Co-occurring Cluster Mining for Damage Patterns Analysis of a Fuel Cell

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Abstract. In this study, we research the mechanical correlations among components of solid oxide fuel cell (SOFC) by analyzing the co-occurrence of acoustic emission (AE) events which are caused by damage. Then we propose a novel method for mining patterns from the numerical data such as AE. The proposed method extracts patterns of two clusters considering co-occurrence between clusters and similarity within each cluster at the same time. In addition, we utilize the dendrogram obtained from hierarchical clustering for reduction of the search space. We applied the proposed method to AE data, and the damage patterns which represent the main mechanical correlations were extracted. We can acquire novel knowledge about damage mechanism of SOFC from the results.

Keywords: clustering, co-occurrence pattern, damage evaluation

1 Introduction

The fuel cell is regarded as a highly efficient, low-pollution power generation system that produces electricity by direct chemical reaction. However, a crucial issue in putting SOFCs into practical use is the establishment of a technique for evaluating the deterioration of SOFCs in the operating environment. Since SOFCs operate in harsh environments (i.e., high temperature, oxidation and reduction), the reaction area is decreased by fracture damage, and the cell performance is reduced as a result[1]. Two of the co-authors have succeeded in observing mechanical damage to SOFCs using the acoustic emission (AE) method[2]. Acoustic emission is an elastic wave (i.e., vibration, sound waves, including ultrasonic wave) produced by damage, such as cracks in the material, or by friction between materials. Depending on the "fracture mode" (i.e., opening or shear), the type of material, the fracture energy, the shear rate, and other factors, distinct AE wave forms are produced[3, 4].

Because AE data is enormous and high dimensional, data mining techniques have been applied for AE data in order to help SOFC experts discover the type and cause of damage. Fukui et al. used kernel self-organizing map (kernel SOM) to succeed in understanding the overview of damage process visually[5]. Also Kitagawa et al. used KeyGraph and density estimation combining with kernel SOM to identify the damage transition and rare essential events[6]. However, little knowledge about the mechanical correlation of damages has been obtained.

Hence, this paper aims to extract damage patterns which represent major mechanical correlation among components in SOFC. For such purpose, this paper proposes a novel method of co-occurrence pattern extraction against numerical data such as AE events. The proposed method determines the area (or the components) of two co-occurring clusters considering co-occurrence between clusters and similarity within each clusters. The experiments show that we can acquire novel knowledge about damage mechanism of SOFC from damage pattern, even for the SOFC experts.

2 The proposed method: *Co-occurring Cluster Mining*

2.1 Problems of the conventional methods

The task to extract co-occurring AE events is equivalent in some part to the well researched frequent pattern mining. Frequent pattern mining is to extract item sets appering frequently. An item is mainly symbolic data, however, there are also methods such as QLIQUE[8] and mining quantative frequent itemsets[9], which can handle numeric item. In [8] and [9], frequent item sets are extracted by searching frequent subspace clusters. However, the purpose is different from our work, because the above works do not search co-occurrence between clusters.

The straightforward approach to extract co-occurrence patterns from numerical data is first to execute clustering, and then to extract patterns. For example, Honda and Konishi quantized by SOM the image data of clouds obtained from the satellite, and then extracted association rules about the climate change[10]. Also, Yairi et al. extracted association rules about anomaly detection after clustering from time series data transmitted by the satellite[11]. After clustering, the correlation pattern extraction method among clusters are used in these researches, namely, two steps pattern extraction method.

However, the above works do not consider the co-occurrence among clusters during clustering process. As a result, clusters may contain data points which are not related to the co-occurrence patterns. To the contrary, clusters may not contain data points which are related to the co-occurrence patterns. For example, in SOFC, a glass seal changes its state according to the temperature, and the feature of caused AE events also changes gradually. We aim to extract a part of AE events caused by the damage of the glass seal which co-occur with other components of SOFC.

2.2 The requirements of a co-occurrence pattern

In this section, we define the characteristics of data this work handles, then define the requirements of the co-occurrence pattern.

Definition 1 (*numerical event sequence*). Suppose N numerical data $\mathbf{x}_i = (x_{i,1}, \cdots, x_{i,v})$, $(i = 1, \cdots, N)$ in v dimensional space are obtained in order $\mathbf{x}_1, \cdots, \mathbf{x}_N$.

