Computers and Chemical Engineering 201 (2025) 109237

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Sustainable recovery of Cu, Ag and Au from the waste printed circuit boards and process optimisation by machine learning

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ARTICLE INFO

Keywords:
Chip manufacturing
Precious metal recovery
Machine learning
Sustainable AI
Electronic Waste Management

ABSTRACT

The sustainable supply of metals, especially precious metals, is critical for the manufacturing of the electronic chips used in the printed circuit boards of mobile phones. At the same time, the large volume of waste printed circuit boards (WPCBs) of mobile phones is a serious environmental issue that requires developing sustainable processes for the recovery of metals and to handle the waste in a resourceful manner. To address the two challenges of sustainable material supplies for chip manufacturing and waste management of WPCBs of mobile phones, we present a machine learning (ML) powered process optimization framework for the sustainable recovery of Cu, Ag and Au from the WPCBs. The process employs NH_4Cl and low-temperature roasting for the recovery of metals for designed experimental conditions. The input-output data obtained from the experiments is deployed to make approximations of the metal recovery profiles for Cu, Ag and Au by Gaussian Process (GP) models. The GP models trained for the three metals are embedded in the objective function of an optimisation problem for determining the optimised experimental conditions that maximise the recovery of the metals from the WPCBs. The verification of optimized experimental conditions, obtained after solving the optimization problem, in made in the lab that confirms 99 %, 90 % and 80 % respectively recovery of Cu, Ag and Au from the WPCBs. This demonstrates the effectiveness of the developed ML powered analysis workflow that improves the material utilisation efficiency and supports sustainable AI by considering material requirements for chip manufacturing and waste management.

1. Introduction

The rapid pace of technological advancement has significantly accelerated the obsolescence of electrical and electronic devices, leading to an unprecedented surge in electronic waste (e-waste) generation (Naik and Eswari, 2022). The recent wave of AI that is founded on electronic chips to process the data and train the large language models can produce huge volumes of electronic waste that requires global attention to ensure the material supplies for chip manufacturing and eco-friendly waste management to support sustainable AI (Lannelongue, 2024; Wang et al., 2024). The improper disposal of e-waste through landfilling and open burning has dire consequences for the environment, human health, and wildlife (Kiddee et al., 2014). Considering the importance of environmental protection, resource conservation, and material reuse, the eco-friendly recovery of metals from e-waste is crucial (Stein, 2024).

At present, hydrometallurgy and pyrometallurgy techniques are the most widely used methods for recycling e-waste (Ashiq et al., 2019; Wang et al., 2017). Hydrometallurgical methods, involving a two-step leaching process with mineral acids and solvents, are effective for metal extraction but generate significant toxic effluents requiring costly neutralization, posing environmental concerns (Chauhan et al., 2018). Pyrometallurgical processes, widely adopted for their straightforward mechanisms, operate at high temperatures (>1000 °C) and may emit hazardous gases due to halogenated compounds in e-waste, leading to high energy consumption and potential environmental hazards (Khaliq

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https://doi.org/10.1016/j.compchemeng.2025.109237
Received 14 March 2025; Accepted 7 June 2025
Available online 8 June 2025

et al., 2014; Xiao et al., 2021; Zhang and Xu, 2016). Both methods necessitate improvements to reduce operating temperatures, toxic effluents, and hazardous emissions to ensure sustainable e-waste recycling.

In our efforts to find a more sustainable alternative, ammonium chloride roasting has emerged as an advantageous, non-toxic, and non-corrosive chlorinating agent (Xiao et al., 2021). Upon decomposition above 200 °C, it produces ammonia and hydrochloric acid. The highly reactive hydrochloric acid reacts with metals to form metal chloride salts, which are highly soluble in suitable solvents, facilitating efficient metal extraction. In comparison to traditional processes, low-temperature ammonium chloride roasting offers several benefits: it is less corrosive, uses less energy, is easier to operate, and is environmentally friendly. Furthermore, the waste gases produced, such as NH_3, can be recycled to generate NH_4Cl, significantly reducing the cost of recovery operations. The ammonium chloride roasting process has proven effective in recovering rare earth metals from FeNdB magnets and metals such as Ni, Cu, and Co from various sources (Xiao et al., 2021). In our previous studies, we successfully applied the ammonium chloride roasting method to recover critical metals from waste printed circuit boards (WPCBs) (Panda et al., 2020; Panda et al., 2021). This approach ensures efficient metal recovery while minimizing environmental impact, making it a popular choice for sustainable metal extraction.

Machine learning (ML) has demonstrated exceptional capabilities in processing and analyzing complex processes, making it an invaluable tool for developing predictive models (Chakraborty et al., 2021; Goswami et al., 2024; Haq et al., 2023; Mann et al., 2024, 2023). Recently, ML has gained traction in environmental science and engineering, particularly in predicting metal recovery from solid waste. The selection of appropriate ML algorithms significantly impacts the prediction accuracy of these models, thereby influencing the analysis of interaction mechanisms among various factors. Deware et al. employed a machine-learning framework to design a recovery process for e-waste sources, optimizing copper recovery by acid leaching from PCBs (Daware et al., 2022). The framework predicted operating ranges for parameters, and achieved reduced cost of operation. Priyadarshini et al. compared five machine learning models for maximum metal recovery of zinc and manganese from spent batteries, finding that the XGBoost regression model was the most efficient, followed by gradient boosting regression, random forest regression, AdaBoost regression, and linear regression (Priyadarshini et al., 2022). The analysis emphasized the importance of hyperparameter tuning and highlighted the stability of these models in predicting metal recovery efficiency. Niu et al. used machine learning to optimize metal leaching from spent lithium-ion batteries (LIBs), achieving high predictive accuracy with the XGBoost algorithm and developing a user-friendly GUI for researchers (Niu et al., 2023). Mokarian et al. used machine learning tools to significantly reduce experimental costs, labor, and environmental risks, paving the way for efficient and sustainable recycling technologies (Mokarian et al., 2022). This study utilized Random Forest Regression (RFR) among 40 regression-based algorithms to predict bioleaching recovery rates using nine input variables. Ashraf et al. maximized Cu and Ni recovery from WPCB of mobile phones using an ANN model integrated with a robust NLP optimization framework, achieving 100 % Cu and 90 % Ni recovery (W.M. Ashraf et al., 2024).

The literature review highlights the significance of ML based modelling algorithms to predict the metal recovery profiles from the electronic waste. A lot of lab-based studies have been reported for the extraction of metals including Cu, Ni, and Zn from the WPCBs. However, a limited attention is paid for the eco-friendly process development to recover precious metals including Ag and Au from the WPCBs. The precious metals in the electronic chips accelerate the data processing and boost the chip performance to ensure the desirable functionality of the electronic devices including mobile phones. Another promising research gap identified in the literature is to integrate the ML model, trained on initial set of experiments, with optimisation framework to estimate the new optimised experimental conditions for the maximum recovery of precious metals from the WPCBs. The optimisation led experimental workflow can reduce the hit-and-trial approach based experimental campaigns and provides a systematic approach to estimate optimised experimental conditions for the metal recovery from the WPCBs.

