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ORIGINAL ARTICLE

Contrastive deep clustering for detecting new defect patterns in wafer bin maps

Insung Baek[1] · Seoung Bum Kim[1]

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Abstract
Wafer bin maps (WBMs) data, presented as images, play a critical role in identifying defects in the semiconductor industry. Thus, accurately classifying WBM defect patterns is essential to maintain high quality and enhance the overall yield. However, the task of labeling and classifying WBM data, which are generated daily in the tens of thousands or more, presents a challenge for experts. Recently, with advancements in artificial intelligence research, there has been a surge in efforts to automatically classify WBM defect patterns. Nevertheless, existing studies have primarily focus on classifying known defect patterns using labels. However, in the real-world semiconductor industry, new defect patterns are constantly emerging in addition to the known patterns. In this study, we propose the contrastive deep clustering (CODEC) for wafer bin maps that identifies new defective patterns in WBMs while simultaneously clustering these patterns into multiple defects without using labels. We use a contrastive loss function to address the challenges associated with a limited number of novel defect patterns. We demonstrate the effectiveness of our proposed methodology in accurately classifying new defect patterns using open data WM-811 k.

Keywords Semiconductor manufacturing · Wafer bin map · Deep clustering · New defect pattern classification · Contrastive learning · Deep learning

1 Introduction

The wafer, integral to the semiconductor manufacturing process, serves as the substrate upon which semiconductor devices are fabricated [1, 2]. A single wafer contains hundreds of semiconductor chips. To ensure high yield and quality, it is crucial to swiftly identify and address defects [3, 4]. Industry engineers conduct inspections, such as electrical die sorting (EDS), to detect defective wafers [5–7]. EDS generates the wafer bin map (WBM) data representing the defect status of each chip on the wafer. As shown in Fig. 1, WBM data is presented as an image, indicating each chip defects or not. These images reveal patterns associated with the causes of defects, aiding in tracing their root causes. However, because of the large volume of WBMs produced daily, it is impractical for engineers to manually classify them. Recent studies have used machine learning and deep learning algorithms to automate the classification of such large volumes of WBM data [8–10].

However, existing studies have limitations in encompassing all practical issues related to the WBM defect classification. First, in the semiconductor industry, both known and new defect patterns constantly emerge in actual WBM data [5, 6, 9]. When a known defect pattern occurs, experts can identify the cause and take appropriate action based on their experience. However, when a novel defect pattern appears, it becomes more challenging to promptly determine its cause. This increases the time required to trace the root cause of the defect and take corrective action, thereby increasing the risk of quality incidents. Hence, models should be capable of detecting both known and new defect patterns. Second, multiple new defect patterns can appear simultaneously. Therefore, the model needs to accurately group and classify identical patterns among the new defects to identify process paths that lead to such defects [11]. By accurately identifying new fault patterns, the root cause of the fault can be pinpointed, minimizing defect occurrence and preventing

✉ Seoung Bum Kim
sbkim1@korea.ac.kr

Insung Baek
insung_baek01@korea.ac.kr

[1] School of Industrial and Management Engineering, Korea University, Seoul 02841, Republic of Korea

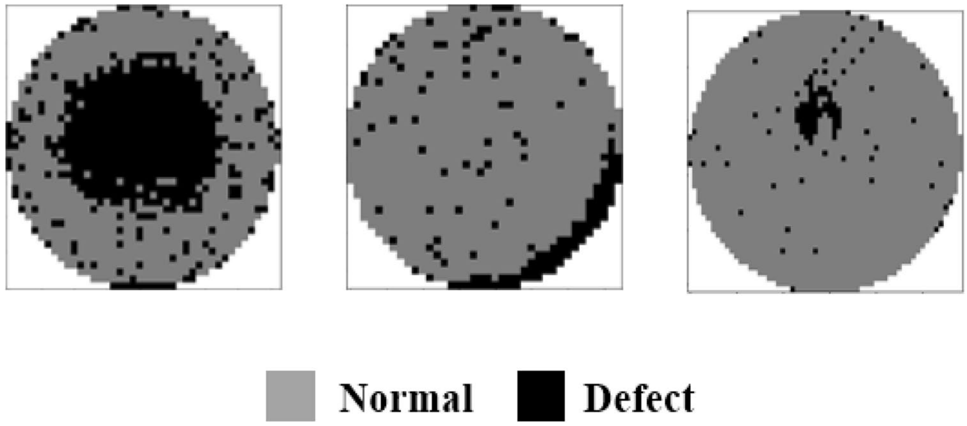

Fig. 1 Examples of a wafer bin map

potential incidents. Finally, unlike known defect patterns that have already been directly inspected by engineers and assigned labels, these new defect patterns lack label information [6, 9]. Ultimately, the timely detection of new defect patterns and the simultaneous clustering of multiple defect patterns are highly important for preventing major quality accidents in the semiconductor industry. Therefore, for the automatic classification of WBM defects, it is important to develop methods that can detect and classify novel defects without labels. However, previous studies on WBM analysis are limited to classifying known patterns using labels or detecting the existence of a new defect pattern [1, 5, 6, 8, 9]. Existing WBM studies focus on enhancing the performance of known defective patterns, even when using unlabeled data [8]. Moreover, in situations involving new defect patterns, some studies focus solely on detecting their presence based on their differences from existing ones [5, 9]. In contrast, this study proposes a method capable of identifying new defect patterns while simultaneously clustering these patterns into multiple defects without relying on label information. In this situation, deep clustering techniques, commonly used in computer vision, can effectively identity and classify new patterns. Deep clustering groups similar patterns based on image features, without using labels, enabling the classification of patterns with different characteristics [12, 13]. Deep clustering uses a deep learning model to extract features from unlabeled images and subsequently conducts clustering. During this process, the clustering performance is enhanced by learning to group similar images together while distinguishing those with different characteristics. Deep clustering differs from zero-shot learning, which involves using labels for learning and subsequently detecting unseen classes that were not included the training set. Deep clustering is typically used for general image data with a sufficient volume of data. However, in the case of real WBM data, the number of new defect patterns is small.

