आयकर विभाग
INCOME TAX DEPARTMENT

सत्यमेव जयते

भारत सरकार
GOVT. OF INDIA

स्थायी लेखा संख्या कार्ड
Permanent Account Number Card

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भारत सरकार

Government of India

आधार

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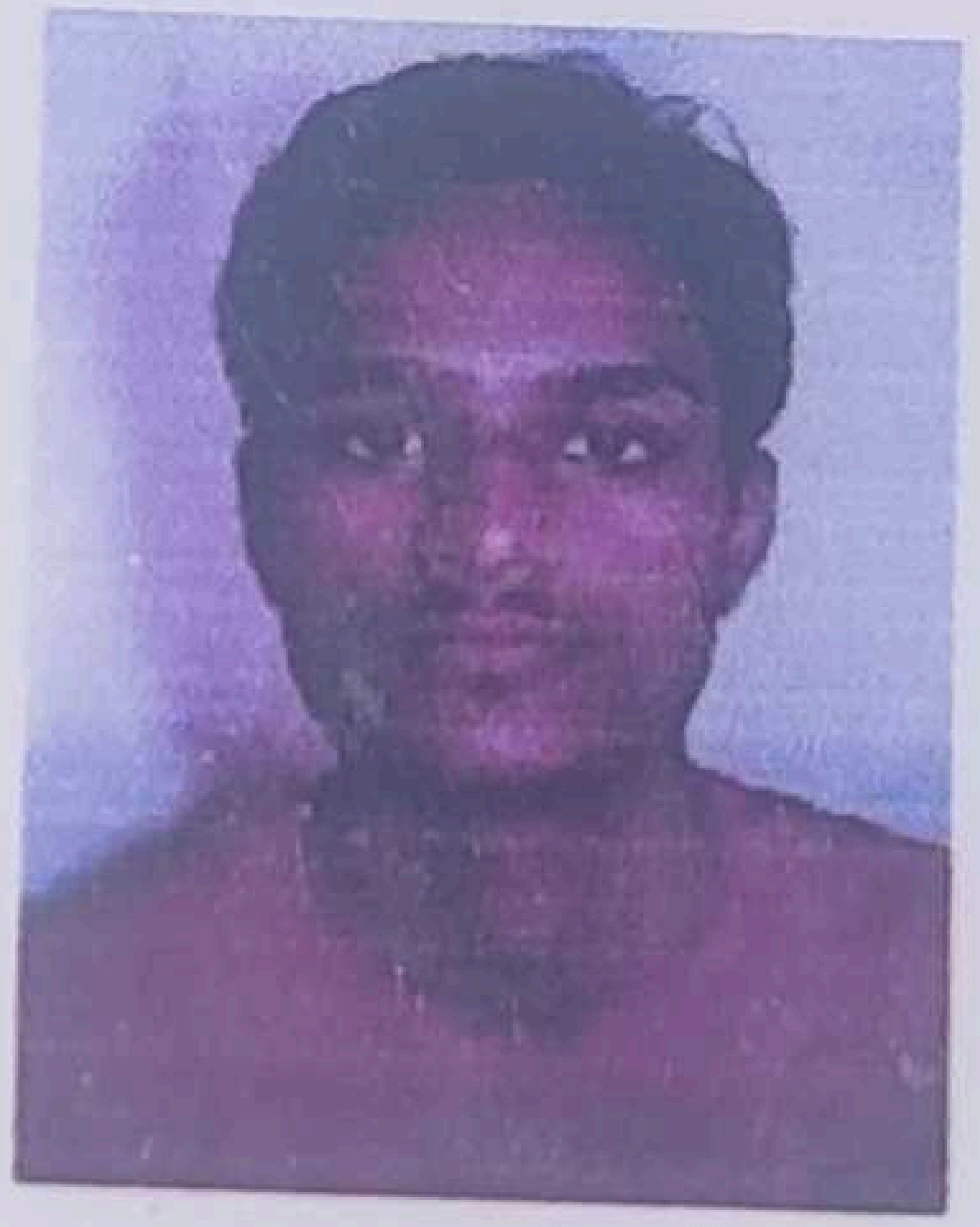

