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Interface and Surface Optical Phonons Spectra in Wurtzite Nitride Quantum Well Wires: Size and Dielectric Effects

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Abstract: By employing the method of electrostatic potential expansion, the interface optical (IO) and surface optical (SO) phonon modes and the corresponding Fröhlich-like electron-phonon-interaction Hamiltonian in a Q1D wurtzite cylindrical quantum well wire (QWW) embedded in nonpolar dielectric matrix are derived and studied based on the dielectric continuum model and Loudon's uniaxial crystal model. Numerical calculations for a wurtzite GaN/AlN QWW are mainly focused on the size- and dielectric-dependent IO and SO phonon spectra and electron-IO (SO)phonons coupling functions. Results reveal that, in general, there are two branches of IO phonon modes and one branch of SO mode in the system. The dispersions of the IO and SO modes are obvious only when the radii ratio β and the dielectric constant of nonpolar matrix ε_d is small. The limiting frequencies of IO and SO modes for very large β have been analyzed in depth from both physical and mathematical viewpoints. The reducing behaviors of some modes have been clearly observed. Via the discussion of electrostatic potential spacial distributions of the IO and SO modes, we find that the QWW structures and dielectric constants of nonpolar matrix have little influence on the low-frequency IO mode, but they can greatly affect the potential distributions of high-frequency IO mode and SO mode. Detailed comparison of the dispersion behaviors of the modes and electron-phonon coupling properties in the Q1D wurtzite QWWs with those in wurtzite QWs and cubic quantum dots has also been made. Furthermore, part of the theoretical results derived in the present paper is consistent with the relatively experimental conclusion.

Key Words: Optical Phonon Vibration Spectra; Wurtzite QWW.

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