COLIBABA, G.V. ZnO doping efficiency by multivalent metals in complex CVT reactionsd. In: Solid State Sciences. 2018, vol. 97. ISSN 1293-2558.

The present investigation is a theoretical study of doping efficiency of ZnO crystals grown by using compound chemical vapor transport (CVT) agents based on HCl and doped by oxides of various metals in the growth process. The thermodynamic analysis for compositions of Me_xO_y –ZnO–ZnCl₂–CO CVT systems in the closed growth chambers was carried out for oxides (Me_xO_y) of all non-radioactive metals of the periodic table, taking into account various types of chloride species. The influence of temperature (1000–1500 K), ZnCl₂ pressure (10^{-2} –10 atm) and Zn pressure (10^{-5} –3 atm) on the total pressure and mass transport rate of doping species (MeCl_n) were investigated. The possibility of increase in the doping efficiency of ZnO by $Me_xO_y + ZnCl_2 + Zn$ CVT reactions is predicted for some multivalent metals. Some calculation results are confirmed experimentally.