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Simulations of resonant Raman response in bundles of semiconductor carbon nanotubes OLEKSIY ROSLYAK, Fordham University, STEPHEN DOORN, ERIK HAROZ, JUAN DUQUE, JARED CROCHET, HAGEN TELG, Los Alamos National Laboratory, ANGELA HIGHT WALKER, JEFFREY SIMPSON, National Institute of Standards and Technology, ANDREI PIRYATINSKI, Los Alamos National Laboratory — This work is motivated by experimental study of resonant Raman response associated with E_{22} exciton state coupled to G^+ -mode vibrational mode in bundles of (6,5) semiconductor carbon nanotubes. In order to provide an insight into 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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