Electronic and optical properties of (Al xGa 1-x) 1-yMn yAs single crystal: a new candidate for integrated optical isolators and spintronics

Abstract

We have explored the electronic and optical properties of cubic $(Al_x Ga_{1-x})_{1-y} Mn_y As$ system using the FP-LAPW method. The unit cell has 64 atoms, so that one manganese (Mn) atom is placed in the position of gallium site, which corresponds to 3.125 % doping concentration with x = 12.5 %. Our calculations, using local density approximation + U (Hubbard parameter) scheme, predict that the ferromagnetic state for AlGaMnAs, with a magnetic moment of about 4.014 μ_B per Mn dopant is more favorable. Despite its electronic properties being strongly affected by inducing small amounts of Mn substitutional atoms in the cationic sublattice of AlGaAs, $(Al_x Ga_{1-x})_{1-y} Mn_y As$ possesses optical properties strictly less than those of $Al_x Ga_{1-x} As$, especially its optical conductivity at the peak 1.256 eV. The results indicate that AlGaMnAs may be agood candidate for optoelectronics when exploited in optical fiber networks, and it can still be of great interest because of its promising potential when used for spintronics.