Perspective of p-conductivity Enhancement in ZnO Nanowires

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We present calculation of electronic structure of impurity in nanowire. Ionization energy of impurities is calculated in dependence on nanowire radius. It is shown that shallow donors are strongly influences by space confinement, which is expressed in sharp increase of ionization energy.

We consider an electron bound to Coulomb-type impurity placed in a ZnO Nanowire of a cylinder form and with an infinite length and radius a_0. The potential outside nanowire is taken to be infinity. Our purpose thus is to solve the effective-mass Schrödinger equation. In the cylindrical coordinates we have

$$\left(-\frac{\hbar^2}{2m^*}\Delta-\frac{q_0 e^2}{\varepsilon\sqrt{z^2+\rho^2}}\right)\Psi(\rho,z,\varphi)=E\Psi(\rho,z,\varphi) \quad (1)$$

In (1) q_0 is the charge of the Coulomb impurity, ε is the static dielectric constant of the material, m^* is the effective mass of the electron and E is the electron energy measured from the bottom of bulk material conduction band.

To solve (1), we replace the real potential by truncated Coulomb potential $2q/(|z|+a)$. The rest of Hamiltonian $V=q/(|z|+a)-q/\sqrt{z^2+\rho^2}$ is accounted by direct diagonalization.

Calculations show that space confinement affects strongly only shallow donor defects. For $a_0=1nm$ radius nanowire the ionization energy of donor, the ground state of which in bulk samples is 50 meV bellow from the bottom of conduction band, is increased up to 234 meV. This ionization energy exceeds the bulk value until $a_0=7nm$.

In the case of deep donors electronic structure is only slightly influenced by space confinement. We calculated energy levels for donor impurity owing 200 meV ionization energy in bulk specimens. It turned out that in 1 nm radius nanowire ionization energy exceeds bulk value by 30 meV only. For acceptor levels space confinement is significant only for small values of nanowire radius, for 2 nm radius nanowire ionization energy is already dropped to its bulk value. Taking into account that acceptors in ZnO are typically deep, while compensating centers are typically shallow, we can expect that for definite values of radius compensation processes can be suppressed.