Definition 2 (*basket*). Suppose an event sequence with numerical value is divided into some sections in time series. Namely, let all data set $\mathcal{D}$ is denoted by $\mathcal{D} = [\mathbf{x}_1, \cdots, \mathbf{x}_i][\mathbf{x}_{i+1}, \cdots, \mathbf{x}_j] \cdots [\mathbf{x}_k, \cdots, \mathbf{x}_N]$, $(i < j < k < N)$, where "$[\cdot]$" refers to a basket.

The baskets are given by a minute, a day and so on, besides the length of baskets is not always regular. The details about SOFC data is described in section 3.2.

Here, extracted co-occurrence patterns must satisfy the following three requirements:

Requirement 1 (*correlation*). As for two sets composed of events $A, B \subset \mathcal{D}$, the co-occurring ration of A and B must be high rate.

E.g., Jaccard coefficient, confidence as in association rule, etc.

Requirement 2 (*frequency*). The number of times of which A and B co-occurs in the time series are over the certain number of times.

E.g., support, etc.

Requirement 3 (*similarity*). As for two event sets A and B, events in each event set is similar each other.

E.g., variance in a cluster, average distance between data points in a cluster, etc.

Requirements 1 and 2 are derived from the co-occurrence between event sets (cluster), and requirement 3 is from the clustering of the events.

Definition 3 (*co-occurring cluster*). If event sets with numerical value $A, B \subset \mathcal{D}$ satisfy the above three requirements, set A is a co-occurring cluster of B.

Definition 4 (*co-occurrence pattern*). With co-occurring clusters A and B which satisfy all three requirements, $P(A, B) = \{A, B | A \cap B = \emptyset\}$ is called a co-occurrence pattern.

We aim to extract the co-occurrence petterns mentioned above. This paper proposes a novel method of co-occurrence pattern extraction called *Co-occurring Cluster Mining*. Note that we do not consider the order of occurrence of AE events in the same basket. The reason is mentioned in section 3.2.

A conventional frequent pattern means an item set appearing frequently, whereas co-occurrence pattern means two sets composed of events that co-occur frequently. Therefore, the proposed method is regarded as a particular kind of clustering method considered the co-occurrence between clusters, rather than frequent pattern mining.

2.3 The objective function

In this section, the objective function is defined to search co-occurrence patterns. In searching, the most complex problem is to make clusters which satisfy the correlation and similarity. We search the pairs of clusters $A, B \subset \mathcal{D}$ which maximize the following objective function:

$$L(A, B) = \{f(A, B)\}^{\alpha} \cdot \{g(A, B)\}^{(1-\alpha)}, \quad (1)$$

where the function $f(A, B)$ denotes the pattern correlation. The higher $f(A, B)$ value is, the more correlative pattern. For example, Jaccard coefficient and confidence as in association rule are used as $f(A, B)$. Jaccard coefficient is used in case of analyzing the ratio of the co-occurrence of event A and B. While confidence is used to the co-occurrence of event B under the situation that event A occurred. Note that because requirement 1 denotes the correlation among many separated baskets, the correlation in the short and sequential period must be excluded. Therefore, even if events A and B co-occur several times in the same basket, this is considered only once.

On the other hand, the function $g(A, B)$ denotes the pattern similarity. The higher $g(A, B)$ value is, the more similar clusters. For example, the distance between clusters, or the variance within each cluster are used as $g(A, B)$. Note that some definitions of the distance between clusters does not guarantee the monotonicity of cluster merge, e.g., centriod and median methods in hierarchical clustering. Therefore, we should avoid using those distances for $g(A, B)$. If only the distance between objects can be calculated, the average distance between objects is used as the variance in a cluster.

Since the co-occurrence patterns must satisfy the requirements of correlation and similarity at the same time, the objective function is defined as the product of $f(A, B)$ and $g(A, B)$. Generally speaking, the range of $f(A, B)$ is different from that of $g(A, B)$. Therefore, by normalizing as $f(A, B), g(A, B) \in [0, 1]$, both requirements of the correlation and similarity can be satisfied equally. The parameter $\alpha \in [0, 1]$ determines whether the correlation or similarity should be considered strongly. If α is close to 1, the similarity is considered more strongly than the correlation, and if α is close to 0, and vice versa. By maximizing the objective function by eq. (1), the co-occurrence patterns are obtained which satisfies the requirements of correlation and similarity. In addition, the requirement of frequency can be satisfied by extracting patterns which have higher support value than the pre-defined minimum support.