In this study, we propose the contrastive deep clustering (CODEC) for wafer bin maps that combines deep clustering with contrastive learning to enhance the classifying performance of very few new patterns [14, 15]. Our methodology extends the work of Huang et al. (2022), which used two different loss functions to train a deep clustering model [16]. They implemented an approach where samples with similar characteristics are trained to be closer, while the centers of dissimilar clusters, based on the pseudo labels, are trained to move apart. However, their study had limitations in that the performance was good only on general image data with a substantial number of samples. Consequently, we propose a methodology that incorporate a contrastive loss function to improve the classifying performance of new patterns. The use of a contrastive loss function with negative samples enhances the effectiveness of classifying a small number of novel patterns. We use a traditional convolutional neural networks (CNN) model to classify whether a pattern is known or new. Subsequently, the proposed CODEC is applied to the data predicted by the new patterns to group several of them. There are studies that classify previously new classes through multiple stages [17–19]. Ren and Li (2021) proposed a two-stage method for addressing the open-set problem in acoustic scene classification (ASC). After identifying the unknown scenes, the classification process proceeds to categorize the defined acoustic scene [17]. Wu et al. (2022) proposed a two-stage object detector that first determines whether a new object class or an existing object class and then distinguishes between multiple new class objects [18]. Guo et al. (2019) proposed a study to classify new classes in the radio frequency and Twitter data using a multi-stage deep classifier [19]. We conduct experiments across various scenarios to confirm the effectiveness of our proposed methodology in accurately classifying effectively classifies novel patterns when the number of new defect patterns is small. Specifically, with the use of the open data WM-811 K, we select certain classes as new patterns and conduct experiments by sampling a small number of them. Consequently, we demonstrate that the proposed methodology effectively classifies several new patterns, even in the absence of label information and with few new patterns data. The main contributions of this study are as follows:

- A hybrid loss function that combines contrastive loss function with a deep clustering algorithm is proposed. The use of a contrastive loss function with negative samples enhances the effectiveness of classifying a small number of novel patterns. Given the limited quantity of new patterns in the WBMs, the probability of choosing negative samples with the same attributes as the input data is reduced. Consequently, the inclusion of negative samples facilitates the efficient classification of novel patterns by distinguishing data belonging to a distinct class from the input image.
- The proposed method enables the classification of new patterns solely based on WBM image characteristics without label information. By using a deep clustering strategy that does not require label information, it facilitates the grouping of WBM data with similar characteristics.
- Before applying the proposed CODEC algorithm, it is necessary to classify patterns as either known or new. The traditional CNN model used for these classification tasks can be used without requiring any additional modifications to the existing model.

The structure of this paper is as follows. Section 2 reviews existing studies on WBM classification and deep clustering. Section 3 illustrates the details of the proposed CODEC method. Section 4 presents the qualitative and quantitative experimental results. Section 5 contains our concluding remarks and directions for future research.

2 Related works

2.1 Wafer bin map classification

The classification of WBMs is significant in the semiconductor industry, and various algorithms have been used for studying this issue. Wu et al. (2015) publicly released the "WM-811 K" WBM dataset and used a support vector machine algorithm for classifying wafer defects [1]. Piao et al. (2018) used a radon transform to extract wafer features and used a multiple decision tree ensemble method for defect classification [20]. However, these methods face challenges in maintaining classification precision as the complexity of wafer defect patterns increases. Recently, substantial advancements have been made in using CNN for the analysis of WBM image data. Lee et al. (2017) accurately identified wafer defect patterns using a CNN model [21]. Nakazawa and Kulkarni (2018) achieved promising results in recognizing intricate patterns in both real and simulated wafer map image data using a CNN model [19]. Kyeong and Kim (2018) proposed a strategy for defect classification that considers multiple patterns on a wafer, in contrast to conventional methods that focus on a singular pattern [22]. However, these studies used supervised learning, requiring labels, and did not consider potential new defect patterns in the WBM. In the semiconductor industry, new defect patterns without labels constantly appear, making it essential to develop an approach that can accommodate them.

Shim et al. (2020) demonstrated that using uncertainty-based sample selection methods that prioritize samples with the highest influence on performance can yield high classification results even with limited labeled data [23]. Kahng and Kim (2021) proposed using pretext-invariant representation learning, which is one of the self-supervised learning frameworks incorporating CNNs for efficient classification using unlabeled data [8]. While these studies leverage unlabeled data, they overlook the potential emergence of new patterns in real-world scenarios. Jang et al. (2020) addressed this issue by proposing the support weighted ensemble model, specifically designed to detect new patterns [5]. Jang and Lee (2023) introduced an open-set recognition model using probability scores obtained from computed reconstruction errors and random network errors [6]. Although these studies make progress in identifying new patterns within WBMs, they are less effective in simultaneously classifying multiple new patterns. Jin et al. (2019) proposed a pattern clustering technique for WBMs using density-based spatial clustering of applications with noise (DBSCAN) [24]. Park et al. (2021) introduced a classification method that includes label reassignment based on a Siamese network approach [11]. While pattern clustering and label reassignment methods have shown potential in identifying new patterns, there is a lack of classifying new defect patterns tailored to the unique characteristics of WBMs, such as feature similarity across classes and limited quantities of new pattern data. In this study, we propose a CODEC that can accurately classify multiple new patterns by effectively solving the problems caused by the similarity between WBM classes and the scarcity of new pattern data.