In this paper, we provide an ML based process optimisation workflow to maximise the recovery of Cu, Ag and Au from the WPCBs of mobile phones. An eco-friendly low-temperature roasting process is developed for the recovery of metals from the WPCBs. The process input variables include roasting time (h), roasting temperature (°C), NH_4Cl dose (g/g) and leaching solvent (M), and a wide operating range of the process variables is established to design the experiments. The recovery of Cu, Ag and Au corresponding to the experimental conditions is recorded for all designed experiments. The compiled input-output dataset of the metal recovery is deployed to train gaussain process (GP) models to predict the percentage recovery of Cu, Ag and Au from the WPCBs. Shapley Additive exPlanations (SHAP) are made for the trained GP models to investigate the significance of process input variables on the metal recovery.

An optimisation problem is formulated that attempts to maximise recovery of Cu, Ag and Au from the WPCBs subjected to the operating bounds on the process input variables and embedding the trained ML models in the optimisation environment (Gueddar and Dua, 2012, 2011). The optimisation problem is solved by genetic algorithm solver and optimised experimental conditions are obtained which are verified in the lab. A good agreement is observed between the estimated percentage recovery of three metals with the experimental percentage recovery made from the WPCBs. This paper provides an ML powered analysis workflow to maximise the metal recovery including precious metals from the WPCBs in an environmental-friendly approach. The recovery of precious metals from the WPCBs improves the material utilisation efficiency, reduces the strain on the natural resources for their demand for chip manufacturing and its utilisation on printed circuit boards. The ML powered and eco-friendly recovery of metals also support the sustainable AI development by metal circular economy and handling the electronic waste in a resourceful manner.

2. Materials and methods

2.1. Experimentation, data collection and importance of data-visualization

In this study, a machine learning (ML) approach is employed to optimise the experimental conditions for maximum recovery of Cu, Ag and Au from the WPCBs of mobile phones using low-temperature roasting process. The experimental setup that generated this data is detailed here. The roasting experiments are conducted using a batch quartz reactor with an air flow rate of 100 mL/min to assess the corrosive effects of HCl formed during roasting. For each experiment, 10 g of WPCBs sample is thoroughly mixed with a measured amount of NH_4Cl and placed in the reactor. The process input variables such as roasting temperature (200–300 °C), roasting time (1–3.5 h), and NH_4Cl dosage (1–3 g/g) are varied in a wide operating range to find the optimal process conditions for the maximum recovery of metals. After chlorination, samples are cooled to room temperature and HCl is used to dissolve the metal chlorides, with concentrations ranging from 0 to 3 M for maximum efficiency. The unreacted HCl and NH_3 from the chamber are scrubbed with water, and ammonium chloride obtained through evaporation can be reintroduced into the roasting process. This creates a closed-loop system that reduces processing costs. By utilizing low roasting temperatures, this method not only conserves energy but also mitigates the challenges of metal recovery encountered in pyrometallurgical processes. Metal concentration of samples is calculated using a microwave plasma atomic emission spectrometer (MPAES, Agilent

4210). Solid samples are digested in a microwave digester (Anton Parr, Multiwave Go) using aqua regia before analysis.

The one-factor-at-a-time scheme is applied to investigate the significance of the process input variables on the metal recovery from the WPCBs. A total of 19 experiments designed on the different operating levels of the process input variables are carried out and the percentage recovery of Cu, Ag and Au is recorded. The collected dataset provides the metal recovery profiles built on the operating levels of the process input variables and also captures the relationships built between the process input and output variables.

Data visualisation is crucial in ML-based studies as it provides a clear and intuitive understanding of the data collected from experiments (Tariq et al., 2022). Visualising data allows researchers to explore the distribution densities across variable operating ranges, which is essential for gaining insights into how variables interact and influence outcomes. Techniques such as histograms, violin plots, partial dependent plots, and box plots are commonly employed in the ML community to visualise dataset characteristics effectively (W.M. Ashraf et al., 2024). For instance, box plots not only offer a visual summary of statistical information like median, quartiles, and outliers but also facilitate the identification of data anomalies (Ashraf and Dua, 2023). In the context of research on metal recovery datasets, using box plots ensures that the data distribution associated with variables is presented conveniently, flexibly, and clearly, aiding in comprehensive analysis and interpretation of experimental results.

At one side, data visualisation provides crucial insights into the operating behaviour of the system under consideration. On the other side, it is equally important to investigate the strength of the relationships or dependencies among the variables. In the literature, statistical metrics such as the Spearman and Pearson correlation coefficients are commonly used to quantify monotonic or linear relationships between variables, respectively. The Pearson correlation coefficient (PCC) is particularly valuable because it measures the linear relationship between pairs of variables, offering a precise and quantifiable method to understand their interactions (Ishfaq et al., 2023). The PCC not only indicates the strength of the relationship but also reveals whether the variables are associated by direct or inverse relationship. Mathematically, the PCC between two variables x and y is given by:

$$R_{xy} = \frac{\sum_{i=1}^{N}(x_i - \overline{x_i})(y_i - \overline{y_i})}{\sqrt{\sum_{i=1}^{N}(x_i - \overline{x_i})^2}\sqrt{\sum_{i=1}^{N}(y_i - \overline{y_i})^2}} \tag{1}$$

Here, R_{xy} denotes the PCC, ranging from -1 to $+1$, signifying a strong inverse and direct relationship between the variables, respectively. A value of $R_{xy} = 0$ indicates no linear association, although their main-effect profiles might be nonlinear, confirming the independent nature of the variables. The utilisation of PCC for understanding the variables dependencies is crucial because it provides an quantifiable measure of linear dependence, which is a key aspect in many scientific and engineering applications. Visualising these relationships using heat map, which maps the computed PCC values between pairs of variables, offers an intuitive and comprehensive way to identify patterns and strengths of relationships. This visual approach is essential for uncovering the patterns and strengths underlying data structures, guiding feature selection, and informing subsequent analytical or modelling efforts in ML-based studies.

