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Data Driven Design of Gas Sensors Parameters Optimization by Tailoring the Catalytic Metal Alloy Contacts

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Abstract— Currently, low power Metal Oxide Gas Sensors (MOXs) are widely employed in gas detection because of its benefits, such as high sensitivity and low cost. However, MOX presents several problems, as well as lack of selectivity and environment effect. Semiconducting Zinc Oxide was used for sensing methane, where alloys of noble metals, mostly pure or binary alloys, were used to increase the sensor parameters of the device. Experimental results of such noble metals or their binary alloys were used to develop the corresponding artificial neural network model describing the three pivotal attributes of the sensor device, viz. response magnitude, response time and recovery time. The models were used in a novel approach to design ternary alloys with superior performance using multi-objective optimization technique, where the Pareto front thus developed was used for designing ternary catalysts. The present scheme of prescriptive data analytics seems to provide some definite clue for experimental study aiming the pre-determined set of sensor parameters.

Keywords— Gas Sensor parameters, Ternary Alloy Design, Artificial Neural Network, Multi-Objective Optimization.

I. INTRODUCTION

A highly volatile hydrocarbon such as Methane (CH_4), if combines with ambient air, it can form a highly explosive mixture and can damage the safety in coal mine environment. A reliable sensor is thus required to be developed for the early detection of the harmful mixture present in the atmosphere. It is important to observe the emission of Methane in the atmosphere to reduce the environmental pollution [1]. It is proved that various kinds of oxide semiconductor materials are successful in detecting the presence of CH_4 [2-7]. Semi-conductor ZnO can be efficiently used to sense the reducing gases of different types at low temperature [8]. ZnO acts as very promising catalyst, in detection of methane , when the sensing temperature varies between 200 °C and 250 °C (depending on the ZnO synthesis route) [9-11]. The contact electrodes (alloys of noble metals) are used in gas sensor devices for improving the device sensitivity, i.e. response time, response magnitude and recovery time. Noble metals acting as a catalyst by itself is kept inert to the reactions comes in handy in this type of gas sensors. A direct interaction between the promoter and the semi-conductor surface brings a sensitization in these type of sensor devices. The electronic state of the semiconductor changes with the change in the oxidation state of the promoter. In presence of air, two promoters of Ag and Pd form stable oxides (Ag_2O and PdO), but get reduced to metals quite easily in presence of a combustible gas [5]. Each promoter in the oxidised form produces a strong electron-depleted space charge inside the semi-conductor, and is indicated in the work function by the corresponding shifts [12]. The electronic interaction jeopardized, when it is reduced to metal [12]. Hydrogen gas (inflammable gases) is highly susceptible in coal mines , for the improvement of the system properties of the sensor device for the detection of leakage of methane gas , different metals and binary alloys with varying combination and composition have been tried by the earlier researcher [9,11,13,14]. In the present work, since ternary alloys were never used for this purpose, to explore the possibility of developing ternary alloys which can improve the performance of the gas sensor devices, an information based approach has been adopted. The three key sensor parameters for quantifying the performance of a sensor device are: Response magnitude, Response time, Recovery time, but in the optimization parameters they often found to have varying requirement. Genetic algorithm (GA) [16], plays a significant role in cases of multi-objective optimization [15], and is used for the design of alloys with varying objectives successfully [17, 18]. A data driven model from the data generated on binary alloys by the earlier researchers has been evolved by using Artificial Neural Network (ANN) [19, 20] for the three aspects mentioned above, in the absence of any suitable analytical model correlating the properties and the alloy composition. An ANN map [21, 22] is used to outline the input-output spaces of complex

materials systems. The objective functions for the optimization process utilizes the developed ANN models.
The earlier researchers have successfully used the ANN models as objective functions for GA based optimizations in materials systems [23, 24]. In the current case, for designing ternary alloys a novel computational design was adopted by using a database consisting of pure metal and binary alloys. To detect the trend of combinations and compositions to finally design the alloy there is an application of an outcome of the optimization process developed The" Pareto fronts"[16] consisting non-dominated optimal solution.