2.4 The algorithm

The proposed method searches the pairs of clusters maximizing $L(A, B)$. The proposed method is based on an aggregative clustering, because of high computational complexity when using partition clustering like k-means. Partition clustering needs to be executed every time variables in the search are changed, in order to generate the candidate clusters of A and B. On the contrary, in aggregative clustering, once the merge process of clustering is obtained, co-occurrence patterns can be searched on the merge process. However, even in aggregative clustering, the pair of $Seeds$(starting point of clustering) is $O(N^2)$, and the expansion from each $Seed$ will be $O(N)$. Therefore, the total computational complexity is $O(N^4)$. For the reduction of search space, we utilize a dendrogram from the result of hierarchical clustering and search co-occurrence patterns on the obtained dendrogram. By using the dendrogram, although the degree of freedom about the decision of cluster shape decreases, the benefit is a great reduction of the search space to $O((N \log N)^2)$.

The algorithm of the proposed method is presented below. Here, assume a dendrogram by some hierarchical clustering has been obtained in advance.

Co-ocuurring cluster mining algorithm

Input: $L_{min}(A, B)$, $Supp_{min}(A, B)$, dendrogram by hierarchical clustering (HC), baskets of numerical event sequence $\mathcal{D} = \{Object_k\}_{k=1}^{N}$.
Output: Co-occurrence patterns $\{P(A, B)\}$.

```
BEGIN
  FOR i from 1 to N DO
    FOR j(≠ i) from 1 to N DO
      Cluster A ← Object_i, Cluster B ← Object_j;
      Initialize L_Best(A, B) ← 0;
      WHILE (TRUE) DO
        IF L(A, B) > L_Best(A, B) THEN
          L_Best(A, B) ← L(A, B);
          Cluster A_Best ←Cluster A, Cluster B_Best ←Cluster B;
        END IF
        IF all pairs of clusters satisfying A ∩ B = ∅ have been searched THEN
          BREAK;
        END IF
        Cluster A ← Expand_Cluster(A, HC);
        IF A ∩ B ≠ ∅ THEN
          Cluster A ← Object_i, Cluster B ← Expand_Cluster(B, HC);
        END IF
      END WHILE
      IF L(A, B)_Best > L_min(A, B) and Supp(A, B) > Supp_min(A, B) THEN
        Output P(A, B) = {A_Best, B_Best};
      END IF
    END FOR
  END FOR
END
```

Here, Fig. 1 represents an example of the process of $Expand\_Cluster()$. $Expand\_Cluster()$ moves the current merge state from a certain node to the upper parent node, all leaf nodes (objects) which are children of this node belong to new cluster A. By the expansion of cluster A, label A is given to objects 1 and 6. And A and B co-occur in baskets 1 and 3, namely, a co-occurrence pattern (A, B) appears twice.

3 Application to AE data

3.1 Damage evaluation test of fuel cells

A schematic diagram of the apparatus used to perform the SOFC damage test is shown in Fig. 2. The test section was initially heated up to 800°C in order to melt a soda glass ring and was then gradually decreased to room temperature. Note that this damage evaluation test was to rupture the cells intentionally while lowering the temperature. Therefore, the knowledge obtained through this experiment is not directly available to actual running the SOFC. However, it is sufficient to demonstrate and confirm the reasonableness of the proposed method.

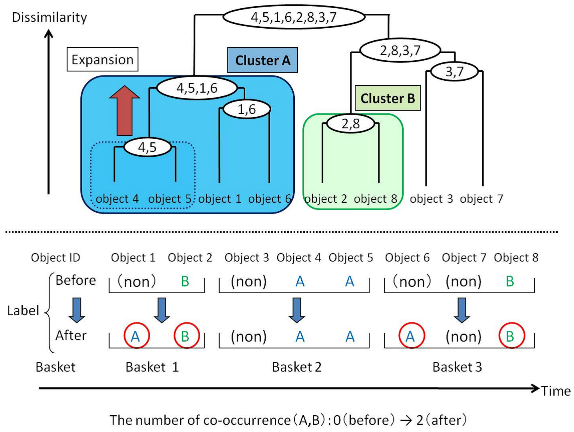

Fig. 1. The process of the proposed method. The above shows the dendrogram in the data space, and the below shows baskets in the time series.

The AE measurement was performed using a wide-band piezoelectric transducer. The AE transducer was attached to an outer Al_2O_3 tube away from the heated section. The sampling rate is 1 MHz, and so the observable maximum frequency is 500 KHz. Running the SOFC for over 60 hours, 1,429 AE events were extracted using the burst extraction method[12, 5].