2.2 Deep clustering

Deep clustering methods extract vectors that summarizes the high-dimensional data such as image data using deep learning algorithms [25]. Xie et al. (2016) introduced deep embedded clustering that applies k-means clustering to vectors representing image features obtained from an autoencoder model [26]. Gou et al. (2016) proposed an improved version of the deep embedded clustering that incorporates a clustering loss in addition to the reconstruction loss computed in the autoencoder [27]. Huang et al. (2020) proposed the partition confidence maximization (PICA) algorithm that maximizes confidence by forming clusters with similar samples [28]. The PICA algorithm assigns a confidence value of one when all images in a cluster belong to the same class, while the confidence value decreases if the cluster includes images from diverse classes. Therefore, they essentially aim to maximize this confidence value by effectively creating clusters. However, this study has a limitation in that it solely relies on clustering by confidence and disregards both the distances between distinct clusters and the distances between disparate clusters.

Recently, the advancement of self-supervised learning methods, capable of extracting salient features from input data without labels, has improved the performance of deep clustering. Especially, in computer vision area, self-supervised learning has demonstrated it effectiveness in extracting feature vectors for clustering. This is achieved by brining similar samples closer together in the embedding space while keeping dissimilar sample far apart. Li et al. (2021) introduced contrastive clustering (CC) that integrates contrastive learning at both the sample and cluster levels [29]. They performed contrastive learning using vectors and pseudo labels that well-summarized samples within a batch. In the embedding space, different clusters are trained to be farther apart, which improves clustering performance. Huang et al. (2022) identified an issue known as "class collision" in contrastive learning that negatively impacts clustering performance [16]. The class collision problem arises when semantically identical samples are mistakenly included in the negative samples. To address this, they proposed prototype scattering and positive sampling (ProPos) that combines a contrastive learning loss function to separate clusters and a bootstrap your own latent (BYOL) loss function for to aggregate similar samples [30]. While these methods have demonstrated strong performance on large datasets such as CIFAR-10, CIFAR-20, STL-10, and ImageNet, they may not be well-suited for clustering new patterns in WBM because of the limited amount of data. Therefore, in this study, we propose CODEC that combines the contrastive loss function with the two loss functions used in ProPos. This approach aims to accurately distinguish new patterns occurring in small numbers.

3 Proposed method—CODEC

In practical industrial settings, it is crucial to determine whether newly collected test data represents a novel defect pattern or one that is already known. This uncertainty necessitates a reliable approach to distinguish between the two. To address this, we initially develop a standard CNN model based on ResNet-18, specifically designed for the classification of both known defective patterns and potential new patterns. The CNN model is trained using labeled data of previously known defective patterns. During the prediction phase, the CNN model generates a logit vector, which is then used to determine whether the test data represents a new defect pattern or one of the known patterns. To make this determination, we calculate the median of the logit vector for each class. Next, we compute the distance between this median and all data points within the corresponding class. These distances are then sorted by class. To establish a reference distance, we identify any distance that exceeds 70% from the center. If the new test data surpasses this reference distance for all classes, it is identified as new defect pattern data. This method provides a systematic way to discern whether the test data represents a novel defect pattern or one that is already known, aiding in the accurate classification of the data.

The proposed CODEC aims to cluster and differentiate multiple new defect patterns in the WBM process of the semiconductor industry. An overview of the CODEC method is presented in Fig. 2. The loss function used in CODEC builds upon the ProPos method, which has demonstrated superior performance among deep clustering methods for general image data [16]. The ProPos loss function combines two components: the prototype scattering loss (PSL) and positive sampling alignment (PSA), both of which contribute to improving clustering performance. The PSL encourages the centers of different clusters to be more distant from each other while ensuring that the calculated centroids of the same cluster, as derived from the query encoder and key encoder, learn to be close to each other. Concurrently, the PSA enables samples with similar characteristics to cluster together. However, the effectiveness of the ProPos algorithm on new and rare defect patterns in WBM, which are inherently scarce, may not be optimal. To address this limitation, we propose the CODEC loss function, which combines the ProPos loss function with a contrastive loss component [14–16]. The inclusion of the contrastive loss function aims to enhance the clustering of a small number of new pattern data in WBMs. Equation 1 represents the loss function of the proposed CODEC method, with α_{psl}, α_{psa}, and α_c representing hyperparameters that can be adjusted to control the importance of each component in the overall loss function. Below, we provide a more detailed explanation of each component of the loss function.

$$L = \alpha_{psl}L_{psl} + \alpha_{psa}L_{psa} + \alpha_c L_c, \tag{1}$$

The first loss function used in the CODEC is the PSL. The PSL function calculates the distances between the centroids of clusters formed during the learning process. Pseudo-labels for PSL are generated using the k-means algorithm applied within a batch. In our study, we set the value of "k" in the k-means algorithm to seven, which corresponds to the total number of predicted new defect patterns. The

