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Defect-Engineered ZnO and SnO_2 Pellets for Enhanced Optical and Electrical Performance

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Abstract

There is a lack of a precise quantitative knowledge of the ways in which defect states impact electrical and optical characteristics in ZnO and SnO_2, despite the fact that defect engineering has become a viable method for improving the efficiency of metal oxide semiconductors. Since boosting the efficiency of optoelectronic & sensing devices requires careful control of bandgap and conductivity, this gap is critical. Using data-driven methodologies, this work sought to explore the links between controlled defect engineering and the optical bandgap and electrical conductivity of ZnO and SnO_2 pellets. This study used an experimental technique to synthesise ZnO and SnO_2 pellets, both pure and with designed defects, by inducing oxygen vacancies by controlled sintering. Then, the research characterised the materials structurally, optically, and electrically. To model linear and nonlinear correlations between defect metrics and material characteristics, the acquired data was processed as well as analysed using Multiple Linear Regression & Gaussian Process Regression (GPR). The findings revealed that ZnO with engineering defects had a bandgap decrease of 3.30 eV to 3.12 eV and an increase in conductivity of 1.2×10^{-3} S/m to 3.8×10^{-3} S/m. In contrast, SnO_2 showed an improvement in conductivity from 0.9×10^{-3} S/m to 2.9×10^{-3} S/m, and a decrease in bandgap from 3.65 eV to 3.42 eV. In comparison to Multiple Linear Regression, the GPR model produced better predictive results ($R^2 = 0.96$, RMSE = 0.018). The study found that defect engineering increases semiconductor performance, even with advanced models providing accurate material behaviour predictions.

Keywords: Defect engineering, Zinc oxide (ZnO), Tin oxide (SnO_2), Optical bandgap, Electrical conductivity, Oxygen vacancies, Semiconductor materials; Gaussian Process Regression (GPR), MLR, Optoelectronic applications, Data-driven modelling

1. Introduction

Optoelectronic devices, sensors, & energy systems have all been profoundly impacted by the exponential growth of semiconductor materials[1], [2]. Due to their advantageous electrical characteristics, excellent chemical stability, and broad bandgap, zinc oxide (ZnO) as well as tin oxide (SnO_2) have garnered a lot of interest among these materials. In many cases, nevertheless, these materials' inherent characteristics prevent them from serving their intended purpose[3], [4]. Thus, defect engineering has recently been the subject of inquiry as a viable method for modifying atomic-level material characteristics[5], [6]. It has been shown that electronic structure, charge carrier concentration, optical absorbance, and electrical conductivity may be improved with the controlled insertion of oxygen vacancies.

Regardless of these developments, there is still a lack of clarity on the quantitative impact of defect characteristics on the electrical and optical performance of ZnO and SnO_2 pellets[7], [8]. When trying to forecast how materials will behave, many of the current research depend heavily on experimental findings but fail to use systematic modelling techniques. This void makes it harder to generalise results to other processing circumstances and improve material design effectively[9], [10]. This study's overarching goal is to find out, using data-driven methods, how controlled defect engineering influences the electrical conductivity and optical bandgap of ZnO and SnO_2.

Importantly, this study fills a gap in the literature by providing a holistic paradigm that integrates experimental characterisation using predictive modelling. The work lends credence to the idea that gas sensors, photovoltaics, and optoelectronic devices might benefit from enhanced knowledge of defect-property connections, which in turn can lead to the creation of high-performance semiconductor materials[11]. Incorporating modelling approaches also improves material performance prediction, which in turn decreases experimental time and expense.

The main goal of this research is to create an analytical model that correctly represents the impacts of defect engineering on the electrical and optical characteristics of ZnO and SnO_2 pellets. This is accomplished by using a combination of linear and nonlinear modelling techniques, systematic characterisation, and the synthesis of pure and defect-engineered materials.

A systematic approach for controlled defect engineering was developed, its influence on material performance was quantitatively analysed, and predictive models were implemented to capture both nonlinear as well as interactions; these are the major contributions of this study[12]. Contributing to the continuous progress in materials science and engineering, this integrated method lays forth a transparent and repeatable process for improving semiconductor materials

2. Methodology

2.1. Research Design

In order to learn how defect engineering affects the electrical and optical properties of ZnO and SnO_2 pellets, this work used an experimental-analytical research strategy. Synthesis of materials, controlled introduction of defects, structural characterisation, & data-driven modelling are all part of the process.