Then, the same as the research by Fukui et al.[5], the AE events obtained from damage evaluation test are transformed into frequency spectrum data by Fast Fourier Transform (FFT). We obtained 1,429 frequency spectrum data each of which consists of 3,968 discrete points.

3.2 Division into basket

Assume that the potential stress in a composite material is released after a large-energy AE event occurs, i.e., interactions of internal forces are reset. In this research, the observed AE event sequence was divided into baskets followed by the research of Kitagawa et al.[6], assuming a sequence until a large-energy AE event occurs to be a chain of damage progression. These baskets are used in the proposed method. Note that because the damage process of SOFC is a complicated system, it is difficult to extract co-occurrence patterns considering the order of occurrence or the time intervals between AE events exactly. Therefore, we do not consider the order of occurrence of AE events in the same basket, or the time intervals between AE events.

In this research, the energy threshold is $1,500\text{mV}^2$, which is also used in the research[6]. Then the AE event sequence is divided into 123 baskets. Fig. 3 shows an example of division into baskets.

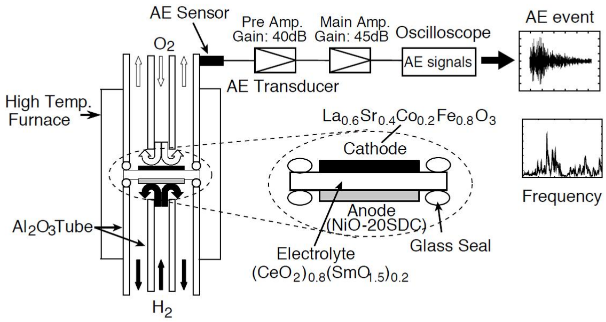

Fig. 2. SOFC damage test apparatus.

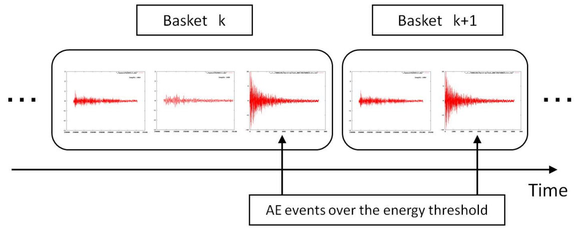

Fig. 3. An example of division into baskets (damage segments).

3.3 Calculation of distance between AE events

This work utilizes the result of the research by Fukui et al.[5] obtained by the kernel SOM. We regard the objects used for hierarchical clustering as the codebook vector (prototype). The self-organizing map[13] is an unsupervised neural network and a visualization technique by mapping the high dimensional feature space into the lower dimensional space (mainly two dimension). Kernel SOM[14] is the extended method of conventional SOM by improving the ability to express distribution of data with kernel method, which extends linear analysis method to non-linear method by mapping higher dimension. According to the earlier research, because the major damage types are already known on the kernel SOM, we can visually understand damage types with this result. Furthermore, the number of data points N is replaced to the number of prototypes $M (N >> M)$ by the quantization of the data space, the computational cost of searching co-occurring patterns is significantly reduced.

The distance between prototype vectors for the requirement of similarity (requirement 3) can be culculated as follows. Let M neurons of the prototype vectors be $\{\mathbf{m}_1, \cdots, \mathbf{m}_M\}$, where $\mathbf{m}_j = (m_{j,1}, \cdots, m_{j,v})$. In addition, let the position of M neurons in the topological layer be $\mathbf{r}_j = (\xi_j, \eta_j) : j = 1, \cdots, M$. The number of neurons and the layout of the topological layer must be predefined, and a regular or hexagonal grid is normally used. Also, let a function $\phi : \Omega \to \mathcal{H}$ maps an original data space Ω to a high dimensional feature space $\mathcal{H}$. Then the prototype vector $\mathbf{m}_i$ is calculated by:

$$\mathbf{m}_i = \gamma_i \sum\nolimits_n h_{c(n),i} \phi(\mathbf{x}_n), \tag{2}$$

where $\gamma_i = 1/\sum_n h_{c(n),i}$ refers to the normalization factor. The neighborhood function $h_{i,j}$ is the Gaussian function: $h_{i,j} = \exp(-\|\mathbf{r}_i - \mathbf{r}_j\|^2/2\sigma^2)$, where σ refers to the radius which represents the influence range of neighborhood.