The data visualization offers the ML practitioner to understand the data-specific strengths, information and distribution. In real-life engineering systems and lab-based test benches, the operating ranges of the process related variables are significantly different. The ML models construct the functional map between the input-output variables that are strengthened by the dataset associated with the variables to predict the state of the output variable. The very different operating range and variable associated value can dominate the marginally small value of the variables – the small-value based variable can be a significant variable affecting the performance of the system. Thus, it becomes important to scale the operating ranges of the variables on the same range to avoid the variable bias and imperfect functional mapping. Among various data scaling techniques, data normalization method maps the operating values on the same scale for all the variables. The mathematical expression on scaling the operating value on $[a, b]$ scale is given as:

$$X_i^* = \frac{(X_i - X_{min}) \times (b - a)}{X_{max} - X_{min}} + a \tag{2}$$

here, X_i^* is the scale-transformed observations for X_i. We have scaled the data on $[-1, 1]$ in this research.

2.2. Machine learning model development and evaluation metrics

The Gaussian Process (GP) model is one of the powerful algorithms of ML (Rasmussen, 2003) for modelling the lab-based experimental data, particularly due to the non-parametric nature and capacity of the algorithm to handle uncertainty effectively. One of the key strengths of GP models is their flexibility in capturing complex, non-linear relationships without requiring a predefined functional form (Bradford et al., 2021). This adaptability is crucial when dealing with experimental data where underlying processes may be intricate and not well understood. GP models are built on the assumption that function to be learnt from the dataset is drawn from the Gaussian process that allows to compute the well-defined uncertainty around the model-based predictions (Bradford et al., 2018). Furthermore, the GP's ability to incorporate prior knowledge through the choice of kernel functions allows for fine-tuning of the model to reflect specific domain insights, enhancing the predictive performance (Williams and Rasmussen, 1995). In the context of metal recovery from the WPCBs, GP models can robustly interpolate the data and optimise experimental conditions to maximise the metal recovery. The use of non-parametric GP models thus ensures a comprehensive, data-driven approach to understanding and optimising complex systems providing the competitive edge over the parametric models which are prone to overfitting and may lead to the inaccurate model-based analyses.

Consider a set of input data points $x_1, x_2, x_3, \ldots, x_n$ where each $x_i \in \mathbb{R}^d$ represents a D-dimensional vector. Corresponding to these inputs, we have output values $y_1, y_2, y_3, \ldots, y_n$ where each $y_i \in \mathbb{R}^d$ is a scalar. In GP regression, we model the relationship between inputs and outputs using a Gaussian process characterized by a mean function μ and a covariance function κ. The function f that relates the inputs to the outputs is assumed to be drawn from this Gaussian process. At a set of test points x^*, the distribution of f is given by:

$$f(x^*) \sim \mathcal{N}(\mu(x^*), \kappa(x^*, x^*)) \tag{2a}$$

The mean function and covariance function are typically defined using kernel functions. For example, the commonly used squared exponential kernel is defined as:

$$\kappa(\mathrm{x_i}, \mathrm{x_j}) = \exp\left(-\frac{1}{2}\|\mathrm{x_i} - \mathrm{x_j}\|^2\right) \tag{3}$$

Given a set of training data (x, y), the GP regression model employs Bayesian inference to determine the distribution of the function f. This process involves computing the posterior distribution of f given the data, which is expressed as:

$$p(f|x, y) = \frac{p(y|x, f)\, p(f)}{p(y|x)} \tag{4}$$

where $p(y|x, f)$ is the likelihood function, representing the probability of observing the data given the function f, $p(f)$ is the prior distribution of f, and $p(y|x)$ is the marginal likelihood of the data.

Once the posterior distribution of f has been learned, the model can make predictions at new test points x^* by computing the posterior predictive distribution, defined as:

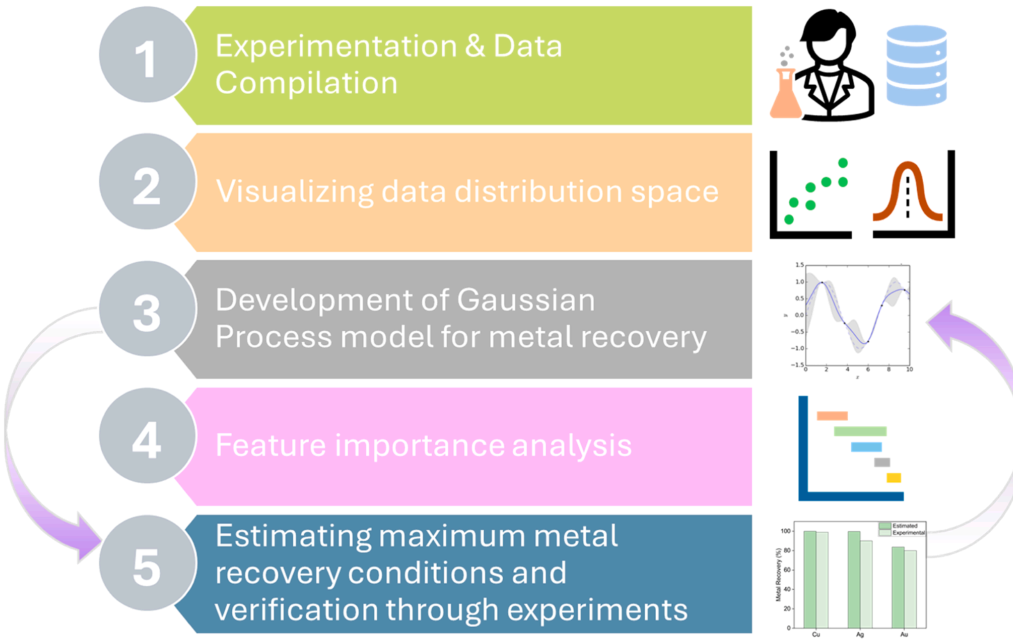

Fig. 1. ML powered workflow developed to maximise Cu, Ag and Au recovery from the WPCB. The experiments are designed and carried out to collect the data on the metal recovery against the process input conditions. The collected dataset is visualised to understand the characteristics of the metal recovery process followed by the development of GP based models for Cu, Ag and Au on the experimental data. The feature importance analysis is caried out by the SHAP and the trained GP models are integrated in the multi-objective function to determine the optimised process conditions for the maximum metal recovery from the WPCB by GA. The solution determined by the GA is verified in the lab, promoting the effectiveness of the workflow for the higher metal recovery rate and circular economy.

$$p(f^*|x^*, y, x) = \int p(f^*|x^*, f)\, p(f|y, x) df \quad (5)$$

This distribution provides a measure of the uncertainty of the prediction, which is beneficial for tasks such as active learning and uncertainty-aware decision making. GP regression is particularly effective for small data sets and provides predictions with uncertainty quantification (Deringer et al., 2021). The kernel hyperparameters are optimized during the fitting process by maximizing the log-marginal likelihood using an optimiser (Damianou and Lawrence). This maximisation problem is non-convex, leading to multiple local optima, so the optimiser is typically restarted multiple times. The initial iteration begins with the specified initial hyperparameters, while subsequent iterations use randomly selected hyperparameters within the allowed range.