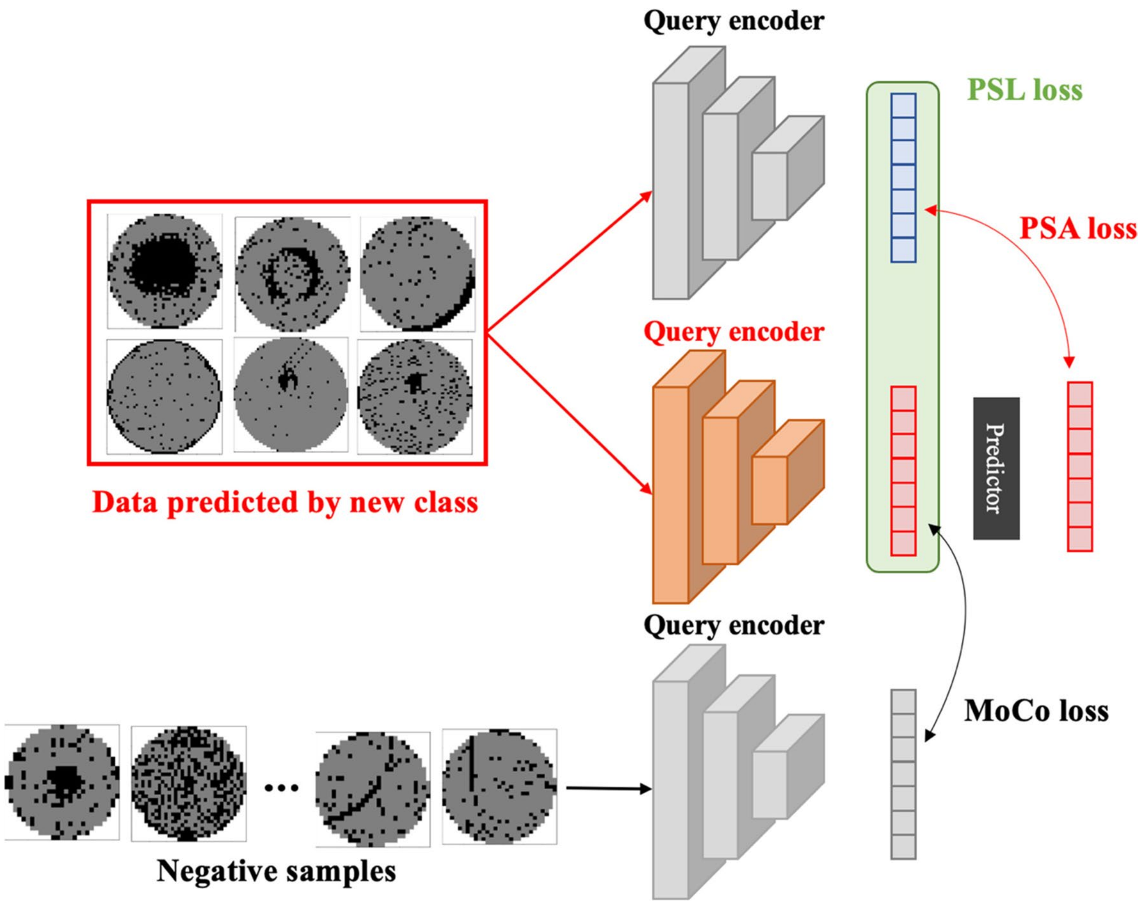

Fig. 2 Overview of the CODEC algorithm

computation of PSL is defined by Eq. 2, which incorporates the values of μ_k and μ_k'. Here, μ_k represents the cluster center computed using the vector of the query network, while μ_k' corresponds to the cluster center calculated using the vector of the key network. Similar to the loss used in traditional contrastive learning, the PSL aims to minimize the distance between μ_k and μ_k' for samples within the same cluster. Simultaneously, it encourages the centers derived from different clusters to be distant from each other. This encourages distinct clustering of samples belonging to different defect patterns while promoting compactness within each cluster.

$$L_{psl} = \frac{1}{K}\sum_{k=1}^{K} -log\frac{\exp\left(\frac{\mu_k^T\mu_k'}{\tau}\right)}{\exp\left(\frac{\mu_k^T\mu_k'}{\tau}\right) + \sum_{\substack{j=1 \\ j\neq k}}^{K}\exp\left(\frac{\mu_k^T\mu_j}{\tau}\right)}, \quad (2)$$

$$\mu_k = \frac{\sum_{x\in\beta}p(k|x)f(x)}{\|\sum_{x\in\beta}p(k|x)f(x)\|_2}, \quad (3)$$

$$\mu_k' = \frac{\sum_{x\in\beta}p(k|x)f'(x)}{\|\sum_{x\in\beta}p(k|x)f'(x)\|_2}. \quad (4)$$

In addition to the PSL, the CODEC incorporates the PSA loss function, which aims to bring samples with similar characteristics closer together in the embedding space. The formulation of the PSA loss function is inspired by the loss function used in BYOL (bootstrap your own latent), one of the noncontrastive-based self-supervised learning methods [30]. The PSA loss function, as depicted in Eq. 5, calculates the mean squared error loss between the vector generated by the predictor in the overall model architecture and the vector produced by the target network. Notably, these vectors represent augmented versions of the same source image. By minimizing the PSA loss, the model learns representations that encourage samples with similar attributes to cluster together in the embedding space. This promotes the grouping of samples sharing common characteristics, facilitating effective pattern recognition and clustering of defect patterns in the WBM process.