Although the mapping function $\phi(\mathbf{x}_n)$ cannot be calculated directly, a kernel function can be defined as $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$, where $\langle , \rangle$ refers to the scalar product.

In this research, we use Kullback-Leibler (KL) kernel which was validated against the waveform data by Ishigaki et al.[15] and Fukui et al.[5].

Finally, the distance between prototype vectors $\mathbf{m}_i$ and $\mathbf{m}_j$ is culculated by:

$$\begin{aligned} d_{i,j} &= \|\mathbf{m}_i - \mathbf{m}_j\|^2 = \gamma_i^2 \sum_k \sum_l h_{c(k),i} h_{c(l),i} K(\mathbf{x}_k, \mathbf{x}_l) \\ &\quad - 2\gamma_i \gamma_j \sum_k \sum_l h_{c(k),i} h_{c(l),j} K(\mathbf{x}_k, \mathbf{x}_l) + \gamma_j^2 \sum_k \sum_l h_{c(k),j} h_{c(l),j} K(\mathbf{x}_k, \mathbf{x}_l) \end{aligned} \tag{3}$$

Since batch learning is used for kernel SOM, the neighborhood radius σ gradually decreases as learning is iterated. In calculating the distance of the codebook vector from the map obtained after the learning, we cannot decide the value of σ definitely. Therefore, the optimal neighborhood radius σ^* used for extraction of co-occurrence patterns is supposed to maximize the variance of the distances between the prototype vectors: $\sigma^* = \arg\max_\sigma V(d_{i,j})$. $\sigma^* = 0.1$ was linearly searched at intervals of 0.01. We use this $d_{i,j}$ as the distance between individual events.

3.4 The design of the object function

This paper focuses on the co-occurrence relationship in certain damage period, namely about two sets of AE events A and B, we aim to extract damages co-occurring at the high probability. Therefore, we use Jaccard coefficient as $f(A, B)$:

$$f(A, B) = \frac{count(A \cap B)}{count(A \cup B)}, \tag{4}$$

where $count(A)$ is the number of baskets where event A appears.

Moreover, we cannot obtain the centroid of clusters but can obtain the distance between codebook vectors with d_{ave} as the average distance among all pairs of codebook vectors in the cluster. Hence, $g(A, B)$ is:

$$g(A, B) = 1 - \sqrt{d_{aveA} d_{aveB} / d_{aveALL}^2}, \tag{5}$$

Table 1. The average values of the objective function of the extracted 100 patterns in different hierarchical clustering methods; single linkage, complete linkage, group average, centroid, median, and Ward's method.

Method	Single	Complete	Average	Centroid	Median	Ward
Average	0.443	0.494	0.482	0.444	0.459	0.487

Table 2. The number of extracted damage patterns. The alphabets of damage types are listed in Table 3, and the inter-regions damage types are represented with ",".

Pattern	Number	Pattern	Number	Pattern	Number
(B)-(B)	2	(D)-(D)	1	(E)-(D),(E)	1
(B)-(C)	3	(D)-(E)	1	(F)-(A),(D)	1
(B)-(D)	2	(E)-(E)	4	(F)-(D),(E)	1
(B)-(E)	2	(E)-(F)	5	(A),(D)-(D),(E)	1
(C)-(C)	1	(E)-(A),(D)	3	(D),(E)-(D),(E)	1

where d_{ave} is normalized divided by d_{aveALL} of the largest cluster so that $g(A, B) \in [0, 1]$. To consider the corrrelation and similarity of patterns as equally as possible, the parameter α in eq. (1) is set to 0.5.

3.5 The results of extracted damage patterns

The topology of kernel SOM is two dimensional square grid, and the number of neurons is 15×15.

First, Table 1 shows the average values of the objective function in different hierarchical clustering methods. The values are averaged by the extracted 100 patterns when the minimum support is 0.04. The complete linkage method shows the best result. The following all results are obtained by using the complete linkage method in the hierarchical clustering.

Next, the representative extracted damage patterns are explained. Two experts of SOFC of the co-authors interpreted damage patterns. Table 2 shows the estimated interpretation of extracted damage patterns. As the parameters of pattern extraction, the minimum object function is 0.47, the minimum support is 0.04, 29 patterns were extracted. The computational time when using 1429 individual objects was 888.7 (sec) with Intel Xeon CPU 2.66GHz and 6GB RAM. While, when using prototypes of the kernel SOM, the computational time in 225 objects was 25.6 (sec).