We have incorporated two statistical terms namely coefficient of determination (R^2) and root-mean-squared-error (RMSE) to evaluate the predictive performance of the GP regression model trained for the metal recovery from the WPCBs (Shboul et al., 2024; Ashraf and Dua, 2024). The mathematical expressions of R^2 and RMSE are given as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \widehat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \overline{y}_i)^2} \quad (6)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\widehat{y}_i - y_i)^2} \quad (7)$$

here, y_i and $\widehat{y}_i$ are the actual and model-based responses respectively while $\overline{y}_i$ is the mean of y_i for observations $i = 1,2,3,\ldots, N$. R^2 computes the accuracy measure that varies from zero to one. On the other hand, RMSE is the mean error associated with the model-based prediction. A low-RMSE indicates a good function fitting on the data for the model-based predictive tasks and thus, should be minimised for the selection of model.

2.3. Feature importance analysis

Feature importance analysis is an important aspect of interpreting and understanding machine learning models, especially in applications where decisions have significant impact for the real-life applications like metal recovery from the WPCBs (Wu et al., 2023). It helps identify which input feature(s) influence the model's predictions the most, providing insights into the underlying data patterns and the model's decision-making process (Daware et al., 2022). Additionally, feature importance can help in diagnosing model biases and ensuring that the model does not rely on spurious correlations or irrelevant features.

SHAP (SHapley Additive exPlanations) is recurringly used in literature for feature importance analysis due to its strong theoretical foundation and practical benefits (Feng et al., 2021). Derived from cooperative game theory, SHAP values attribute the contribution of each feature to a prediction by considering all possible combinations of features, ensuring a fair distribution of importance (Marcílio and Eler). This results in a consistent and intuitive explanation of feature impacts (Meng et al., 2020). SHAP values are also model-agnostic, making them applicable across different types of models like GP regression (Chau et al., 2024). Furthermore, SHAP provides local interpretability by explaining individual predictions, and global interpretability by summarizing feature importance across the entire dataset. This dual capability enhances both the depth and breadth of model interpretability, making SHAP a robust and versatile tool for understanding and explaining the pattern of metal recovery from the WPCBs.

2.4. Maximising Cu, Ag and Au recovery from the WPCB by genetic algorithm

The metal recovery from the WPCBs of mobile phones is a complex process that is influenced by the operating levels of the process input variables. The sensitivity of the process to the process input conditions requires to formulate an optimisation problem that can provide optimised experimental conditions for the maximum recovery of metals from the WPCBs of mobile phones. Genetic algorithm (GA) for the

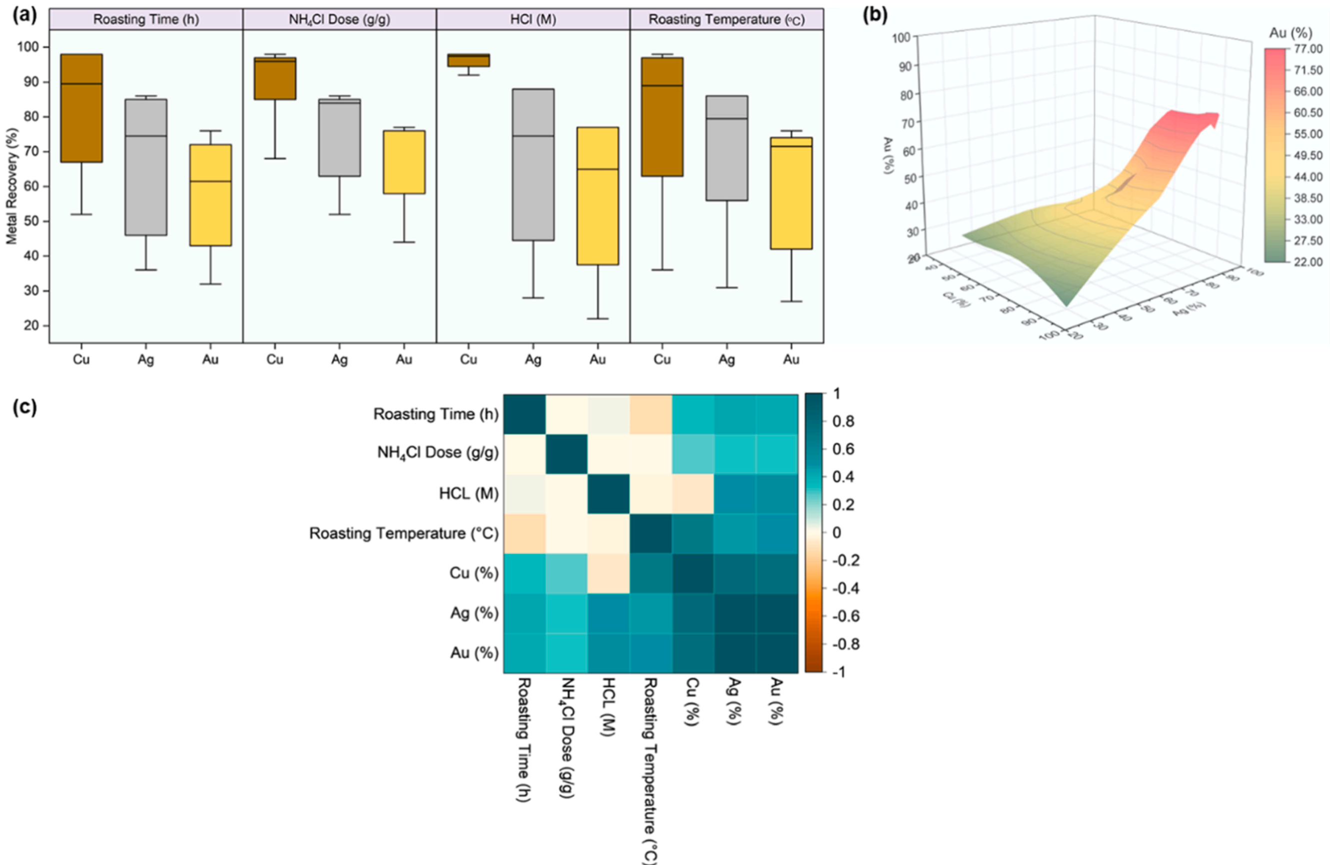

Fig. 2. Visualising the data-distribution associated with the process input conditions and metal recovery from the WPCB. (a) Box plots present impact of process input conditions on percentage recovery of Cu, Ag and Au, (b) the function space built for Cu, Ag and Au recovery from the WPCB, and (c) variable inter-dependence analysis by the PCC based heat map plotted for the process conditions and metal recovery from the WPCB.

maximum recovery of Cu, Ag and Au from the WPCBs is an efficient approach to tackling nonlinear, and multi-dimensional maximisation problem (Mirjalili and Mirjalili, 2019). The inherent advantage of GA lies in its capacity to handle non-linear, multi-modal objective functions effectively (Sivanandam et al., 2008). In the context of metal recovery from the WPCB, this capability is particularly valuable, as it allows the GA to explore the intricate and often non-linear relationships between various input variables of the system (Whitley, 1994). The iterative process of selection, crossover, and mutation in GA enables the algorithm to progressively refine solutions, thereby avoiding local optima and converging towards the global maximum metal recovery from the WPCB (Dehghanian and Mansour, 2009).

