Machine Learning Models for Diffused Copper Doping Profiles in CdTe Solar Cells

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It is well known that Cu plays an important role in CdTe solar cells for back contact formation and providing p-type doping. Therefore, an important outcome of the simulation effort of the DOE PREDICTS project was to gain insight into the formation and evolution of doping during the annealing process and the cool-down. In the work presented here, we use machine learning to shed light on the Cu profiles that result from the diffusion and cool-down process in the fabrication sequence of CdTe solar cells. The calculation of the profile of the majority holes in the absorber of the CdTe solar cells will be described in a subsequent study. In this paper, we establish the methodology of neural networks machine learning (ML) as applied to the diffusion and cool-down process steps. The big dataset was generated using the PVRD-FASP Solver [1].

Artificial Neural Network models (ANN) have been widely used to model complex problems. In material science, neural network algorithms have been used to search for a total energy minimization and material parametrization. In this work we interpolate from one multi-dimensional space (slow variables, nslow ~ 100) to another multidimensional space (fast variables, nfast ~ 10). For such problems, it is difficult to determine an adequate number of hidden layers and number of neurons. An alternative way is to implement an ANN using keras with backend TensorFlow that uses Radial Basis Function (RBF) network and has only three layers. Hence, its training is much simpler. This approach is able to approximate any multivariate continuous function on a compact domain to a desirable accuracy by using a sufficient number of units. In this work, the ANN and RBF approaches are used. In other words, we have developed and implemented a machine learning model based on neural networks designed to predict the Cu diffusion profile given input parameters (temperature and duration of the diffusion process with subsequent cool-down). Excellent agreement is found between the test and predicted datasets, the difference between the two being smaller than 0.009 μm.

[1] Abdul R Shaik, Daniel Brinkman, Igor Sankin, Christian Ringhofer, Dmitry Krasikov, Hao Kang, Bedrich Benes, Dragica Vasileska, "PVRD-FASP: A Unified Solver for Modeling Carrier and Defect Transport in Photovoltaic Devices", IEEE J. Photovoltaics, Vol. 9(6), pp. 1602-1613, November 2019.

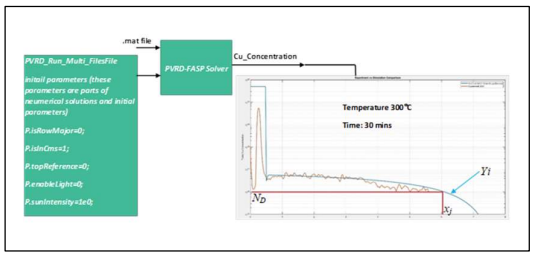

Fig.1: Generation of the dataset to be used in machine learning. In the graph that depicts the copper concentration vs. depth, the blue line is the doping profile generated with the PVRD-FASP solver and the red line are the experimental data provided to us by First Solar. Parameters in these curves are the temperature 300C and the duration of the diffusion process 30mins.

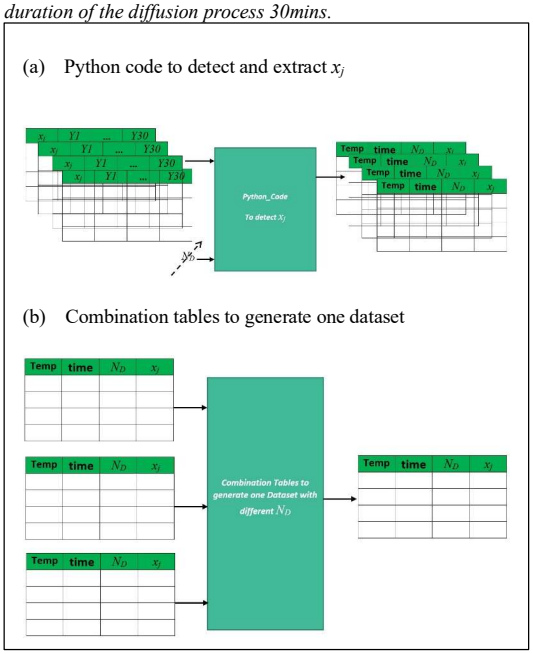

Fig.2: (a) Python code used to detect xj for different input parameters. (b) Generation of one dataset.