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भारतीय विशिष्ट पहचान प्राधिकरण

Unique Identification Authority of India

AADHAAR

Download Date: 08/09/2022

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MSE360: Capstone Project

Department of Materials Science and Engineering

IIT Kanpur

1. Project Title

"Estimation of the dimensions and weight of sintered ZnO through machine learning techniques, coupled with the prediction of its mechanical properties. Additionally, an in-depth analysis of its optical properties and bandgap will be conducted using Raman spectroscopy, along with a detailed study of grain density variation in the sintered ZnO samples"

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2. Team Name: The Ferrite Frontiers

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3 Background and Motivation

Zinc Oxide (ZnO) is a versatile material with significant applications in electronics and structural components, where properties like hardness and fracture toughness are crucial. Traditional methods to determine these properties are time-intensive, motivating the use of machine learning to predict them efficiently using minimal data. Raman spectroscopy complements this by offering a non-destructive way to study ZnO's optical properties and bandgap, providing insights into its electronic structure. This project aims to develop a machine learning model for predicting mechanical properties while leveraging Raman spectroscopy for optical characterization. Together, these methods enhance the efficiency and depth of ZnO material analysis.

- **What is the problem you aim to solve?**

1. **Efficient Prediction of Mechanical Properties**: Traditional methods to determine hardness and fracture toughness are time-intensive and resource-heavy. The project aims to develop a machine learning model to predict these properties efficiently using minimal data.
2. **Comprehensive Optical Characterization**: Accurate understanding of ZnO's optical properties and bandgap is crucial for its applications. Raman spectroscopy will be employed as a non-destructive method to analyze these characteristics effectively.

- **Why is it significant in the field of Materials Science?**

This project advances Materials Science by applying machine learning to predict critical mechanical properties like hardness and fracture toughness, reducing reliance on extensive experiments. It also utilizes Raman spectroscopy for non-destructive analysis of ZnO's optical properties and bandgap. This integration enhances efficiency and understanding in material design and application.

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4. Objectives

- **To analyze the optical properties of ZnO using Raman spectroscopy**
- **Create the triangular relationship between bulk density, temperature and mechanical properties of samples .**
- **To do a dialometry analysis of sintered materials and predict the linear coefficient of the ZnO sample.**
- **Develop machine learning models to predict critical properties such as mass, dimensions, and mechanical characteristics from experimental inputs.**
- **Extract thermal expansion coefficients from the experimental data to evaluate material behavior under thermal stress.**
- **Derive activation energy values from the experimental data to understand the sintering process and material behavior at elevated temperatures.**

Proposed Methodology

Production of Zinc Oxide (ZnO) Samples via Powder Metallurgy

- Zinc oxide powder will be compacted into desired shapes using uniaxial pressing techniques under controlled pressure.

- The green compacts will be sintered at varying temperatures to achieve densification and optimize mechanical properties.
- Bulk density and compaction percentages of sintered samples will be recorded for analysis.
- The study involves varying the temperature from 800˚C to 1200˚C, holding a sample at each temperature for 30, 60, 90, and up to 180 minutes.

Analysis of Optical Properties Using Raman Spectroscopy

- Raman spectroscopy will be employed to examine the optical properties of the sintered ZnO samples.
- Key parameters such as **vibrational modes** and the **bandgap** will be extracted from the Raman spectra to understand the material's optical behavior.

Mechanical Property Evaluation

- The **hardness** and **fracture toughness** of the sintered ZnO samples will be measured using standard mechanical testing techniques such as Vickers hardness tests.
- The mechanical properties will be evaluated for samples sintered at different temperatures to establish trends.