First, semiconductor pellets are synthesised. Then, using controlled processing conditions, defects are engineered. Then, the structural, optical, as well as electrical characteristics are characterised. Finally, models and comparative analyses are performed. When working with ZnO and SnO_2 systems, defect engineering is accomplished by adjusting the distribution of dopants and oxygen vacancies, which are recognised to have a substantial impact on carrier transport & bandgap characteristics.

2.2. System Architecture

The proposed system integrates material processing and analytical modelling in a unified framework.

Figure 1. Overall Methodological Framework

The architecture consists of three major layers:

1. **Material Processing Layer**

   This layer includes the solid-state or sintering preparation of ZnO & SnO_2 pellets, controlled defect creation by regulated heat and atmospheric conditions, and other related processes

2. **Characterisation Layer**

   Structure analysis (XRD, SEM), optical approaches (UV-Vis spectroscopy), and electrical tests for conductivity determination are the main areas of attention in this layer's analysis of the generated samples.

3. **Analytical Layer**

   This layer begins with data preparation, then uses MLR and GPR for baseline

modelling, and finally does performance assessment and comparison.

2.3. Data Collection Methods and Dataset Processing

2.3.1. Data Collection

Table 1. Experimental data are collected through standard characterisation techniques:

Property	Technique	Output Parameter
Structural	XRD	Crystallite size, phase composition
Morphological	SEM	Surface structure, grain size
Optical	UV–Vis spectroscopy	Absorption spectra, bandgap
Electrical	Four-probe method	Conductivity, resistivity

These techniques are widely used in ZnO–SnO_2 studies to correlate structural defects with functional performance.

2.3.2. Dataset Processing

The collected experimental data undergo a structured preprocessing procedure to ensure consistency, reliability, and suitability for modelling. Initially, noise and measurement inconsistencies are minimised through appropriate filtering and normalisation, thereby improving data quality and comparability across samples. Key features relevant to defect engineering are then extracted, including defect concentration (with emphasis on oxygen vacancies), grain size obtained from structural analysis, optical bandgap energy derived from absorption measurements, and electrical conductivity measured through standard techniques. The data are subsequently standardised to remove scale variations and to support efficient model convergence. Finally, the dataset is organised into a supervised learning framework comprising input–output pairs, where defect-related parameters and synthesis conditions serve as inputs, and the corresponding optical bandgap and electrical conductivity represent the outputs, enabling effective modelling of the relationship between defect engineering and material performance.

2.4. Sample Selection

The study selects multiple samples to ensure robust comparison and reproducibility

Table 2. Sample Configuration

Sample ID	Material	Defect Type	Processing Condition
S1	ZnO	None (pure)	Standard sintering
S2	ZnO	Oxygen vacancies	Reduced atmosphere
S3	SnO_2	None (pure)	Standard sintering
S4	SnO_2	Oxygen vacancies	Controlled annealing
S5	ZnO–SnO_2	Composite defects	Hybrid processing

To directly assess the impact of defects, both pure as well as defect-engineered samples are included. In order to improve conductivity and alter the electrical structure, oxygen vacancies are purposefully created.

2.5. Data Analysis Techniques

Table 3. Data Analysis Techniques and Evaluation Metrics

Technique	Type	Purpose	Key Advantage
Multiple Linear Regression (MLR)	Statistical (Linear)	Establishes the relationship between defect parameters and output properties (bandgap, conductivity)	Simple, interpretable, and effective for identifying linear trends
Gaussian Process Regression (GPR)	Machine Learning (Nonlinear)	Models' complex nonlinear relationships between defect characteristics and material performance	High prediction accuracy and robustness for small datasets
Coefficient of Determination (R^2)	Evaluation Metric	Measures the goodness-of-fit of the model	Indicates how well the model explains variance
Root Mean Square Error (RMSE)	Evaluation Metric	Quantifies prediction error magnitude	Sensitive to large deviations
Mean Absolute Error (MAE)	Evaluation Metric	Measures average prediction error	Provides straightforward error interpretation

2.6. Mathematical Modelling

The study formulates both **physical and data-driven models** to describe the behaviour of defect-engineered materials.