$$L_{psa} = \|g(v) - f'\left(x^{+}\right)\|_2^2, \quad (5)$$

$$v = f(x) + \sigma\epsilon, where \epsilon \sim N(0, I) \quad (6)$$

To enhance the model's ability to discriminate a small number of new patterns, the CODEC incorporates a contrastive loss function based on the MoCo algorithm [14, 15]. The contrastive learning process, illustrated in Fig. 3, involves a query encoder and a key encoder. Pairs of data obtained through two different augmentations of the same sample are designated as positive pairs. One pair is processed by the query encoder to generate a query vector, and the other pair is fed into the key encoder to generate a positive key. Furthermore, a subset of the remaining samples is selected as negative samples, and their representations are computed using the key encoder. These representations are stored in a dictionary of negative keys. The learning objective of contrastive learning is twofold: to bring the query and positive keys closer together in the embedding space and to push the query and negative keys apart. By training the model with this objective, the encoder learns representations that facilitate the discrimination of positive pairs from negative pairs. One important consideration in contrastive learning is the selection of negative samples. In our methodology, negative samples are chosen from all other samples, excluding the sample itself that has undergone different augmentations. Given the numerical scarcity of data corresponding to the new patterns per class, the negative samples have a higher likelihood of encompassing data from different classes. This approach proves effective in classifying new WBM defect patterns by training the model to separate a small number of new defect patterns. In Eq. 7, q represents the query representation, k^{+} denotes the representation of the positive key, and k^{-} refers to the representation of the negative keys. τ represents a temperature hyperparameter that controls the scale of the similarity scores in the following contrastive loss function:

$$L_c = -log\frac{\exp(q \bullet k^{+}/\tau)}{\exp(q \bullet k^{+}/\tau) + \sum_{k^{-}} \exp(q \bullet k^{-}/\tau)}. \quad (7)$$

4 Experiments and results

4.1 Data

In our experiments, we use the WM-811 K dataset, which is an open dataset containing real WBM samples. The dataset comprises a total of 811,457 WBMs, out of which 172,950 WBMs have labeled data. To focus on classifying new defect patterns, we exclude the "none" class that represents samples without a specific pattern. We also exclude the "near-full" class, which closely resembles the random class and lacks meaningful patterns. Our experiment involves seven defect patterns: edge-ring, edge-loc, center, loc, scratch, random, and donut. Because the WBM data represent categorical information, where values of zero, one, or two indicate the background or defect status for each chip, we preprocess the data into a one-hot vector representation. Furthermore, we standardize the sample size to 32×32 pixels to ensure

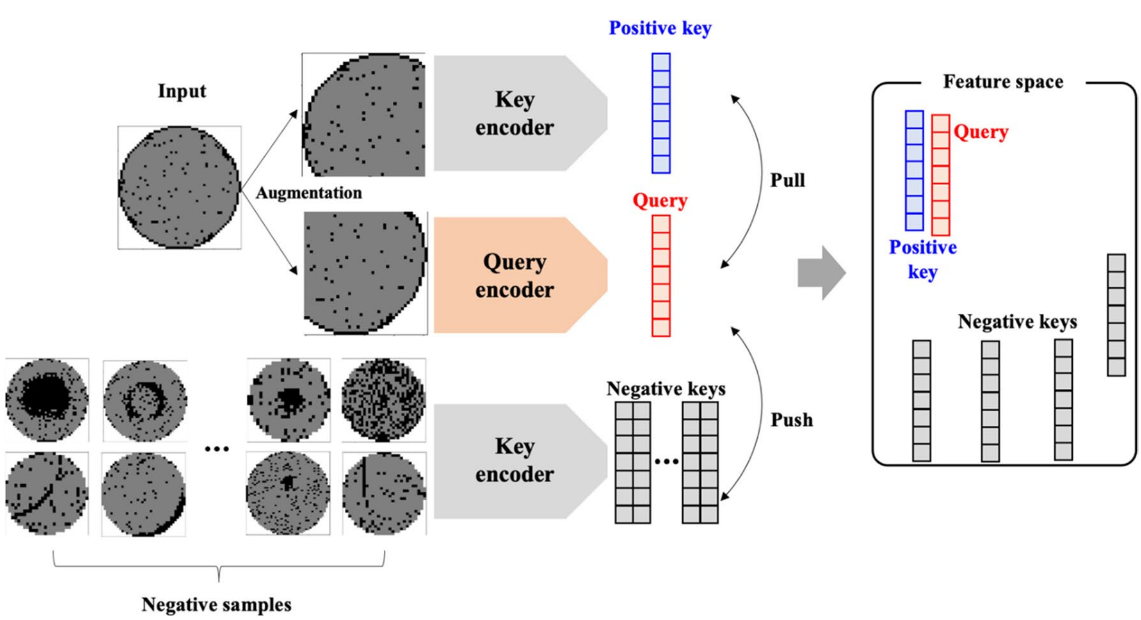

Fig. 3 Structure of contrastive learning in WBM data

consistency across all samples. Finally, each sample is transformed into an image with dimensions of $3 \times 32 \times 32$, which served as the input data for our experiments.

The aim of this study is to achieve accurate classification performance despite the limited availability of new defect pattern data in the semiconductor industry. To simulate this scenario, we sample 3%, 4%, and 5% of the total data for known defect patterns to represent the quantity of new defect pattern data. Furthermore, we establish four different scenarios to simulate various combinations of new defect patterns encountered in real-world situations. In Scenario A, the selected new patterns are scratch, donut, and random. Scenario B includes loc, scratch, and random as new patterns. For Scenario C, we choose center, edge-loc, and loc as new patterns, and Scenario D consists of edge-loc, loc, and random as new patterns. Figure 4 provides an overview of each scenario's known and new pattern dat. To conduct the experiments, we divide the data into training, validation, and testing sets, with proportions of 80%, 10%, and 10%, respectively for each scenario. Table 1 presents the number of samples used for training, validation, and testing in Scenario A, emphasizing the scarcity of data for each new defect pattern compared to the data for known defect patterns used in training and testing. The objective of these experiments is to assess the effectiveness of the proposed methodology in accurately distinguishing new patterns, even when the number of new pattern data is extremely limited.