Establishing the Triangular Relationship

- A correlation will be established between **bulk density, sintering temperature**, and mechanical properties using experimental data.
- Statistical and graphical methods will be used to analyze and visualize these relationships.

Dilatometry Analysis

- Dilatometry will be performed to measure the thermal expansion behavior of the sintered ZnO samples.
- The linear thermal expansion coefficient will be determined to further understand the material's thermal behavior.

Grain Size Analysis:

- Use Scanning Electron Microscopy (SEM) or optical microscopy to determine average grain size and morphology.
- Perform image analysis to measure grain boundaries and grain size distribution.

Correlation with Sintering Parameters:

- Relate measured grain density to sintering parameters such as temperature, holding time, and heating rates.
- Identify trends and analyze how changes in sintering parameters influence grain growth and densification.

Validation:

- Cross-validate grain density results with X-ray Diffraction (XRD) data to confirm phase composition and crystallite size.

Statistical Analysis:

- Perform statistical analysis to quantify the relationship between grain density, sintering parameters, and material properties.

Data Collection:

Measure the initial and final dimensions, mass, density, and porosity of the sintered samples. Conduct additional mechanical tests, such as hardness and fracture toughness, to complete the dataset.

- Material Properties:
    - Type of material (e.g., alloys, ceramics).
    - Particle size distribution.
    - Powder density and additives/alloying elements.
    - Compacting pressure.
- Processing Parameters:
    - Hardness and Fracture toughness.
    - Sintering temperature and duration.
    - Heating and cooling rates.
    - Sintering atmosphere (e.g., vacuum, inert gas).
- Observed Outcomes:
    - Final mass and dimensions.
    - Shrinkage percentage.
    - Porosity and density.
    - Hardness (Tensile Strength and Yield Strength).
    - Fracture toughness.

Feature Engineering:

- Preprocess raw data to eliminate noise and handle missing values.
- Identify critical features influencing final workpiece properties, including:
    - Shrinkage rates.
    - Material-specific coefficients.

    - Temperature-dependent properties.
- Normalize and encode features for optimal model performance.

Model Development:

- Train machine learning models using algorithms such as:
    - Linear Regression (if relationships are linear).
    - Decision Trees and Random Forests (for non-linear relationships).
- Implement hyperparameter optimization techniques to enhance model accuracy.
- Leverage libraries like Scikit-learn, TensorFlow, and PyTorch for implementation.

Validation and Testing:

- Split the dataset into training, testing subsets (e.g., 80:20).
- Evaluate model performance using metrics such as:
    - Mean Absolute Error (MAE).
    - Root Mean Squared Error (RMSE).
    - R-squared (^{2}).

Analysis and Interpretation:

- Compare model predictions with experimental results for accuracy.
- Identify key input parameters affecting mass and dimensions.
- Assess model robustness across materials and conditions.
- Analyze trends between features and outcomes to enhance understanding.

Expected Outcomes and Deliverables

1. **Optical Properties Analysis**: Detailed characterization of ZnO's optical properties, including bandgap and lattice dynamics, using Raman spectroscopy.
2. **Mechanical Properties Evaluation**: Comprehensive evaluation of hardness and fracture toughness of sintered ZnO samples at various temperatures, revealing trends and dependencies on processing conditions.
3. **Triangular Relationship**: Developed a triangular relationship model connecting bulk density, sintering temperature, and mechanical properties, providing insights into the interplay of these parameters.
4. **Dilatometry Insights**: Accurate determination of the linear thermal expansion coefficient of ZnO through dilatometry analysis, aiding in understanding the thermal behavior of the material.
5. **Machine Learning Predictions**: A robust machine learning model capable of accurately predicting the mechanical properties and compaction percentage of ZnO

samples post-sintering, reducing reliance on extensive experimental testing.
6. **Grain Density Trends**: Quantitative analysis of how grain density varies with sintering parameters like temperature, duration, and heating rate, supported by microstructural observations.