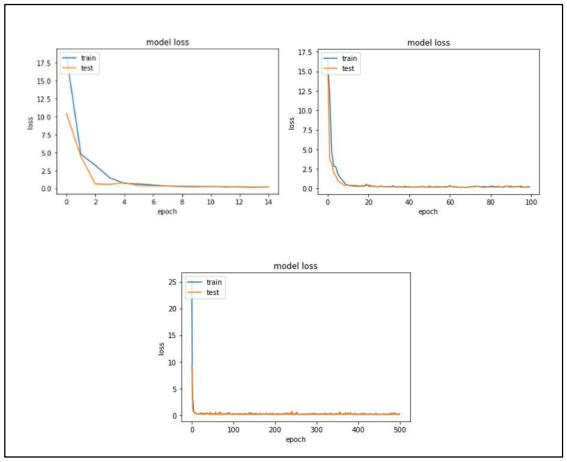

Fig.5: Loss function (error) vs. epoch (number of iterations after which we update the weights and the bias).

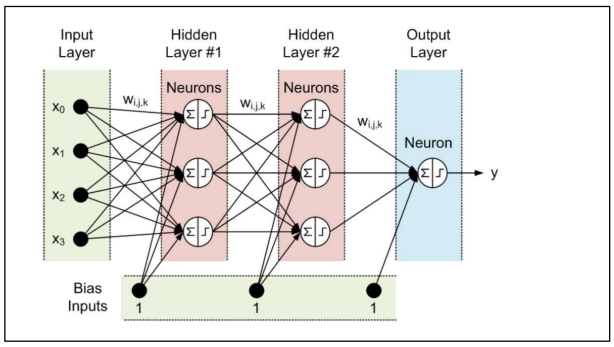

Fig.3: Artificial Neural Network ANN diagram of the machine learning used in this work.

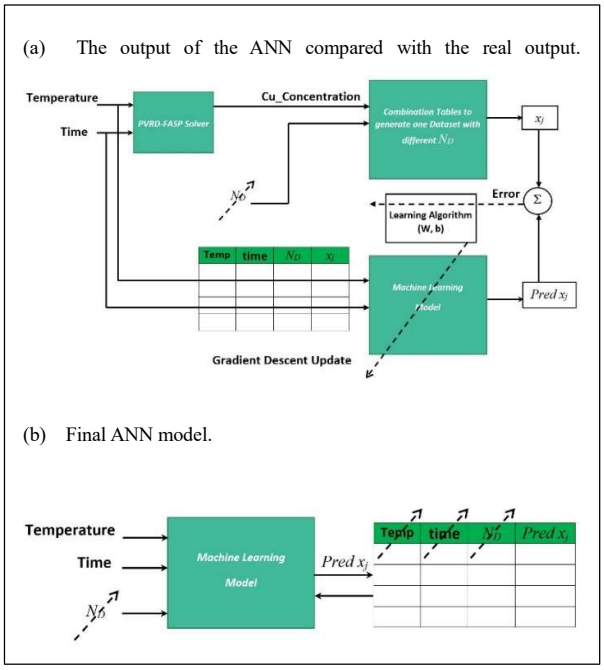

Fig.4: (a) The output of the ANN compared with the real output. (b) Final ANN model.

Table 1: test vs. predicted data

Test (x_j) (μm)	*Predicted x_j (μm)*
8.69000	8.502874
5.66750	5.5411371
10.15250	9.890299
8.93375	8.9742605
6.44750	6.910209
3.96125	3.82681
5.32625	5.2161648
10.00625	9.954606
7.03250	6.982865
8.20250	8.460101
4.74125	4.9217137
6.30125	6.536751