined and compared with the experimental data.

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