

The effects of point defects, hydrogen, and growth conditions on the electronic structure and properties of the (Al,N) codoped p-type ZnO have been investigated using the first principles method. The obtained results showed that the AlZn-NO-VZn complex is a shallow acceptor that can play an important role in achieving the p-type conductivity in the (Al,N) codoped ZnO films. Our results showed also that the electrical conductivity type in the (Al,N) codoped ZnO films strongly depends on the donor/acceptor concentrations ratio. The codoped ZnO films prepared under both Zn-rich and O-rich growth conditions with a donors/acceptors ratio of 1:2 have a p-type conductivity, while those prepared with a ratio of 1:1 cannot be p-type unless if they are prepared under O-rich conditions. The achieved p-type quality depends also on the used nitrogen doping source. To prepare p-type ZnO film of high quality using the (Al,N) codoping method, the use of NO or NO₂ is recommended. The presence of donor defects such as oxygen vacancies and hydrogen will significantly affect the electronic properties of the (Al,N) codoped ZnO films, and if the concentration of these defects in the sample is high enough, the material can be easily converted to n-type.