A multi-objective function integrating the GP regression-based models of Cu, Ag and Au is formulated and is solved by GA to determine the optimised operating conditions for the maximum recovery of metals from the WPCBs. The confirmatory experiments are conducted in the lab on the estimated optimised conditions of the process input variables and the percentage recovery of metals from the WPCBs is recorded. A good agreement between the estimated and experimental recovery of metals from the WPCBs demonstrates the effectiveness of the developed ML based workflow. The graphical representation of the ML based workflow developed in this research is depicted on Fig. 1.

3. Results and discussions

3.1. Understanding Cu, Ag and Au recovery pattern from the WPCB

Ammonium chloride (NH_4Cl) offers a highly effective method for recovering critical metals from electronic waste. Unlike traditional wet chlorinating agents, ammonium chloride is less corrosive and easier to handle, making it safer for operational use (Lorenz and Bertau, 2019). When subjected to high temperatures, NH_4Cl decomposes into ammonia and hydrochloric acid gas. These gases effectively react with metals to form metal chlorides, which can be extracted using a suitable solvent. This method boasts several benefits, including high metal recovery rates, low energy consumption, and minimal toxic and corrosive effluent generation. Its application in recovering metals from e-waste is particularly promising due to its efficiency and simplicity.

Selecting the optimal process variables for the roasting process requires careful consideration about the operating bounds of roasting temperature, roasting time, and ammonium chloride dosage. The decomposition of NH_4Cl begins around 200 °C, but a sharp decrease in its weight is observed near 300 °C, indicating vigorous decomposition and maximum efficiency in converting metals to their chlorides (Panda et al., 2020). Here, all the process input variable ranges derived from Panda et al. are provided and discussed in (Panda et al., 2023). Therefore, maintaining the roasting temperature within the range of 200–300 °C is crucial for metal recovery. The importance of roasting time in NH_4Cl roasting process cannot be overstated. The duration of roasting significantly influences the efficiency of metal recovery. A well-optimised roasting time ensures that NH_4Cl has adequate opportunity to decompose into ammonia and hydrochloric acid gas, which are crucial for the conversion of metals into metal chlorides. Insufficient roasting time may result in incomplete decomposition of NH_4Cl and inadequate formation of metal chlorides, leading to lower metal recovery rates. Typically, a roasting duration of 1 to 3.5 h is found to be effective, allowing for thorough decomposition and maximum recovery of metals. The dosage of NH_4Cl plays a pivotal role in the roasting process for metal recovery. It directly influences the availability of reactive hydrochloric acid (HCl) which is critical for converting metals into their

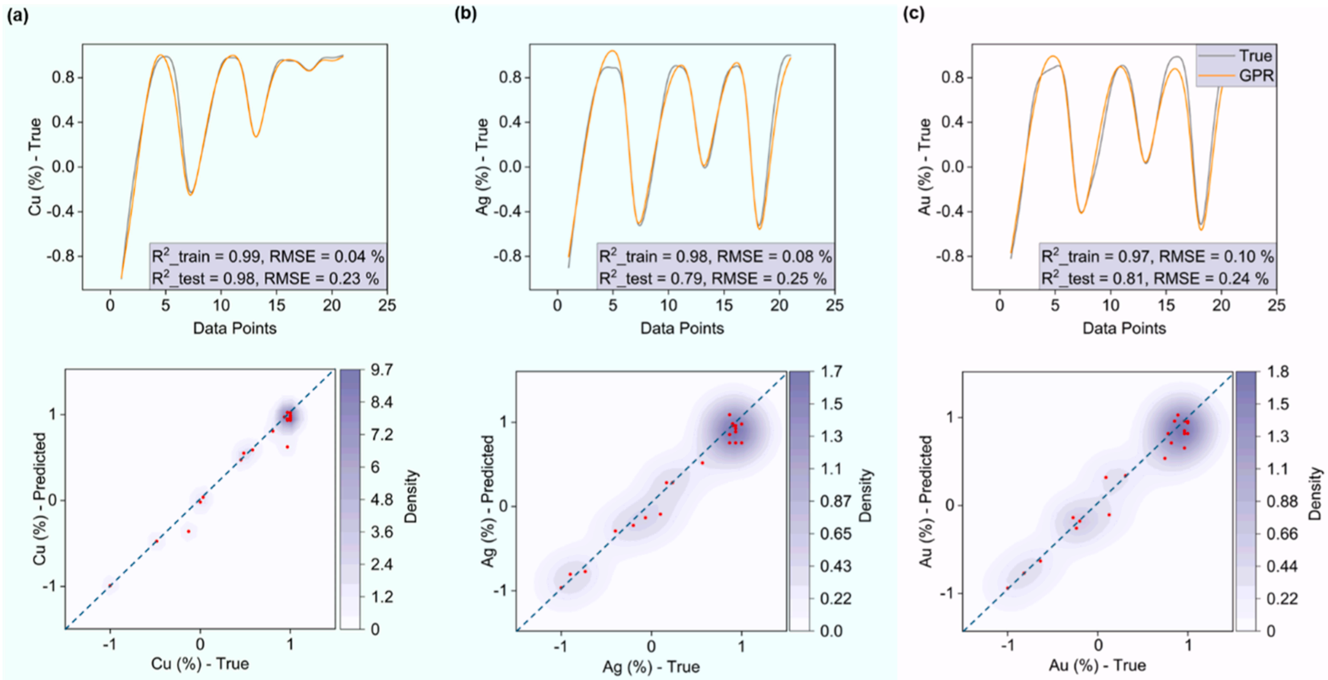

Fig. 3. The modelling performance of the GP Regression model to predict the train and test dataset for (a) Cu, (b) Ag, and (c) Au recovery from the WPCB. The KDE on the parity plots is also plotted to visualise the distribution and agreement between the true and model-predicted responses.

chlorides. The impact of NH_4Cl dosage on metal extraction is examined by adjusting the NH_4Cl dose from 1 to 3 g/g of WPCB. HCl acts as a leaching agent, facilitating the dissolution of metal chlorides formed during roasting. The effectiveness of this extraction process is highly dependent on the molar concentration of HCl. Using HCl ensures high recovery rates, minimises metal loss due to hydration and precipitation, and offers a more efficient alternative to water leaching. Properly managing HCl concentration is essential to maximise metal recovery and ensure the success of the metal extraction process post-roasting. HCl is utilised within a concentration range of 1 to 3 M to investigate the efficient recovery of metals and determine the optimal concentration.