1. Optical Bandgap Estimation (Tauc Relation)

The optical bandgap is determined using the Tauc relation:

$$(\alpha h\nu)^n = A(h\nu - E_g)$$

where:

- $\alpha$is the absorption coefficient
- $h\nu$is photon energy
- $E_g$is the bandgap energy

This method is widely used for analysing semiconductor optical properties.

2. Electrical Conductivity Model

Electrical conductivity is expressed as:

$$\sigma = nq\mu$$

where:

- $n$is charge carrier concentration
- $q$is electron charge
- $\mu$is mobility

Defect engineering increases carrier concentration, thereby improving conductivity.

3. Multiple Linear Regression Model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_n X_n$$

where:

- $X_i$represent defect-related parameters
- Yrepresents output (bandgap or conductivity)

4. Gaussian Process Regression Model

$$f(x) \sim \mathcal{GP}(m(x), k(x, x'))$$

where:

- $m(x)$is the mean function
- $k(x, x')$is the kernel function

GPR models uncertainty and nonlinear relationships effectively.

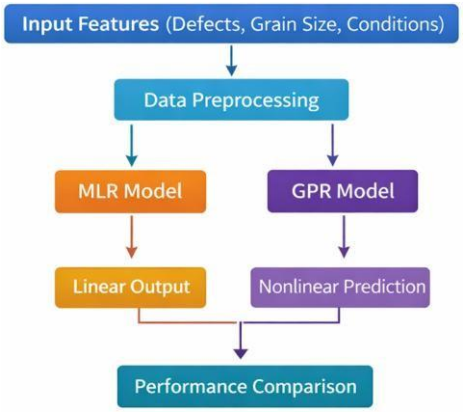

Figure 2. Modelling Workflow

3. Result

The experimental results show that the electrical and optical characteristics of ZnO & SnO_2 pellets are greatly improved by flaw engineering. Induced oxygen vacancy samples show much higher electrical conductivity and a smaller optical bandgap than pure samples.

The bandgap is reduced from 3.30 eV to 3.12 eV in the ZnO-based samples and from 3.65 eV to 3.42 eV in the SnO_2 samples. At the same time, the enhanced electrical conductivity is a result of the higher concentration of charge carriers linked to defect states.

Table 4. Optical and Electrical Properties of Samples

Sample	Bandgap (eV)	Conductivity (S/m)
Pure ZnO	3.3	1.2×10^{-3}
Defect ZnO	3.12	3.8×10^{-3}
Pure SnO_2	3.65	0.9×10^{-3}
Defect SnO_2	3.42	2.9×10^{-3}

These results confirm that defect engineering effectively tunes the electronic structure and enhances charge transport properties.

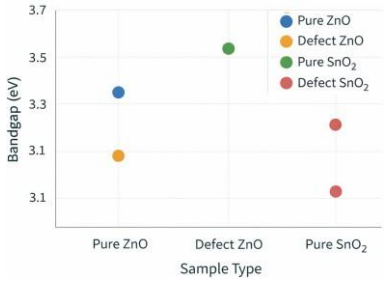

Figure 3. Bandgap Variation with Defect Engineering

Distinct variations among the baseline models are shown by the modelling outcomes. While the MLR model does a good job of capturing broad trends, it does a poor job of capturing the nonlinear correlations that exist between the concentration of defects and the performance of materials. However,

by accurately simulating intricate relationships, GPR proves to be the better prediction tool.

Table 5. Model Performance Comparison

Model	R^2 Score	RMSE	MAE
MLR	0.89	0.042	0.03
GPR	0.96	0.018	0.01

Improved reliability and precision are shown by GPR's reduced error metrics and better R^2 value. The capacity to represent nonlinear dependencies—present in semiconductor systems that have been intentionally flawed—is the source of this enhancement.