II. RELATED WORK

In respect to the traditional way of designing new materials, a trial and error approach , with pre –scheduled performance often leads to a complete drainage of resources is a time consuming process. In attaining the desired goal, the computational materials design, powered by intelligent data analytics techniques conducts lesser experiments and offer faster processing. By reducing the search space computationally, modelling, simulation and optimization reduces the number of trials. To improve the performance of materials the concept of materials informatics is used by generating inherent correlation between the process parameters and its performance based on the available dataset and materials chemistry. To unite scientific information and material discovery Data analytics serves as an effective tool. In the current case, the performance of the device is described through three main elements: Response magnitude, Response time, and Recovery time. They often vary in nature due to which genetic algorithm is used. An optimum balance of response time, response magnitude and recovery time were observed in the current attempts. The objective functions for the optimization study uses three separate ANN models to describe the above three attributes with respect to the input parameters.

III. METHODOLOGY

From the earlier published literatures based on the experimental study done by different researchers, the database was created [9,11,13,14].The database consists of alloy compositions including Methane(CH_4) concentration pure metals and binary combinations of Au, Ag, Pt, Pd, Rh ,testing temperature and size of the ZnO particles as inputs and three attributes : Response magnitude, Response time and Recovery time as output. Table1 consists of the detailed database. As mentioned above the objective functions for the optimization study uses three separate ANN models which is prepared by the data present in the table to describe the above three output parameters with respect to the input parameters.

Table 1: shows the List of inputs for three different output variables with their minimum, maximum, average and standard deviation values [9, 11, 13, 14]

Input variables	Min	Max	Mean	Standard Deviation
CH4 conc. (%)	0.01	1.5	0.524754	0.426081395
Temperature (oC)	100	350	225.4098	64.54517205
ZnO Size (nm)	20	60	57.72131	15.47054314
Pt (wt%)	0	100	8.196721	27.65912729
Pd (wt%)	0	74	34.42623	31.57660474
Rh (wt%)	0	100	22.95082	42.40063924
Ag (wt%)	0	70	27.86885	27.30779828
Au (wt%)	0	100	6.557377	24.95898275
Output variable				
Response Magnitude (%)	20	83.6	45.93888	18.74628351
Response Time (S)	2.69	86	36.11855	18.91098114
Recovery Time (S)	16	102	55.48555	22.39324979

IV. RESULTS AND DISCUSSION

From the database we did the three different Artificial Neural Network plot for each output variable.

Table 2: List of input and output variables with their minimum and maximum value with Response Magnitude

Sl. No.	Input variable	Minimum value	Maximum value
1.	CH4 conc.	0.01	1.5
2.	Pt (wt %)	0	100
3.	Pd (wt %)	0	74
4.	Rh (wt %)	0	100
5.	Ag (wt %)	0	70
6.	Au (wt %)	0	100
7.	Temperature(0C)	100	350
8.	ZnO crystal size (nm)	20	107
Sl.No.	**Output variable**	**Minimum value**	**Maximum value**
1.	Response magnitude	28	88.55