4.2 Experimental setting

During the optimization process, we used the adaptive moment estimation (ADAM) optimizer. Specifically, we set the learning rate to 0.001 and the weight decay factor to 0.00005. The batch size was chosen as 128, and the total number of learning epochs was set to 1000. When incorporating the momentum contrastive learning component,

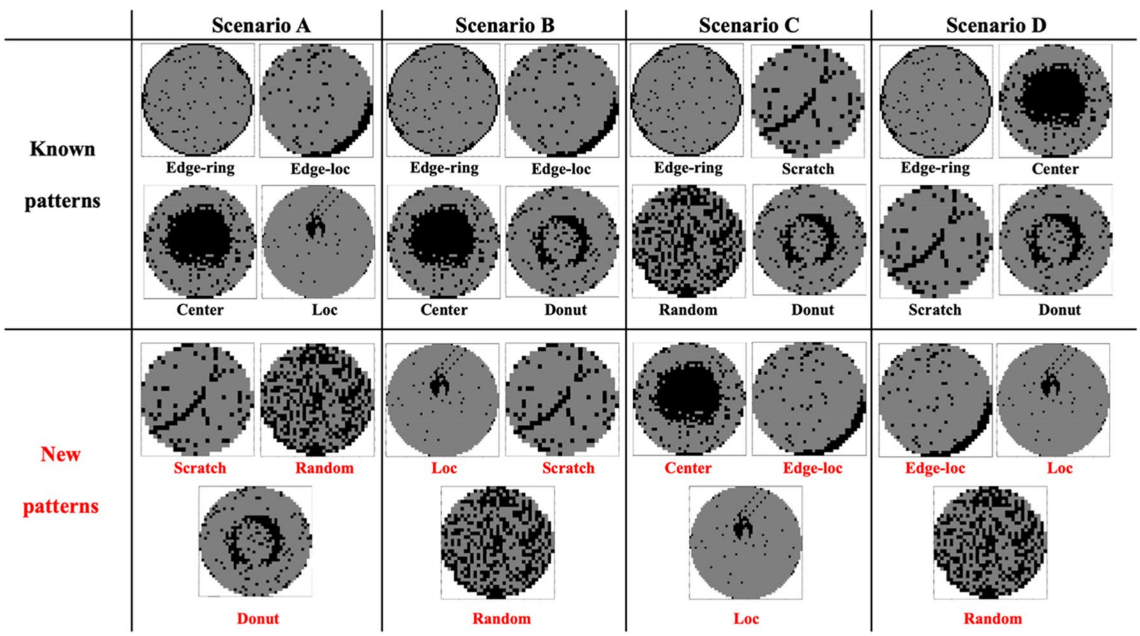

Fig. 4 Overview of known and new patterns in experiment scenarios. The new pattern reflects the possibility of various combinations occurring

Table 1 Number of data in the model that classifies known and new patterns in Scenario A

Known/new	Patterns (classes)	Original data	Train	Validation	Test
Known patterns	Edge-Ring	9680	7744	968	968
	Edge-Loc	5189	4151	519	519
	Center	4294	3434	430	430
	Loc	3593	2875	359	359
New patterns	Scratch	1193	0	0	546
	Random	866	0	0	546
	Donut	555	0	0	546
Total		25,370	18,204	2276	3914

the dictionary size was determined based on the sampling ratio. For a sampling ratio of 0.05, the dictionary size was set to 1024. For sampling ratios of 0.04 and 0.03, the dictionary size was adjusted to 512. These adjustments were made to accommodate the total data volume according to the sampling ratio. To ensure the robustness and reliability of the results, each method was tested five times across different scenarios, with the seed value varied for each run. This variability in the seed value helps account for any potential bias introduced by the random initialization of the model. The hyperparameters α_{psl} and α_{psa} in the loss function of the proposed CODEC were matched with those used in the ProPos study [16]. Additionally, the hyperparameter α_c was set to 0.1 to balance the contribution of the contrastive loss component. For evaluation, we used the accuracy metric, which is widely used in multiclass classification problems. Accuracy is calculated as the ratio of data correctly clustered into their actual class to the total number of data. It provides a measure of the model's performance in correctly classifying samples into their respective defect patterns.

4.3 Results

Table 2 presents the classification performance for both general known patterns and new patterns. The average accuracy for known classes and the accuracy for new classes in each scenario exceeded 0.6, indicating the initial success of the conventional CNN model in distinguishing between known and new patterns. This step is crucial because it isolates the new patterns for further analysis using CODEC. Table 3 provides insights into the quantity of data classified as unknown. As the sampling ratio decreases from 0.05 to 0.03, the volume of data per scenario also decreases. This reduction in data quantity aligns with the nature of WBM data, where new patterns are relatively rare. Hence, Table 2 and 3 collectively demonstrate that the experimental setup is appropriately configured for the classification of minority novel patterns, taking into account the scarcity of such patterns in the WBM data.