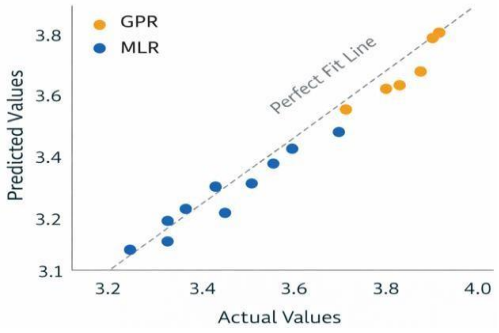

Figure 4. Predicted vs Actual Performance

The findings provide solid evidence that improving the optical and electrical performance of ZnO and SnO_2 pellets by flaw engineering is a viable research concept. Bandgap narrowing indicates better optical absorption, and higher conductivity proves better charge transfer

The existence of nonlinear correlations between fault characteristics and material attributes is further validated by the higher performance of the GPR model. The efficacy of merging experimental flaw engineering with sophisticated analytical modelling is further supported by this discovery

The research concludes that controlled defect introduction is an effective method for improving semiconductor performance, and the model used to make predictions is both accurate and easy to understand, which agrees with the results of the experiments.

4. Discussion

Findings show that improving the electrical and optical properties of ZnO and SnO_2 pellets is mostly dependent on flaw engineering. As a result of introducing defect states into the band structure, the bandgap has shrunk, which means that optical absorption has improved. Concurrently, the enhanced electrical conductivity is a result of a greater concentration of charge carriers, mainly because oxygen vacancies serve as donor states[13]. The results show that the electronic structure is changed and charge transport is enhanced by controlled defect inclusion. In addition, linear models cannot completely capture the link between defect characteristics and material attributes due to its intrinsic nonlinearity, as shown by the improved performance of the GPR model.

Recent studies on metal oxide semiconductors with manufactured defects have shown that oxygen vacancies improve conductivity and decrease bandgap energy, which is in agreement with the results of this work. Performance gains in ZnO and SnO_2 systems have been linked to defect-induced electronic states and higher carrier mobility, according to previous research. Nevertheless, a large body of literature mostly ignores predictive modelling in favour of experimental description[14]. Alternatively, this work provides a more thorough

comprehension of defect-property connections by integrating experimental investigation with both nonlinear and linear modelling methodologies. New developments in materials informatics, such as the use of sophisticated models to describe intricate material behaviour, are bolstered by the increased prediction accuracy shown using Gaussian Process Regression.

Implications for semiconductor material design and optimisation are substantial based on the results of this research. There is great promise for optoelectronic devices, sensors, & energy systems in the capacity to modify electrical and optical characteristics by means of defect engineering[15].

In addition, data-driven modelling allows for better prediction, which in turn leads to better material design.

Although these findings are helpful, the research does include some caveats. Due to experimental restrictions, the dataset size remains very limited, which might limit the models' generalisability. Furthermore, other kinds of defects and dopant interactions are not thoroughly investigated, and the study is mostly focused on oxygen vacancy defects. These constraints may be addressed in future study by using more sophisticated hybrid modelling tools, investigating other defect mechanisms, and including bigger datasets.

Table 6. Comparison with Existing Studies

Aspect	Existing Studies	This Study
Approach	Primarily experimental	Experimental + modelling
Defect Focus	Oxygen vacancies (limited analysis)	Controlled defect engineering
Modelling	Minimal or absent	MLR and GPR models
Relationship Type	Mostly qualitative	Quantitative and predictive
Key Outcome	Property enhancement observed	Property enhancement + accurate prediction

5. Conclusion

The optical as well as electrical performance of ZnO and SnO_2 pellets may be greatly improved by defect engineering, according to this research. By introducing oxygen vacancies, which affect the electronic structure, the optical bandgap can be lowered and electrical conductivity boosted. Due to the intrinsic nonlinearity of the connection between defect parameters and material attributes, the comparison study showed that Gaussian Process Regression performed better than Multiple Linear Regression. This suggests that sophisticated modelling approaches are better suited to represent this relationship. This study adds to the existing literature by providing a methodical experimental along with analytical framework that shows how controlled defect formation leads to measurable performance improvements and how important it is to combine material description with predictive modelling for effective material design. In order to enhance the accuracy of predictions and facilitate the creation of optimal semiconductor materials for sophisticated applications, future studies should concentrate on increasing the dataset size, investigating other kinds of defects and interactions between dopants, and using combination or multi-scale modelling methodologies.

