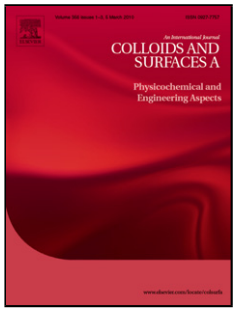

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PII: S0927-7757(17)30371-0
DOI: http://dx.doi.org/doi:10.1016/j.colsurfa.2017.04.038
Reference: COLSUA 21550

To appear in: *Colloids and Surfaces A: Physicochem. Eng. Aspects*

Received date: 28-3-2017
Revised date: 17-4-2017
Accepted date: 19-4-2017

Please cite this article as: B. Ouertani, H. Ezzaouia, B. Theys, Effect of Ruthenium alloy on the band gap value of FeS_2-pyrite, *Colloids and Surfaces A: Physicochemical and Engineering Aspects* (2017), http://dx.doi.org/10.1016/j.colsurfa.2017.04.038

Effect of Ruthenium alloy on the band gap value of FeS_2-pyrite.

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Abstract :

In the aim of increasing the band gap value of FeS_2-Pyrite thin films having good crystallinity, high absorption coefficient (~10^5 cm^{-1}) and a band gap of about 0.95 eV, which were synthesized by a simple and low cost method consisting of sulphuration, under vaccum (≅10^{-4} Pa), of amorphous iron oxide thin films pre-deposited by spray pyrolysis of $FeCl_3.6H_2O$ (0.03 M)-based aqueous solution onto glass substrates heated at 350°C, we draw attention in this work to the fabrication of these films after alloying with Ru. We followed two methods: the first one consists of spraying aqueous $RuCl_3.3H_2O$ solution, during shorter time, on heated pre-deposited oxide layer at the same spray conditions with molar ratio as $RuCl_3.3H_2O$: $FeCl_3.6H_2O$ = x :1-x(x = 0.3966 , 0.1586 , 0.0396 , 0.0317 , 0.0156 and 0.00). The second consists of spraying on heated substrate, an aqueous solution prepared by dissolving ferric chloride ($FeCl_3.6H_2O$) and Ruthenium(III) chloride hydrate ($RuCl_3.3H_2O$) with molar ratio as $RuCl_3.3H_2O$: $FeCl_3.6H_2O$ = x :1-x(x= 0.3171, 0.1586, 0.234, 0.0119, 0.0051, 0.0025 and 0.00). Afterward, the as obtained films are sulphured at the optimum conditions (Pressure ≅ 10^{-4} Pa, duration = 6h, temperature =450°C). Dark layers having granular structure, were obtained. The effect of alloying on atomic structure, as well as optical properties of Ru-alloyed FeS_2-Pyrite films were examined by XRD, optical and MEB characterisations. Our results show that the band gap value of $Fe_{1-x}Ru_xS_2$ layers increases versus the alloy percentage. An optimum band gap value was obtained according to the first method of about 1.48 eV for x = 0.0156 ; which is considered a very interesting result for the photovoltaic applications of our films. An increase of the band gap value versus the Ru concentration with the second method was observed, as well.

Keywords: Ru-alloying FeS_2, spray, sulphuration, photovoltaic cells.