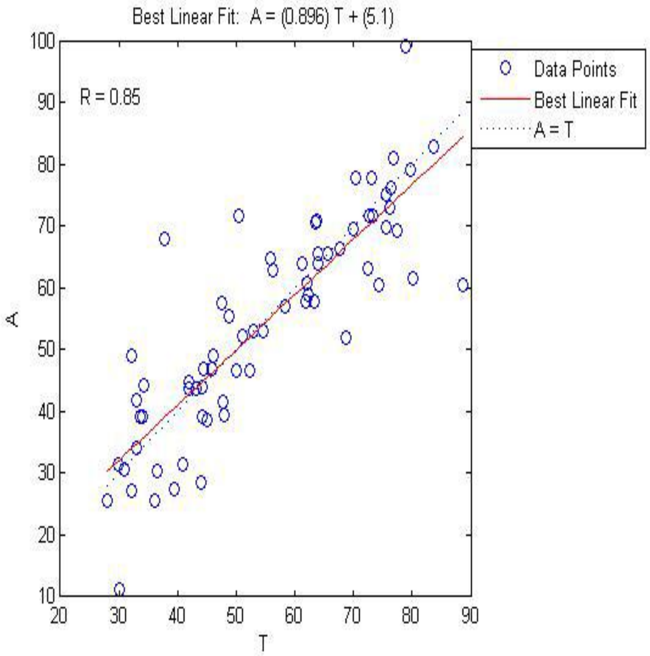

Figure 1: Achieved (A) vs. Target (T) values of Response Magnitude

The plot of target vs. the achieved values of response magnitude, wherein the blue circle represents the data points. The blue dotted line is the A=T (achieved value=target value) line. The red solid line is the best linear fit line. The coefficient of regression (R) is 0.85.

Table 3: List of input and output variables with their minimum and maximum value with Response Magnitude.

Sl.No.	Input variable	Minimum value	Maximum value
1.	CH4 conc.	0.01	1.5
2.	Pt (wt %)	0	100
3.	Pd (wt %)	0	74
4.	Rh (wt %)	0	100
5.	Ag (wt %)	0	70
6.	Au (wt %)	0	100
7.	Temperature(0C)	100	350
8.	ZnO crystal size (nm)	20	107
Sl.no.	**Output variable**	**Minimum value**	**Maximum value**
1.	Response time (s)	0	330

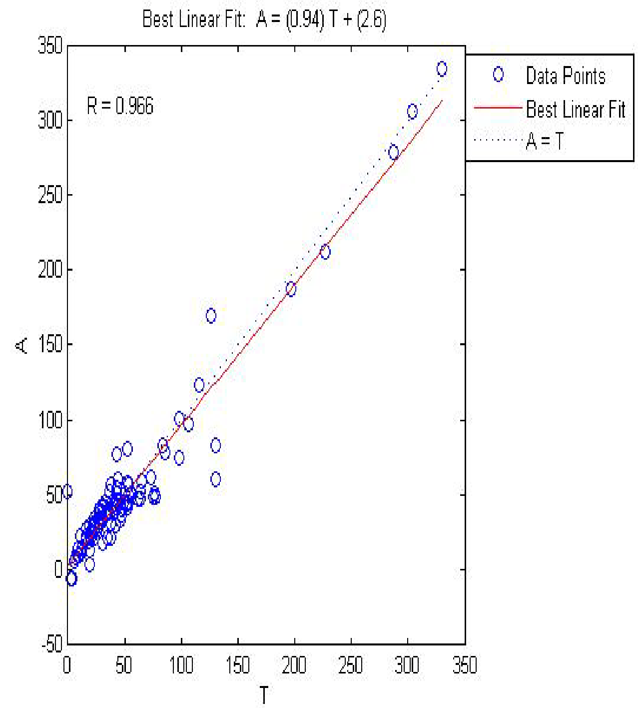

Figure. 2: Achieved (A) vs. Target (T) values of Response Time

The plot of target vs the achieved values of response time, wherein the blue circle represents the data points. The blue dotted line is the A=T (achieved value=target value) line. The red solid line is the best linear fit line. The coefficient of regression (R) is 0.966.

