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The theoretical analysis of the problems of p-type zinc sulfide production by means of silver ion implantation including the calculation of the radiation defects distribution profiles and the thermodynamic calculations of the equilibrium self-compensation under the annealing determines the technological conditions when the p-type conductivity obtaining is possible in this material.

The calculation by Monte-Carlo method has shown that the distribution profiles of implanted silver atoms and the radiation-induced defects namely ones of the vacancies and interstitial atoms ( $V_S$ ,  $S_i$ ,  $Zn_i$ ,  $V_{Zn}$ ) in both sublattices during the ion implantation are more favourable for the formation of the isolated acceptor centres  $Ag_{Zn}$  then for the compensated associators ( $V_S Ag_{Zn}$ ).

It is connected with the fact that the point radiation-induced defects concentration at the maximum of the silver atoms distribution is determined by relations:  $V_{Zn} > Zn_i$ ;  $V_S - S_i < Ag$ . Coulomb and Firsov potentials were used as scattering potentials. Displacement energies of Zn and S atoms out of their lattice sites were taken 15 ev and 9 ev [1] respectively.

For each case of scattering a kind of centre was played by taking into account the difference in differential cross section of scattering.

At the following annealing of the radiation-induced defects it is possible an appearance of the thermodynamically equilibrium self-compensation of acceptor centres by sulphur vacancies. At the usual temperature conditions of the ZnS doping (the temperature above  $1000^{\circ}\text{C}$ ) the self-compensation is determined by the unfavourable relationship between the band-gap and the enthalpy of the compensating native defects formation.

The fulfilled thermodynamical calculations have shown that at the sufficient low temperatures of doping the formation of compensating vacancies becomes disadvantageously from the energy point of view. The intensive self-compensation processes start at the temperatures above  $500^{\circ}\text{C}$ . Hence this temperature is a limit one for the annealing of the ion implanted zinc sulphide in the sulphur vapours.

The experimental data confirm in general the correctness of these calculations. The specially unoriented ZnS single crystals grown from the melt with resistivity of order  $10^{13}$  Ohm.cm were implanted by Ag-ions with the 50-60 kev energy and the dosage  $10^{14}$ - $10^{16}$  cm $^{-2}$ . The sample temperature was  $50$ - $70^{\circ}\text{C}$  throughout the implantation.

In the  $400$ - $450^{\circ}\text{C}$  temperature range of annealing in sulphur vapours the implanted samples were of hole conductivity with the resistivity  $10^3$  -  $10^5$  Ohm.cm. At the annealing temperature above  $450^{\circ}\text{C}$  the n-type of conductivity is observed. The annealing in argon vapours results in the p-type but at the same annealing temperatures and dosages the resistivity is one or two order higher than after the annealing in the sulphur vapours.

#### Reference.

1. F.A.Kröger, "The Chemistry of Imperfect Crystals"  
North-Holland Publishing Company - Amsterdam, 1964