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Prediction of optimal operating conditions to grow $CuGa_{0.3}In_{0.7}Se_2$ thin using CSVT technique

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Abstract:

This work deals with a theoretical and experimental investigation of CSVT process for the preparation of $CuGa_{0.3}In_{0.7}Se_2$ thin films. This study was performed using the SOLMIX software which gives the composition of the chemical system at the thermodynamic equilibrium. The model is based on the minimization of the Gibbs energy of a multiphase mixture containing 51 chemical compounds derived from the combination of the simple elements of (Cu, In, Ga, Se, I). The results highlight the influence of the temperature and pressure on the growth of $CuGa_{0.3}In_{0.7}Se_2$ thin films. The different compounds of the solid phase were predicted for various source temperature and iodine pressure. The conditions of quasi-stoichiometric deposition are [400; 600℃] and [3.10^{-4}; 0.14 atm].The optimal conditions were tested experimentally. The samples grown of $CuGa_{0.3}In_{0.7}Se_2$ have been analyzed by X-ray analysis and the SEM micrographs. The thin films grown in the optimal conditions are of good quality (see figures 1 to 4). The model results validated by our experiments demonstrate that the described thermodynamic model is a helpful tool to the prediction of the optimal conditions of CSVT process.

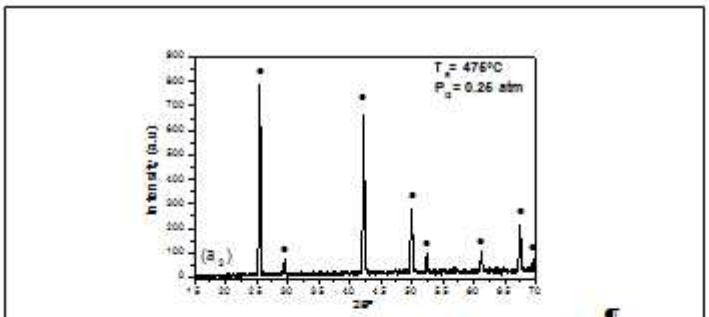

Fig.1.XRD patterns of the deposit at T_3 = 475°C and P_{I2} = 0.25 atm (bad quality)

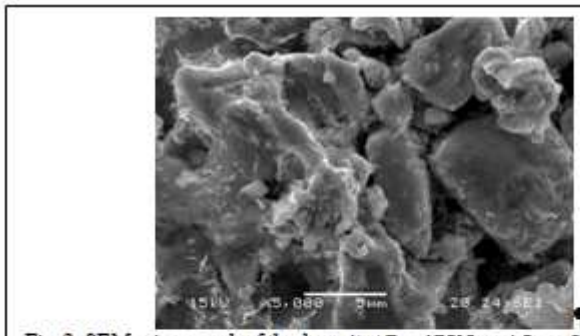

Fig.2.SEM micrograph of the deposit at T_3 = 475°C and P_{I2} = 0.25 atm (bad quality)

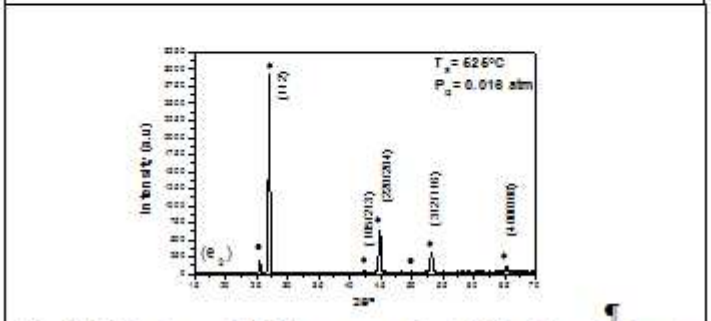

Fig.3.XRD patterns of CIGS layer grown at T_3 = 525°C and P_{I2} = 0.016 atm (good quality)

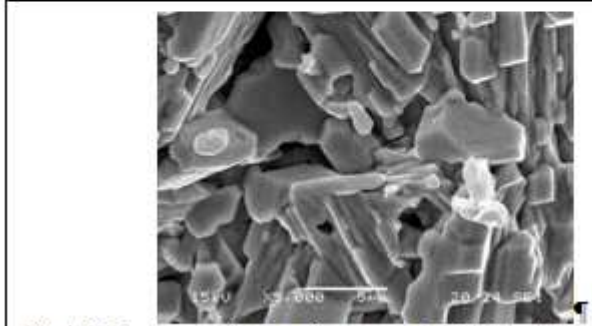

Fig.4.SEM micrograph of sample grown at T_3 = 525°C and P_{I2} = 0.016 atm (good quality).

Key words: Modeling ; CSVT ; SOLMIX ; Thermodynamic Equilibrium; Thin Solid Films ; $CuGa_{0.3}In_{0.7}Se_2$