【NII-03】

Structure of the Ultra-thin Nanorods and Nanowires

강정원, 황호정
중앙대학교 전자공학과

We have investigated the structures and the properties of the ultra-thin polyhedral nanorods and ultra-thin multi-shell nanowires, which composed of a core atomic strand and multi-shells, using a classical molecular dynamics simulation and a many-body potential function of the second-moment approximation of tight-binding scheme. This investigation showed the relation between the ultra-thin multi-shell nanorods and the tetrahedron. The ultra-thin multi-shell nanorods have only the hexagonal-like surface lattice, and are composed of the sequence of the different outer rings in order to form the tetrahedron, the sub-unit of nanorod. When one ring has Nr atoms and the shell number is Ns, the total tetrahedron number of the polyhedron nanorods is $(3n-2)\ p$, where subtracting one from the number of outer ring is equal to n multiplied of Ns, and the unit number of tetrahedron, $p = N\mathrm{r} / N\mathrm{s}$. The structural properties of the pentagonal multi-shell nanorods and nanowires, which have the square surface lattice and diameters of several nanometers, are close to those of fcc as the sub-units composed of both a triangular and a quadrangular pyramids oriented in the <100> directions. The decagonal multi-shell nanorods are another structure related to the pentagonal multi-shell nanorods.