Table 4 displays the accuracy results for each scenario and sampling ratio using the applied methodology. Notably, CODEC achieved the highest performance in 11 out of the 12 scenarios, demonstrating its superiority over other methods. PICA [28], which used confidence values within clusters, exhibited the weakest performance across most scenarios. Similarly, CC [29], which incorporated contrastive learning for both samples and clusters, demonstrated relatively low performance in most scenarios, except for Scenario A. These results suggest that both PICA and CC are not well-suited for situations with a small number of class-specific data. Although ProPos [16] outperformed PICA and CC in the majority of scenarios, its performance remained inferior compared to the proposed CODEC. This indicates that ProPos may not be the optimal choice for clustering new WBM patterns when dealing with limited data per class. In contrast, the CODEC consistently demonstrated superior performance in most scenarios. This highlights the effectiveness of CODEC in accurately classifying a small number of new patterns into their respective clusters in the WBM process. These findings affirm the superiority of CODEC over other methods and its potential to handle the challenges posed by limited data for new defect patterns in the semiconductor industry.

To provide qualitative validation of the classification ability of CODEC, t-SNE visualization was used. Figure 5 displays the t-SNE visualization results for PICA, CC, ProPos, and CODEC. These results align with the quantitative findings, illustrating the performance of each method in classifying patterns when data volumes are limited per class. PICA and CC struggled to achieve effective classification, as evidenced by the substantial overlaps observed in their t-SNE visualizations. This indicates a difficulty in achieving clear class differentiation when faced with limited data. ProPos demonstrated relatively better classification compared to PICA and CC, but there were still noticeable overlaps, suggesting a certain level of ambiguity in class separation. In contrast, CODEC exhibited improved class separation compared to ProPos, as indicated by the t-SNE visualization.

Table 3 Number of data predicted by new patterns

Sampling ratio	Scenario A	Scenario B	Scenario C	Scenario D
0.05	2197	2118	1270	1790
0.04	1975	1825	1113	1453
0.03	1859	1464	969	1204

Table 2 Known and new class accuracy by sampling ratio

Sampling ratio	Known/unknown	Scenario A	Scenario B	Scenario C	Scenario D	Average
0.05	Known class	0.620	0.660	0.767	0.750	0.699
	New class	0.584	0.616	0.669	0.734	0.651
0.04	Known class	0.648	0.693	0.717	0.722	0.695
	New class	0.564	0.676	0.687	0.638	0.641
0.03	Known class	0.609	0.708	0.673	0.726	0.695
	New class	0.609	0.629	0.642	0.688	0.642

Table 4 Accuracy of the predicted unknown class by methodology and sampling ratio (For each sampling ratio, the accuracy of the best-performing deep clustering method in each scenario is highlighted in bold, and the value in parentheses represents the standard deviation from five repetitions.)

Sampling ratio	Methodology	Scenario A	Scenario B	Scenario C	Scenario D	Average
0.05	PICA	0.384 (0.02)	0.384 (0.05)	0.410 (0.02)	0.440 (0.02)	0.404
	CC	0.482 (0.03)	0.448 (0.03)	0.395 (0.03)	0.398 (0.03)	0.431
	ProPos	0.468 (0.04)	0.442 (0.04)	0.429 (0.05)	0.419 (0.03)	0.439
	CODEC (proposed)	**0.484 (0.03)**	**0.477 (0.04)**	**0.430 (0.05)**	**0.448 (0.03)**	0.460
0.04	PICA	0.411 (0.03)	0.347 (0.02)	0.455 (0.05)	0.428 (0.07)	0.410
	CC	0.513 (0.04)	0.450 (0.03)	0.426 (0.03)	0.420 (0.03)	0.452
	ProPos	0.468 (0.01)	0.443 (0.02)	0.460 (0.06)	0.512 (0.08)	0.471
	CODEC (proposed)	**0.522 (0.04)**	**0.452 (0.03)**	**0.487 (0.05)**	**0.520 (0.09)**	0.495
0.03	PICA	0.414 (0.04)	0.327 (0.01)	0.452 (0.06)	0.437 (0.03)	0.407
	CC	**0.544 (0.02)**	0.458 (0.02)	0.465 (0.04)	0.442 (0.07)	0.477
	ProPos	0.483 (0.02)	0.473 (0.01)	0.562 (0.04)	0.452 (0.04)	0.492
	CODEC (proposed)	0.519 (0.03)	**0.475 (0.01)**	**0.571 (0.04)**	**0.504 (0.04)**	0.517

This qualitative validation further supports the effectiveness of CODEC in accurately clustering new patterns in the WBM process, even when the data quantity for each class is small. The t-SNE visualizations provide additional evidence of CODEC's ability to handle the challenges posed by limited data and reinforce its superiority over other methods in achieving robust and distinct class separation.

5 Conclusions and future research

The detection and accurate classification of new defect patterns in the semiconductor industry are of utmost importance to prevent quality failures and ensure product reliability. This study has highlighted the significance of timely identification and resolution of these new patterns. By effectively applying the contrastive loss method, we have demonstrated the capability to classify new patterns even when the number of samples per class is limited. The use of contrastive loss enables tracking shared histories among wafers exhibiting new patterns, thereby preventing potential quality issues. This research marks a pioneering application of deep clustering, a commonly used method in general image analysis, to the specific domain of WBM data. Leveraging the WM-811 K open dataset, we have successfully showcased the feasibility of classifying emerging patterns, even with a scarcity of samples. Specifically, our proposed CODEC algorithms showcase enhanced classification of a limited number of new patterns through the application of the contrastive loss. This enhancement is attributed to the reduced probability of selecting a small set of new pattern data as the negative sample. As a result, when compared to established deep clustering methods, we provide both quantitative and qualitative evidence supporting the effectiveness of our approach in effectively distinguishing and classifying each minority new pattern. The findings of this study make a valuable contribution to the advancement of quality control processes in the semiconductor industry. The early identification and resolution of emerging issues facilitated by the accurate classification of new defect patterns can significantly improve overall product quality and reliability. This research serves as a stepping stone toward enhancing quality assurance practices, enabling proactive measures to ensure the continued excellence of semiconductor products.

