Surface States of The Wurtzite Type Nanowires

NATALIA MALKOVA, CUN-ZHENG NING, NASA Ames — We study the surface states at the lateral facets of the wurtzite type nanowires. As particular example we consider nanowires with the same symmetry for all the lateral facets. Our approach is based on the transfer matrix technique within the semi-empirical tight-binding approximation. We calculate the surface states at (1100), (1210) and (0001) surfaces of the semi-infinite crystal first. Then using the cyclic boundary conditions, depending on the radius of the nanowire, we find the quantized spectrum for the surface states in question. We present the result for the surface states of GaN, ZnO, CdS, CdSe and AlN wurtzite nanowires with the (1100) and (1210) lateral surfaces. The dangling bonds are shown to give a set of the states inside the band gap of the semiconductors studied. The orbital character and decay length of the states are calculated. We analyze the symmetry of the quantized surface states and possible optical dipole transitions between them.