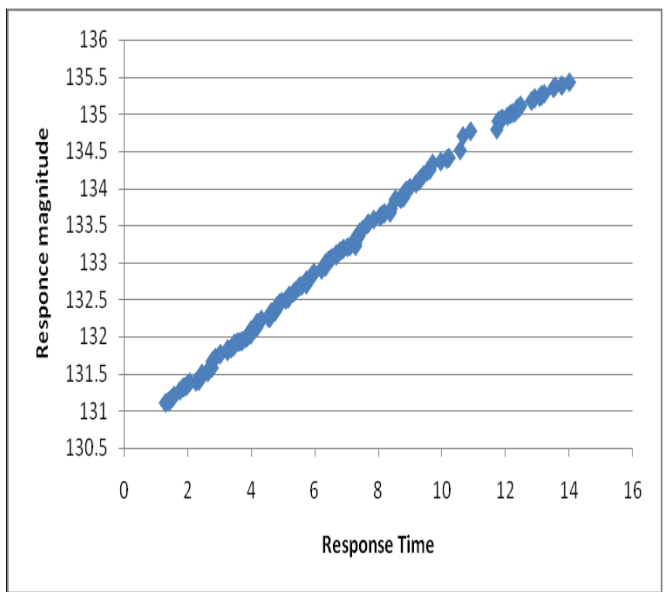

Figure.3: Pareto front of Response Magnitude vs. Response time considering generation and population as 500.

The results obtained from GA are plotted as follows. The X-axis had the Pareto solutions numbers for response magnitude arranged in ascending order and the y-axis had the compositional input variables and testing temperature.