In addition, Fig. 4 shows an example of the result of extracted damage pattern on the result of kernel SOM. The correspondence of the regions on the map to damage types is shown in Table 3. This damage types and frequent period are already known by the research of Fukui et al.[5]. Each damage pattern is distinguished by using different colors, and the typical waveforms and spectra of the damage type are shown.

Table 3. The major damage types corresponding to the map in Fig. 4.

Region	Damage type
(A)	squeaking of the members during heating
(B)	progression of the initial cracks
(C)	squeaking of the members followed by (B)
(D)	cracks in the electrolyte
(E)	cracks in the glass seal
(F)	cracks in and exfoliation of the electrode

Valid results based on the knowledge of SOFC experts: Damage pattern 1 is a co-occurring pattern of (B) the progression of the initial cracks and (D) cracks in the electrolyte. In pattern 1, AE events on the top of map are a part of (B) of which these AE events occur in the latter period. Therefore, damage pattern 1 is interpreted that the progression of the initial cracks causes cracks in the electrolyte. According to table 2, we can know that progression of the initial cracks co-occurs with various damages. So we estimate that progression of the initial cracks is the starting points of various damages.

Next, damage pattern 2 is the co-occurring patterns of the cracks in the glass seal and cracks in and exfoliation of the electrode. Especially, the damage type which influences cracks in and exfoliation of the electrode are cracks in the glass seal which occurs in the latter period of cracks of the glass seal. The glass seal changes its state by the temperature, and in the period mentioned above, the temperature is decreasing and glass seal is congealed at the temperature of damage pattern 2. The glass seal and the electrode are not connected directly, but it is supposed that the shrinking and transformation of the cell due to the congelation of the glass seal produces the indirect mechanical effect.

Novel results: According to Table 2, no damage patterns which include both regions (D) and (F) are extracted. In spite of the fact that the electrolyte and the electrode are connected, damage patterns which include them were not extracted at all. This result was interesting to SOFC experts.

Next, since damage pattern 3 exists in the inter-regions, damage pattern 3 may contain novel damage types. Since these damages cause AE events contain high peaks in the low frequency of the spectrum, the damages between regions (A) and (D) are estimated as the exfoliation of the electrolyte, and the damages between regions (D) and (E) are estimated as the exfoliation of the electrolyte or the glass seal. Damages of pattern 3 have never discovered from the earlier research based only on the occurrence frequency of each AE event. Taking the co-occurrence relationship of AE events into consideration, damage pattern 3 is discovered for the first time.

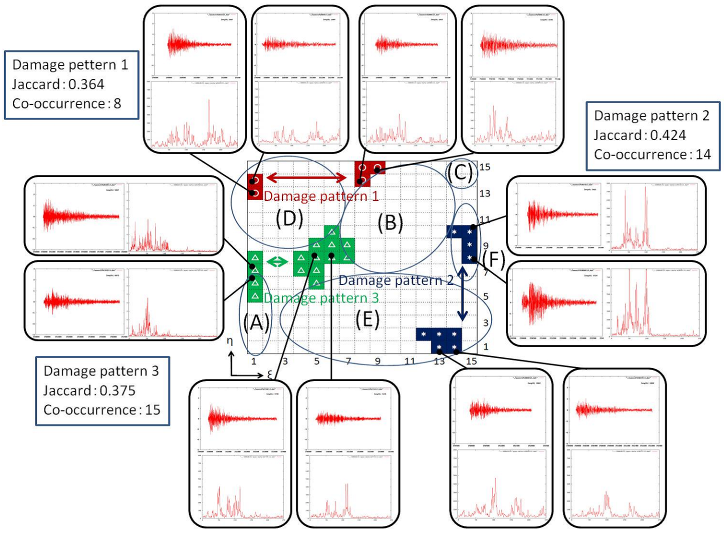

Fig. 4. An example of extracted damage patterns. The central map is the classification result by the kernel SOM.

4 Conclusion

In this paper, we proposed the novel extraction method of co-occurrence patterns against numerical data: *Co-occurring Cluster Mining*. The proposed method determines the area (or the components) of two co-occurring clusters considering co-occurrence between clusters and simultaneously similarity in each cluster. We applied the proposed method for AE events obtained from damage evaluation test of SOFC. As a result, damage patterns which demonstrate major mechanical correlations of SOFC were extracted, including unexpected but valuable damage patterns.

Furthermore, we will apply the proposed method for various numerical data such as earthquake wave or the track of point on dynamic image, and demonstrate the general-purpose of the proposed method.

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