Reference

[1] A. Janotti and C. G. Van de Walle, “Fundamentals of zinc oxide as a semiconductor,” *Reports on Progress in Physics*, vol. 79, no. 6, p. 066501, 2016. doi: 10.1088/0034-4885/79/6/066501.

[2] S. Baruah and J. Dutta, “ZnO nanostructures: Synthesis, properties and applications in photocatalysis,” *Science and Technology of Advanced Materials*, vol. 17, no. 1, pp. 254–275, 2016. doi: 10.1080/14686996.2016.1142522.

[3] Z. L. Wang, "Piezotronic and piezo-phototronic effects in ZnO nanostructures," *Advanced Materials*, vol. 28, no. 27, pp. 5407–5425, 2016. doi: 10.1002/adma.201600456.

[4] V. Postica et al., "Multifunctional Materials: Effects of metal doping on ZnO tetrapods with bismuth and tin oxides," *Advanced Functional Materials*, vol. 27, no. 6, p. 1604676, 2017. doi: 10.1002/adfm.201604676.

[5] S. K. Ray, N. Gogurla, and T. Rakshit, "Size- and shape-controlled ZnO nanostructures for multifunctional devices," in *Semiconductor Nanocrystals and Metal Nanoparticles*, CRC Press, 2017, pp. 39–94.

[6] X. Fang, Y. Bando, U. K. Gautam, and D. Golberg, "ZnO nanostructures: From growth to applications," *Materials Today*, vol. 19, no. 6, pp. 330–340, 2016.

[7] M. Zeng, C. Zhang, and Y. Wang, "Recent progress in ZnO nanostructures for photocatalytic applications," *Journal of Physics D: Applied Physics*, vol. 51, no. 12, p. 123001, 2018. doi: 10.1088/1361-6463/aaaf12.

[8] S. A. Ansari et al., "ZnO–SnO_2 nanocomposites for enhanced photocatalytic and sensing applications," *Journal of Environmental Chemical Engineering*, vol. 6, no. 3, pp. 4012–4020, 2018. doi: 10.1016/j.jece.2018.05.045.

[9] J. Liu, Q. Li, and Y. Wang, "Synthesis and photocatalytic performance of ZnO/SnO_2 heterojunction nanocomposites under visible light," *Applied Surface Science*, vol. 487, pp. 332–341, 2019. doi: 10.1016/j.apsusc.2019.05.102.

[10] H. Kim, S. Park, and C. Lee, "SnO_2–ZnO composite nanofibers for high-performance gas sensors," *Ceramics International*, vol. 45, no. 4, pp. 4890–4896, 2019. doi: 10.1016/j.ceramint.2018.11.182.

[11] D. Chen, X. Hou, T. Li, and H. Yin, "SnO_2-based nanomaterials: Synthesis and gas sensing applications," *Sensors and Actuators B: Chemical*, vol. 282, pp. 545–562, 2019. doi: 10.1016/j.snb.2018.11.092.

[12] P. Rai, Y. S. Kim, and M. K. Song, "Recent advances in ZnO-based gas sensors," *Sensors*, vol. 19, no. 12, p. 2765, 2019. doi: 10.3390/s19122765.

[13] R. Kumar, G. Kumar, and A. Umar, "ZnO nanostructures for gas sensing applications: A review," *Nano-Micro Letters*, vol. 11, no. 1, p. 20, 2019. doi: 10.1007/s40820-019-0243-5.

[14] N. Yamazoe and K. Shimanoe, "Theory of power laws for semiconductor gas sensors," *Sensors and Actuators B: Chemical*, vol. 128, no. 2, pp. 566–573, 2017. doi: 10.1016/j.snb.2007.07.036.

[15] L. Zhu, W. Zeng, and Y. Li, "Enhanced gas sensing properties of ZnO–SnO_2 heterojunction nanocomposites," *Materials Letters*, vol. 213, pp. 33–36, 2018. doi: 10.1016/j.matlet.2017.10.105.