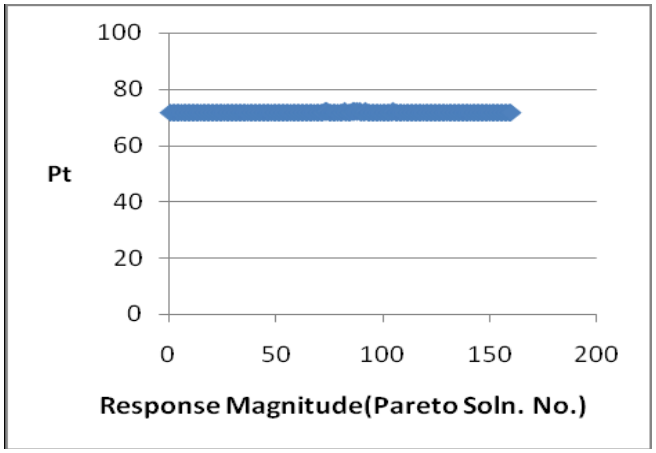

Figure.4: Variation of Pt in the Pareto Solution of Response Magnitude

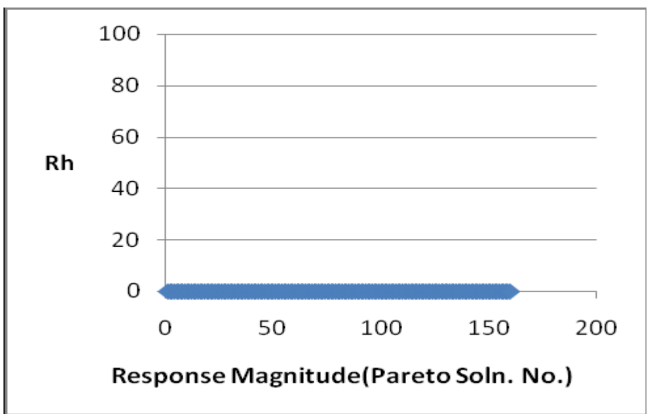

Figure. 5: Variation of Rh in the Pareto Solution of Response Magnitude

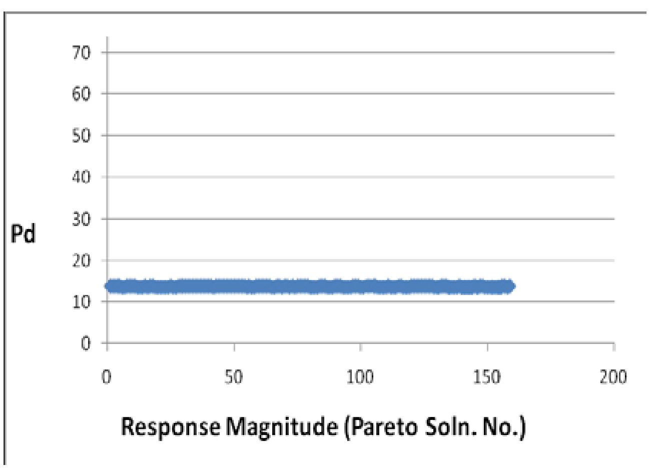

Figure.6: Variation of Pd in the Pareto Solution of Response Magnitude

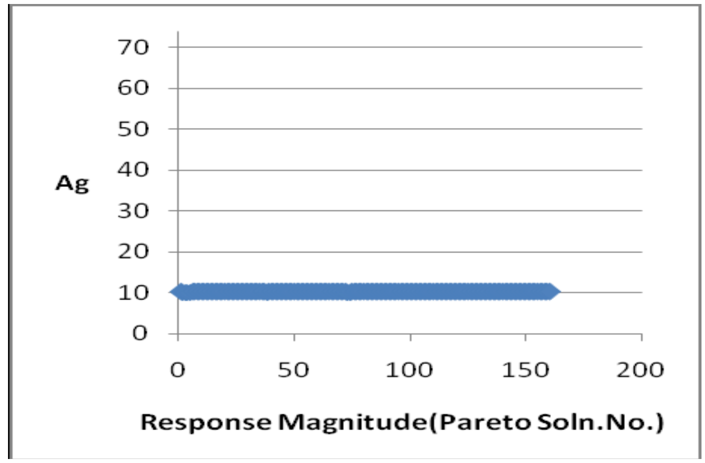

Figure.7: Variation of Ag in the Pareto Solution of Response Magnitude

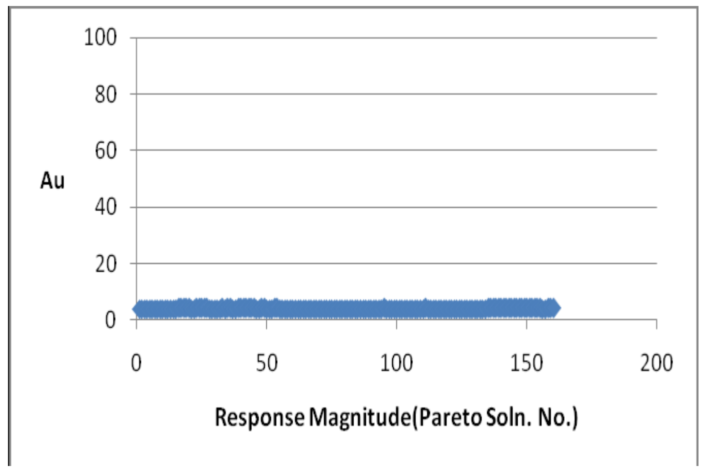

Figure. 8: Variation of Au in the Pareto Solution Of Response Magnitude

The role of compositional variables extracted from the Pareto front are presented below:

i) In Fig 4 there is no effect of Platinum addition on the response magnitude, i.e. for low to high values of response magnitude there is practically no variation in the amount of Platinum addition, it is nearly equal to seventy one.
ii) The optimized solution shows that Rh takes a value nearly equal to zero for all values of response magnitude, which suggests that Rh might not be required in the composition in Fig 5.
iii) In Fig 6 Pd takes a value of nearly 13 for response magnitude, magnitude.
iv) Ag takes a value close to its highest value 11 for all values of response magnitude, in Fig 7

v) In Fig 8**,** Au takes a value close to its highest value 4 for all values of response magnitude.

