

A statistics modeling approach for the optimization of thin film photovoltaic devices

António T. Vicente¹, Manuel J. Mendes¹, Hugo Águas¹, Elvira Fortunato¹ and Rodrigo Martins^{1*}

¹*CENIMAT/I3N, Departamento de Ciência dos Materiais, Faculdade de Ciências e Tecnologia, FCT, Universidade Nova de Lisboa and CEMOP/UNINOVA, 2829-516 Caparica, Portugal*

²*Laboratory of Organic Electronics, Linköping University, Department of Science and Technology, 601 74 Norrköping, Sweden.*

The growing interest in exploring thin film technologies to produce low cost devices such as *n-i-p* silicon solar cells, with outstanding performances and capability to address the highly relevant energy market, turns the optimization of their fabrication process a key area of development. The usual one-dimensional analysis of the involved parameters makes it difficult and time consuming to find the optimal set of conditions. To overcome these difficulties, the combination of experimental design and statistical analysis provides the tools to explore in a multidimensional fashion the interactions between fabrication parameters and expected experimental outputs.

Design of Experiment and Multivariate Analysis are demonstrated here for the optimization of: 1) the low temperature deposition (150 °C) of high quality intrinsic amorphous silicon (i-a-Si:H); and 2) the matching of the *n*-, *i*-, and *p*- silicon layers thickness, to maximize the efficiency of thin film solar cells. This method allowed a rapid screening for the optimization of both intrinsic thin films and the thickness structure for a simple *n-i-p* solar cell at 150 °C, thus saving time and resources by cutting the number of experimental sampling iterations needed. The information provided by the statistical models revealed to be paramount to assist decision-making for subsequent experiments and to support the development of robust and reliable protocols to produce high efficiency solar cells at low temperature.

High quality intrinsic layers at the transition a-Si:H/ μ c-Si:H were engineered from the statistical model, which also highlights the importance of low power density in the fabrication of these device-quality films. The optimum *i*-layers have a photo-to-dark conductivity ratio of 10^7 and ideal band gap ($E_g = 1.73-1.75$ eV). The optimum output provided the necessary active layer for the subsequent study of the SC thickness. From the initial sample poll of 8 devices, the model predictions allowed the improvement of solar cell efficiency by 24% and FF by 13%, when compared with the best sample from the initial set. Such result demonstrates the capacity of the technique to successfully pin-point the optimum combination of thicknesses.

Keywords: Thin films, solar cells, PECVD, Multivariate Analysis, Design of Experiment.