Week Wise Project Plan

Week 2–3: ZnO Sample Production and Data Collection

- Produce ZnO samples using powder metallurgy, varying sintering temperatures and other parameters.
- Collect data on bulk density, compaction percentage, and process conditions for model training.
- Start pre-processing the collected data and feeding it into the ML pipeline for early iterations.

Week 4–5: Mechanical Properties Evaluation and Model Feature Integration

- Measure hardness and fracture toughness of ZnO samples, adding results to the dataset.
- Integrate relevant optical features into the dataset and refine the ML model.
- Train the model incrementally using new data and assess preliminary prediction accuracy.

Week 6–7: Optical Properties analysis and Model Enhancement

- Analyze the optical properties of samples using Raman spectroscopy, recording bandgap and spectral data.
- Refine the ML model by incorporating mechanical properties and additional sample data.
- Use feature engineering to explore relationships between inputs (e.g., temperature, density) and outputs.

Week 8–9: Dilatometry Analysis and Grain Density variation

- Perform dilatometry analysis to determine the linear thermal expansion coefficient of ZnO samples
- Measure grain density of ZnO samples sintered at different temperatures and durations, ensuring consistent data collection.
- Analyze grain density trends, correlate with sintering parameters, and validate results with microstructural observations.

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Week 10–11: Triangular Relationship and Model Optimization and Validation

- Analyze experimental data to establish a triangular relationship between bulk density, temperature, and mechanical properties.
- Use insights from the relationship to improve the model's feature set and prediction accuracy.
- Optimize the ML model through hyperparameter tuning and cross-validation.

Week 12: Final Model Deployment and Testing

- Finalize the ML model for predicting mechanical properties and compaction percentage.
- Test the model on unseen data and validate its performance against experimental results.
- Prepare model documentation, including its development process, features, and limitations.

Week 13: Project Report and Presentation

- Compile a comprehensive report with experimental and ML-based results, highlighting key findings.
- Present the results, including the predictive capabilities of the ML model and insights into ZnO characterization.

Resources Required

1. Experimental Resources

- **Materials**
  - Zinc Oxide (ZnO) powder (high purity grade).
  - Binder for powder metallurgy (e.g., polyvinyl alcohol or equivalent).
  - Lubricants for die pressing.
  - Etching agents for microstructural analysis.
- **Equipment**
  - Uniaxial press for compaction.
  - Sintering furnace with temperature control (up to 1200°C or higher).
  - Raman spectrometer for optical analysis.
  - Vickers hardness tester for mechanical property evaluation.
  - Microstructure analysis tools (e.g., optical microscope, SEM if required).
  - Optical Microscope/SEM: To measure and analyze grain size and boundaries.
  - X-ray Diffractometer (XRD): For phase identification and crystallite size analysis.
  - Image Analysis Software: For processing SEM or optical microscopy images.

2. Computational Resources

- **Software and Libraries**
  - Python or R for machine learning development.
  - Machine learning libraries: Scikit-learn, TensorFlow, or PyTorch.
  - Data analysis libraries: Pandas, NumPy, Matplotlib, Seaborn.
  - Statistical tools for correlation analysis.
  - Visualization software for plots and graphs (e.g., Matplotlib, ggplot2).
- **Hardware**
  - High-performance computer for data processing and ML model training.
  - Storage devices for experimental and computational data.

3. Laboratory and Workspace Resources

- **Lab Facilities**
  - Clean and controlled environment for sintering and Raman spectroscopy analysis.
- **Safety Resources**
  - Personal protective equipment (PPE): gloves, lab coats, safety goggles.
  - Fume hood or ventilation system for handling binders and etching agents.