Fig. 2(a) illustrates the variations in process input conditions designed to investigate their impact on the metal recovery rate from WPCBs. It is observed that metal recovery is significantly influenced by process input variables such as roasting time (h), NH_4Cl dose (g/g), HCl concentration (M), and roasting temperature (°C). It appears that variation in roasting temperature causes fluctuation in the metal recovery profiles and also drives higher metal recovery in comparison to other process input variables. To further explore the intricate and nonlinear characteristics associated with the metal recovery process, a function profile made for percentage recovery of Cu, Ag, and Au is constructed and shown on Fig. 2(b). The metal recovery profile exhibits nonlinear characteristics as evidenced by the non-convex nature of the function. Numerous local minima are observable in the function profile for Cu, Ag, and Au recovery, indicating that the metal recovery process is inherently complex. This nonlinearity poses a significant challenge for optimisation solvers tasked with identifying the optimal process conditions to maximise the metal recovery rate.

Pearson correlation coefficient (PCC) values is computed between pairs of variables and shown as heat map on Fig. 2(c) that presents the information about the variable dependencies associated with the metal recovery from WPCBs. Notably, the PCC values between pairs of process input variables are around zero that confirms that the process input variables are not linearly dependent on each other and are independent in their effects on metal recovery from WPCBs. However, the recovery of Cu, Ag, and Au shows high correlation (PCC $>$ 0.78), suggesting that these metals can be extracted under similar process conditions. This high correlation underscores the fact that the dataset contains sufficient information to determine process conditions that can simultaneously maximise the recovery of multiple metals from WPCBs.

The comprehensive data visualisation associated with the metal recovery process calls for applying the machine learning based algorithms to accurately capture the complex, nonlinear relationships for Cu, Ag and Au recovery from the WPCB. Consequently, the data-visualisation supports the use of sophisticated optimisation techniques such as genetic algorithm, which can effectively estimate an effective solution for maximum recovery of metals from the WPCBs.

3.2. Gaussian process regression models for Cu, Ag and Au recovery from the WPCB

A well-trained GP regression model requires the efficient parameters estimation associated with the algorithm. Covariance and the mean function process the data during the GP regression model training and can be defined by the user or identified by the hyperparameters tuning (Liu et al., 2020). The acquisition function samples the space for the function evaluation and exploration, and is integrated with the optimization solver to estimate the best parameter-settings for the training of the GP regression model. To further generalise the training of the GP regression model, we have embedded the five-fold cross validation technique during the hyperparameters tuning carried out by Bayesian optimization and the mean values of the performance metrics are computed. Constant mean function and squared exponential as covariance function are found to be best hyperparameters for the GP regression models for the training of Cu, Ag and Au models.

Fig. 3(a-c) depicts the modelling performance of the GP regression-based models trained for Cu, Ag and Au recovery from the WPCBs respectively. The true and model-based predictions are mapped for the three metals recovered from the WPCBs. The GP regression model trained for Cu recovery exhibits excellent modelling performance on the test dataset with R^2 value of 0.98 and RMSE of 0.23 %. The predictive accuracy on the test dataset for Ag and Au recovery is computed to be around 80 %, and the RMSE are also comparable, i.e., 0.25 % and 0.24 % respectively. Overall, the performance metrics computed for the

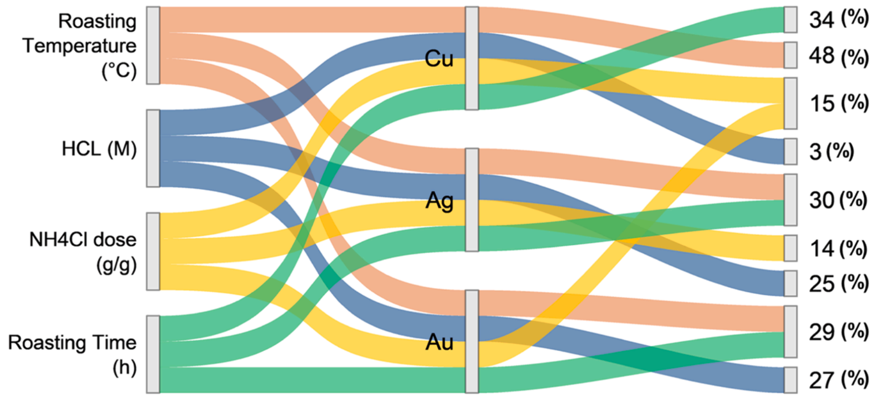

Fig. 4. SHAP based feature importance analysis for the recovery of Cu, Ag and Au from the WPCB. Roasting temperature appears to be relatively more important feature impacting the metal recovery from the WPCB.

predictive proficiency evaluation of the trained GP regression-based models for Cu, Ag and Au demonstrate good mapping constructed within the models for the process conditions and metal recovery from the WPCB.

Furthermore, the parity plots presenting the visualisation of distribution and agreement between the true and model-based predictions along with kernel density estimate (KDE) are also plotted. The kernel density exhibits the likelihood of observing the value of variable, while the area under the KDE curve integrates to unity. The dotted line ($y = x$) represents the perfect match between the true and predicted responses. The model-based prediction for Cu recovery is well aligned with dotted line and KDE curves are compact confirming the excellent predictive capacity and lower uncertainty for the point-predictions from the trained model. The relatively large spread-out of the KDE curves, compared with those of Cu, attempts to explain the likelihood of observing the model-based predictions for Ag and Au recovery as they are constructed based on the predictive performance of the trained models. However, a good degree of agreement between the true and model-based predictions for Ag and Au is apparent along with the identification of the KDE density associated with the model-based predictions.

3.3. Feature importance analysis for the metal recovery process

The ML models are trained to learn the relationships between the input-output variables and the models' learning is based on the dataset collected for each variable. Once the ML models have been trained and the acceptable degree of accuracy of the models has been ensured, it becomes imperative to investigate the feature importance, impacting the point-predictions of the output variables from the ML models. In this regard, SHAP is an excellent technique that constructs the different possible combinations of the input variables corresponding to the observed observations and the constructed experiments are simulated form the ML models to establish the significance order of the input variables.

Fig. 4 presents the percentage significance of process input conditions on Cu, Ag and Au recovery from the WPCBs of mobile phones. Roasting temperature is turned out to be the most significant process input variables, contributing 48 %, 30 % and 29 % respectively for the predictions made by trained GP models for Cu, Ag and Au recovery from the WPCBs. Whereas, roasting time is the second significant variable for the metals recovery from the WPCBs.