In our future studies, we plan to investigate techniques that can enhance the selection of negative samples for improved identification and categorization of novel patterns. Currently, the contrastive loss function considers all samples, excluding the input data itself, as potential negative samples. However, this approach has limitations because the negative samples may still include data from the same class as the input, which can hinder accurate classification. To address this limitation, we intend to develop a strategy for selecting negative samples that possess

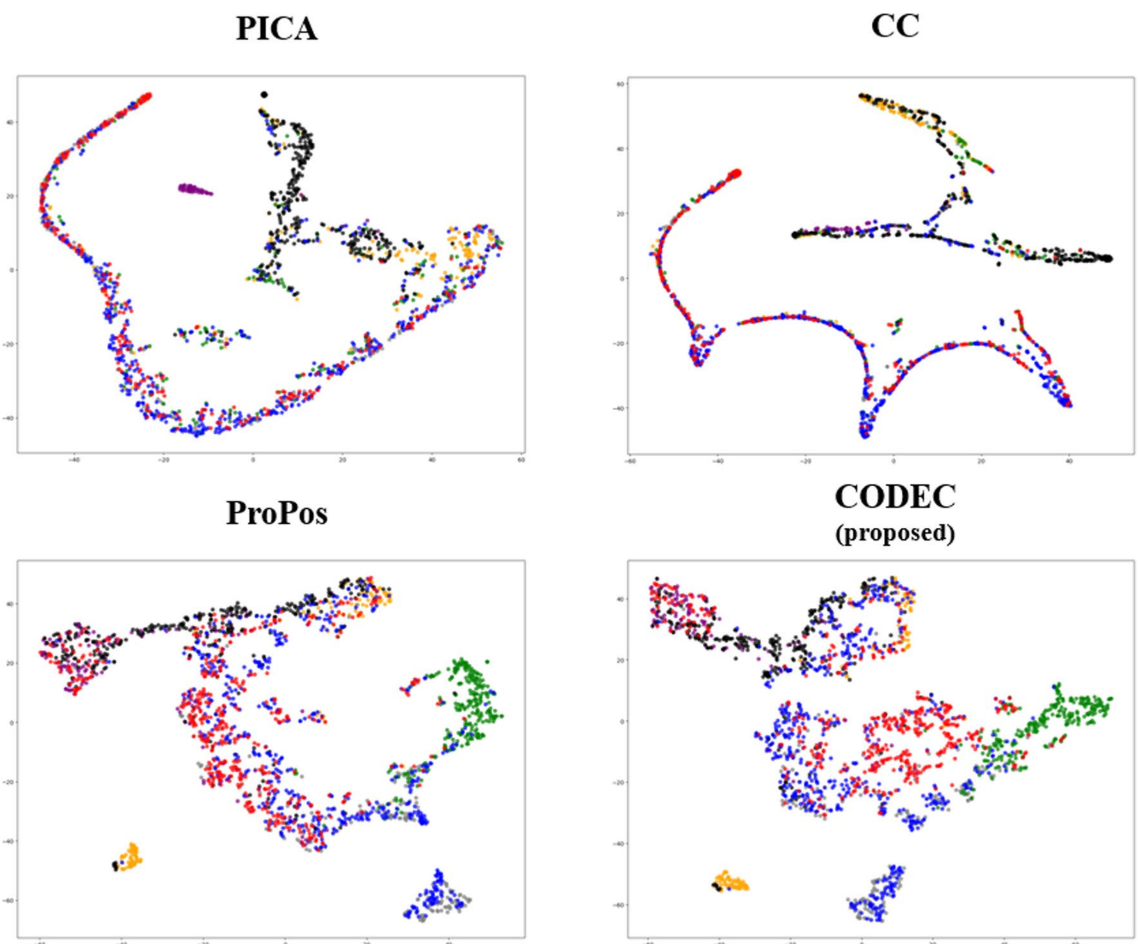

Fig. 5 Comparing representations of PICA, CC, ProPos, and CODEC using T-SNE

significantly contrasting properties compared to the input data. The contrastive loss function becomes meaningful when data points with different labels but close distances in the embedding space are separated. Therefore, we aim to approach this by generating pseudo-labels based on deep clustering. Initially, we intend to select data with different pseudo-labels and then calculate the similarity to designate data within a certain distance as negative samples. By incorporating this refined selection method into the contrastive loss function, we anticipate an enhanced ability to identify and classify unfamiliar patterns. This approach will enable the model to focus on learning discriminative features that differentiate between the input data and negative samples, leading to improved performance in detecting and categorizing novel patterns. Through these future research efforts, we aim to advance the state-of-the-art in pattern recognition and contribute to the development of more robust and effective methodologies for the detection and classification of new defect patterns in the semiconductor industry.

Author contribution All authors equally contributed to this study: design, experiment, and data analysis.

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Data availability All data are fully available without restriction. The dataset used in this study is available from the following website: https://www.kaggle.com/datasets/qingyi/wm811k-wafer-map.

Declarations

Ethics approval Not applicable.

Consent to participate We hereby voluntarily agree to participate in this research.

Consent for publication We all give our consents for this research to be published in IJAMT.

Competing interests The authors declare no competing interests.

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