Material and Sample Information Table

Material	Quantity	Purpose
Zinc Oxide (ZnO) Powder	1 kg	Sample preparation via powder metallurgy.
Binder (e.g., PVA)	0.5 kg	Aiding compaction during the pressing process.
Lubricants	250 g	Reducing friction in die pressing.
Etching Agents	500 ml	Microstructural analysis post-processing.

Sample	Quantity	Description
Green Compacts	**50 samples**	**Initial pressed ZnO samples before sintering.**
Sintered Samples	**50 samples**	**ZnO samples sintered at varying temperatures.**

Lab Coordinators

Coordinator	Week	Purpose
A. K. Verma	2,3,4	Assistance required for operating the uniaxial press and managing the sintering furnace.
S. K. Agnihotri	4,5,6	help with Vickers hardness and fracture toughness tests.
S Kant	7,8	Support for setting up and calibrating the Raman spectrometer for optical property analysis.
G. P Bajpai	8,9	assist with XRD setup and interpretation for phase analysis and guide grain density measurements to correlate with sintering and material properties

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Work Distribution

Week	Akshay Kumar	Aman Nigam	Aman Kumar Sriwastav	Ajay Panwar	Dheeraj Kumar Yadav	Anjali Ratgore
2	Sample Preparation	Model creation and literature-based data	Sample Preparation	Model creation and literature-based data	Sintering	Sintering
3	Sintering	Sample Preparation	Sintering	Sample Preparation	Model preparartion	Model preparartion
4	Model Feature integration/ Sintering	Hardness testing	Hardness Testing	Model Feature integration/Sintering	Tensile strength testing/ Sample preparation	Tensile strength testing/ Sample preparation
5	Hardness test	Study the hypertuning parameters for model/ Sintering	Sample Preparation	Hardness testing	Study the hypertuning parameters for model/ Sintering	Sample Preparation
6	Study Optical Properties of ZnO	Model featuring and adjusting model according to input data	Study Optical Properties of ZnO	Model featuring and adjusting model according to input data	Hardness testing and tensile fracture test	Hardness testing and tensile fracture test
7	Study Optical Properties of ZnO	Band Gap of ZnO	Study the elastic properties of each samples	Study the elastic properties of each samples	Band Gap of ZnO	Study Optical Properties of ZnO
8	XRD	Optical microsccope analysis	XRD	Dilatometry analysis	Optical microsccope analysis	Dilatometry analysis
9	Optical	XRD	Dilatom	Optical	XRD	Dilatome

	microsccope analysis		etry analysis	microscco pe analysis		try analysis
10	Model optimization	Model optimization	Analyze the traingular relationship between studies properties	Analyze the traingular relationship between studies properties	Study of themal parameters of each samples and find them	Study of themal parameters of each samples and find them
11	Analyze the triangular relationship between mechanical properties and temperature	Analyze the triangular relationship between mechanical properties and temperature	Model Validation	Model Validation	Accuracy measurment for different types of model	Accuracy measurment for different types of model
12	Model deployment	Model deployment	Model testing	Model testing	Report prepare	Report prepare

Deliverables:

Upto Midsem:

By the mid-semester, we aim to complete the preparation of all samples and conduct a detailed mechanical properties analysis. Additionally, we plan to develop a basic machine learning model and focus on the feature engineering aspects.

Upto Endsem:

By the end-semester, we aim to develop a machine learning model to predict the mechanical properties and compaction percentage of sintered ZnO workpieces. Additionally, we will prepare a comprehensive report analyzing the mechanical and optical properties, along with the grain density variation influenced by sintering parameters.

Resources:

RESEARCH PAPER:- https://ieeexplore.ieee.org/document/10192469

Scores

JEE (Advanced) roll number	4036384
Candidate name	AKSHAY KUMAR
Chemistry 1	3
Chemistry 2	7
Chemistry Total	10
Physics 1	11
Physics 2	19
Physics Total	30
Mathematics 1	0
Mathematics 2	7
Mathematics Total	7
Total	47
Positive	60

Rank

SC Rank	1881