The proposed method works on roasting WPCB at 260 °C for 2.5 h using NH_4Cl dose of 2 g/g, followed by leaching with a 2 M HCl solution. The combination of optimal temperature, time, and NH_4Cl dosage, along with the precise HCl concentration, ensures high metal recovery rates, highlighting the effectiveness of this approach in metal extraction from electronic waste. When WPCB are roasted with NH_4Cl dose of 2 g/g at 260 °C, NH_4Cl decomposes into NH_3 (g) and HCl (g). The decomposition reaction is as follows:

$$NH_4Cl(s) = HCl(g) + \ NH_3(g) \tag{8}$$

Roasting temperature plays a crucial role in the kinetics of NH_4Cl roasting because it directly influences the rate of the chemical reactions involved. According to the Arrhenius equation, the rate of a chemical reaction increases exponentially with temperature. This means that even a small increase in temperature can significantly speed up the roasting process, leading to quicker and more efficient decomposition of NH_4Cl. Proper control of temperature ensures efficient and cost-effective roasting, making it a critical factor in the process. The sublimation of NH_4Cl occurs at 338 °C. During equilibrium, its decomposition is influenced by the partial pressures of HCl and NH_3. As the partial pressure in the reaction chamber never reaches zero, the decomposition of NH_4Cl begins at temperatures significantly below 338 °C (Lorenz and Bertau, 2019). Panda et al. studied the decomposition of NH_4Cl using TGA (Thermogravimetric Analysis) to gain insight into the roasting temperature range and its behaviour (R. Panda et al., 2021). The temperature range of 200–310 °C shows a sharp decrease in the weight of NH_4Cl powder, with a DTA (Differential Thermal Analysis) minima around 300 °C. The NH_4Cl sample starts to decompose around 200 °C, and as the temperature increases, the NH_4Cl powder decomposes vigorously. The HCl gas reacts with metals present in the T-PCBs to form metal chlorides, which are typically more soluble in water. The general reaction for metal chlorination can be represented as:

$$M(s) + xHCl(g) + \ \frac{x}{4}O_2(g) = MCl_x(s) + \ \frac{x}{2}H_2O(g) \tag{9}$$

At the optimal roasting temperature of 260 °C and the NH_4Cl dose of 2 g/g, the decomposition of NH_4Cl produces sufficient HCl gas to react with the metals in the WPCB, forming metal chlorides such as $CuCl_2$, AgCl, and AuCl. These metal chlorides are crucial intermediates because they are more soluble in acidic solutions, facilitating easier extraction. Using 2 M HCl for the leaching step ensures maximum recovery of Cu, Ag, and Au by efficiently dissolving the metal chlorides formed during roasting.

3.4. Maximising the metal recovery from the WPCB

During experimentation for metal recovery from WPCB, recovery rates reached up to 98 % for Cu, 88 % for Ag, and 77 % for Au which were achieved corresponding different operating levels of the process input variables. It highlights the sensitivity of the reaction kinetics to the operating levels of the process input variables. However, maintaining the same process conditions that maximises the metal recovery offers significant advantages, such as reduced disruptions and lower need of process adjustment for metal recovery operation, improved equipment

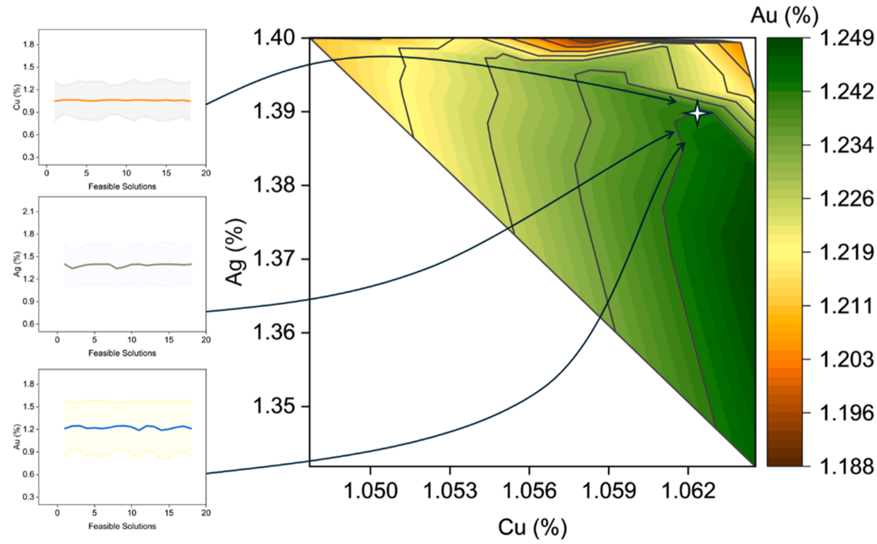

Fig. 5. Estimating the optimised process conditions for maximum Cu, Ag and Au recovery from the WPCB. Genetic algorithm solver is used for solving the maximisation problem and the optimal solution for the metal recovery is selected having the least variance observed out of the candidate solutions.

integrity and safety as well as smooth production scheduling. Moreover, smooth operation of the metal recovery process can decrease equipment wear and maintenance costs, further enhancing operation excellence and good manufacturing practices for the metal recovery from the WPCBs.

The task of finding common optimal process conditions for the recovery of Cu, Ag, and Au is challenging. GA can effectively address this challenge and may estimate optimised operating conditions, maximising the simultaneous recovery rates of all three metals. This approach not only ensures high recovery rates but also supports sustainable and economically viable metal recovery practices. The objective function for the maximisation problem considering the maximum recovery of Cu, Ag and Au from the WPCB is formulated as:

$$\max_{x} : f_{Cu}(x) + f_{Ag}(x) + f_{Au}(x)$$

subject to:

$$h(x) = 0$$

$$x^L < x < x^U$$

here, $h(x)$ is the equality constraint, representing the GP based process models for the metal recovery from the WPCB. While, x^L and x^U represent the lower and upper bounds on the process input variables (x). Considering the bounds on the input variables, the objective function is formulated to integrate the GP based process models for Cu ($f_{Cu}(x)$), Ag ($f_{Ag}(x)$) and Au ($f_{Au}(x)$) that the solver tends to maximise such that optimised process conditions for the maximum metal recovery can be estimated. GA is a global optimisation solver that works well with the experimental datasets to find the global maximum of the objective function and thus, is used in this study. The optimisation analysis carried out in MATLAB 2021 version b.