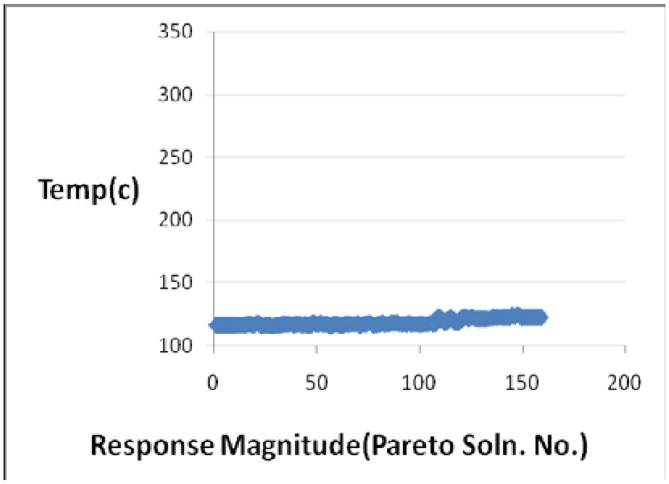

Figure.9: Variation of Temperature in the Pareto Solution of Response Magnitude

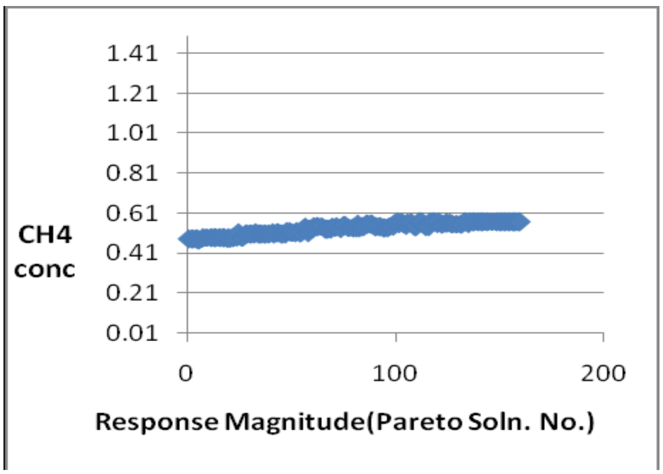

Figure.10: Variation of CH4 in the Pareto Solution Of Response Magnitude.

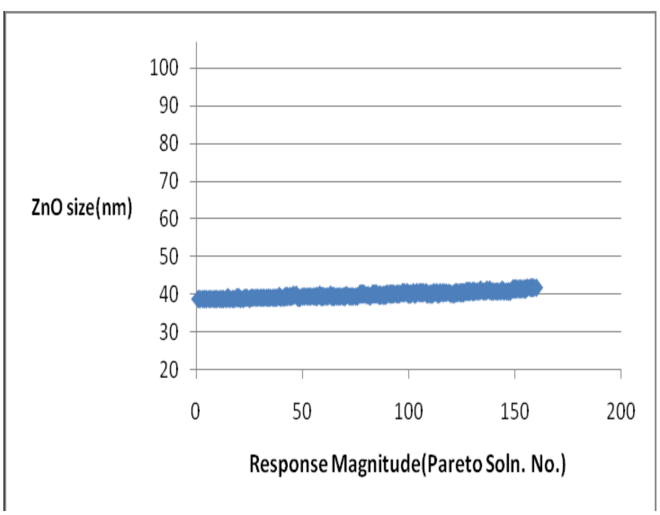

Figure. 11: Variation of ZnO crystal size (nm) in the Pareto Solution of Response Magnitude.

Role of the process variables, gas concentration and size of the metal oxide crystals are presented below:

i) The plot for testing temperature shows some variation in the range 115 to 124, with temperature increasing with increase in response magnitude in Fig 9.
ii) The plot for testing CH_4 concentration shows some variation in the range 0.47 to 0.56, with temperature increasing with increase in response magnitude in Fig 10.

iii) In Fig 11. As well as grain size increase response magnitude will increasing. It takes a small range of variation of 38 to 41 with the Response Magnitude.

Table 4: List of different variables related to the Pareto solutions at lower, medium and higher response magnitude.

CH4 conc.	**Pt (wt%)**	**Pd (wt%)**	**Rh (wt%)**	**Ag (wt%)**
0.482	71.72	13.88	0	10.2
0.556	71.78	14.0	0	10.17
0.56	71.76	13.85	0	10.21
Au (wt%)	**Temp. (deg.C)**	**ZnO crystal Size (nm)**	**Response Magnitude**	**Pareto Solution Number**
4.13	116.82	38.82	131.82	1
4.13	117.34	40.35	133.51	102
4.20	122.35	41.86	135.38	159

The model suggests an alloy composition of Pt- 72, Pd-14, Ag-10 and Au-4 (in wt %) for the optimum property which gives a higher response magnitude (Sensitivity) for ternary alloy composition.

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