Fig. 5 depicts the variance around the maximum recovery of Cu, Ag and Au for the candidate solutions estimated after solving the maximisation problem by GA. The variance around the solution is the measure of the variability of the metal recovery; therefore, the optimal solution is selected having the least variance observed for Cu, Ag and Au recovery from the WPCB. The metal recovery function space is built on the normalised values of the three metals recovered from the WPCB. The maximum recovery of the three metals from the WPCB is mapped on the maximum metal recovery function space by the star. It is important to note that variation in Cu and Ag is reasonably small as estimated on the candidate solutions. However, Au presents a significant potential to be recovered beyond its recovery rate as observed in the dataset since the normalized value for the maximum metal recovery is >1 and is approaching to 1.249. However, the maximum Au recovery has the normalised recovery rate value of 1.242 corresponding to the least variance observed for the three metals recovery rates.

The GA led maximum recovery of metals from WPCBs estimates that roasting time should be maintained for 2.92 h corresponding to NH_4Cl dose of 2.34 g/g, HCl concentration of 2.50 M and roasting temperature of 278 °C to extract Cu, Ag and Au to the maximum recovery of 99.9, 99.7 % and 83.7 % respectively. The metal recovery is estimated to be 2.0 %, 13.3 % and 8.6 % higher for Cu, Ag and Au compared to the metal recovery rate observed during the experimentation. The optimisation analysis presents the potential to extract higher metal recovery rate without controlling the process beyond its operating bounds as well as the same process conditions for the operation of the process equipment.

3.5. Experimental verification of maximum Cu, Ag and Au recovery from the WPCB

The analysis presented in the previous sections is based on data collected from experiments focused on the recovery of Cu, Ag, and Au from WPCB. Data-driven process models were developed to leverage the computational capabilities of ML models, which approximate the patterns of metal recovery rates and are deployed to estimate optimised conditions for maximising metal recovery from WPCB. The data-driven approach minimises experimental costs and resource utilisation compared to traditional trial-and-error methods for process optimisation in the lab.

Model-based estimates of metal recovery rates must be validated experimentally to ensure the accuracy of the model-based optimisation analysis. Significant deviations between model predictions and experimental results highlight gaps in the model's understanding of the system, necessitating adaptive learning based on experimental conditions and observed metal recovery rates. Therefore, adaptive ML approach should be implemented to minimise discrepancies between model predictions and experimental observations. Additionally, adaptive learning enables sequential model-based optimisation, and determine process conditions based on the response surface of metal recovery profiles.

The estimated optimised operating levels of the process input variables are maintained in the lab to investigate the percentage recovery of Cu, Ag and Au from the WPCBs of mobile phones. Similar

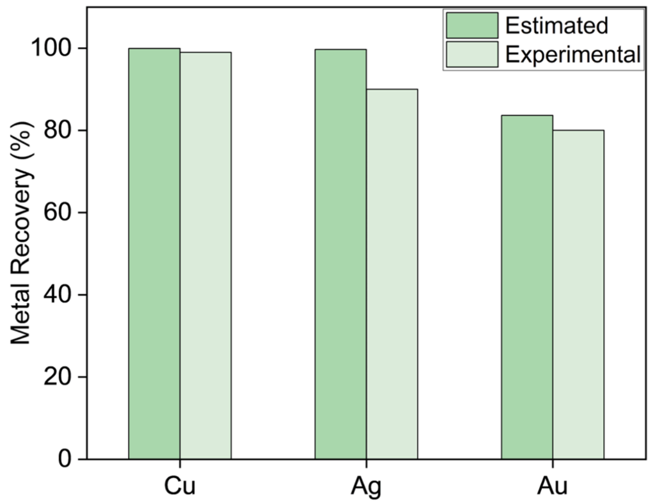

Fig. 6. Comparison of the maximum Cu, Ag and Au recovery from the WPCB corresponding to the optimisation based estimated values and the subsequent experimental extraction of the three metals in the lab.

experimentation protocols are observed during the verification of ML based estimated solution as maintained during the initial experimentation stage for collecting the dataset. The experimental recovery of three metals is measured and compared with the ML based optimisation analysis as shown in Fig. 6. Cu, Ag and Au are recovered up to 99 %, 90 % and 80 % on the optimised operating conditions while the estimated maximum recovery of the three metals have been up to 99.9, 99.7 % and 83.7 % respectively. The mean absolute percentage error is computed to be 0.95 %, 9.7 % and 4.4 % respectively corresponding to the estimated maximum recovery of Cu, Ag and Au. However, the ML based workflow has increased the percentage recovery of Cu, Ag and Au by 1 %, 2.3 % and 3.9 % respectively corresponding to the initial metal recovery rates obtained in the dataset that is deployed to train the GP models. Higher metal recovery rates through ML led optimisation analysis highlights the advantage of the developed workflow to boost the metal recovery rates on the same process conditions, underscoring the capability of ML and optimisation tools for carrying out complex process optimisation tasks effectively.

4. Conclusion

The electronic waste of mobile phones is an environmental burden and pollution. Huge volume of electronic waste of mobile phone is anticipated that requires sustainable solutions to ensure the material supplies and effective waste management for sustainable AI and environmental protection. To address the issue of material supplies for chip manufacturing and waste management of waste printed circuit boards (WPCBs) of mobile phones, an eco-friendly low-temperature roasting process is developed to recover Cu, Ag and Au from WPCBs of mobile phones. Gaussian Process (GP) models are trained on the experimental data to approximate the metal recovery behaviour from the WPCBs. SHAP analysis reveals that roasting temperature (°C) is the most significant input feature that impacts the recovery of Cu, Ag and Au from the WPCBs. An optimisation problem is formulated and solved by genetic algorithm to estimate the optimised experimental conditions for maximising the recovery of Cu, Ag and Au from the WPCBs. The experiments are conducted in the lab and 99 %, 90 % and 80 % recovery of Cu, Ag and Au is achieved from the WPCBs. The ML led workflow can estimate the optimised experimental conditions to optimise the process for the recovery of metals from the WPCBs that enhances the material utilisation efficiency and improves the waste management of WPCBs to support sustainable AI development.

CRediT authorship contribution statement

Waqar Muhammad Ashraf: Data curation, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing. **Ramdayal Panda:** Formal analysis, Investigation, Methodology, Validation, Writing – original draft, Writing – review & editing. **Prashant Ram Jadhao:** Formal analysis, Investigation, Methodology, Validation, Writing – original draft, Writing – review & editing. **Kamal Kishore Pant:** Conceptualization, Funding acquisition, Resources, Supervision, Writing – review & editing. **Vivek Dua:** Conceptualization, Funding acquisition, Supervision, Resources, Writing – review & editing.

Declaration of competing interest

The authors declare no conflict of interest in this research.

Acknowledgement

The authors acknowledge the funding received for the project, "E-waste recycling: Development of green and sustainable technology for recovery of metals from electronic waste" from the UCL-IIT Delhi Strategic Partner Fund, award number MFIRP179.

Data availability

Data will be made available on request.

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