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Evaluation of interactions between two-component self-assembled structures for SEM using multifractal analysis

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Abstract

In this study, a novel method was developed to quantitatively evaluate the interactions between components in multi-component self-assembled structures. By combining multifractal analysis with mutual information from information theory, the effectiveness of this method was validated using simulated images of two-component structures. The analysis showed that the calculated mutual information correlates with changes in structural parameters, demonstrating that this technique can sensitively detect interaction strength. This approach is expected to become a powerful tool for microstructural analysis of multi-component systems, such as composite materials.

Introduction

Image texture analysis is a technique for quantitatively evaluating the spatial distribution patterns of brightness and color within an image, with applications in fields such as medical imaging, materials science, and remote sensing. Complex structures found in nature and the microstructures of artificially created high-performance materials often exhibit heterogeneity and self-similar features that cannot be captured by simple statistics. To mathematically describe and quantify the properties of such complex shapes, fractal geometry, as proposed by Benoit Mandelbrot, opened a new path in image analysis. Using a single index, the fractal dimension, it became possible to quantitatively evaluate the "complexity" of intricate objects such as coastlines, cloud shapes, or material fracture surfaces[1].

However, many natural objects and physical phenomena do not exhibit simple self-similarity (monofractality) described by a single fractal dimension; instead, they have more complex hierarchical structures with varying local scaling laws. Multifractal analysis extends fractal theory to capture such "diverse orders" and "structural heterogeneity"[2]. The shape of the multifractal spectrum reflects the distribution pattern of these diverse orders, providing a more detailed description of the complex statistical properties of an object.

Applied research in multifractal analysis has advanced in various fields due to its powerful analytical capabilities. In materials science, for example, the physical properties of functional materials are strongly influenced by the spatial arrangement and morphology of microstructures such as crystal grains, precipitates, and voids. Microscopic images obtained using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) contain essential information for understanding and controlling material performance. In recent years, attempts have been made to apply multifractal analysis to evaluate the filler dispersion state in composite materials, the pore structure of porous materials, and to quantitatively assess the correlation between microstructural heterogeneity and material functionality [3-5]. These studies suggest that multifractal analysis can serve as a new guideline for quantitatively characterizing the complex microstructures of materials and linking the results to material design and quality control. However, in the multifractal analysis of composite materials, it is common to extract and analyze a single component, and quantitative evaluation methods for the multifractal analysis of multicomponent systems are still in their early stages.

Against this backdrop, multifractal analysis was used in this study as a method of image texture analysis, aiming to establish a quantitative evaluation method for multicomponent multifractal analysis that accounts for changes in the structures within an image, particularly for microscopic images of functional materials. Specifically, a quantitative evaluation of the interaction between two-component structures using simulated images was conducted.

Analysis of Interactions Between Two-component Self-assembled Structures

Theory of Multifractal Analysis

In multifractal analysis, the input image is partitioned by varying the grid size from large to fine. Using the probability of pixel presence in each grid at a given grid size, the particle distribution can be determined in detail at different scales, allowing for quantification of the structural complexity spreading across the entire input image. The equations for multifractal analysis are shown in Equations (1) and (2).

$$P_\varepsilon(i) = \frac{N_\varepsilon(i)}{\sum^n N_\varepsilon(j)} \quad (1)$$

$$D(q) = \frac{1}{q-1} \lim_{\varepsilon \to 0} \frac{\log \sum^n P_\varepsilon(i)^q}{\log \varepsilon} \quad (2)$$

Using the number of pixels contained in each grid, $P_\varepsilon(i)$ is the probability of pixel presence within a partitioned grid, ϵ is the side length of the partitioned grid, and n is the total number of partitions at scale ϵ. q represents the moment order. The moments q=0, 1, 2 have specific interpretations: D0 is called the fractal dimension and evaluates structural complexity; D1 evaluates the density and dispersion of the structure; and D2 evaluates the correlation of the structure[6]. This allows for a detailed evaluation of the morphology of particle groups based on the relationships between these Dq values. In particular, D1 is used to evaluate density and dispersion as the positional entropy of the pixel distribution constituting the structure. The formula used to calculate D1 is shown in Equation (3).

$$D(1) = \lim_{\varepsilon \to 0} \frac{\sum^n P_\varepsilon(i) \log P_\varepsilon(i)}{\log \varepsilon} \quad (3)$$

As shown in Equation (3), the numerator is equivalent to the entropy formula, indicating that D1 captures the change in entropy for each grid size. Thus, the structure was evaluated from the input image using multifractal analysis. However, the target structure in this study was a mixture of two components; therefore, a simple multifractal analysis was insufficient.

In this paper, masks are used to separate each component from the input image, extracting three types of images: "component 1 only," "component 2 only," and a "composite of component 1 and component 2." This enabled us to understand the aggregation or dispersion of each component and its shape. For SEM images in the field of materials engineering, which was the focus of this study, separation of each component is possible using the brightness values of the grayscale image because it is assumed that different components have different brightness levels.

Mutual Information

When performing multifractal analysis on the three types of images—"component 1 only," "component 2 only," and "composite of component 1 and 2"—the result for the composite includes the interaction between the first and second components. This represents a newly ordered structure created by the collision of these structures. In multifractal analysis, D1 represents entropy. Through entropy, the information generated by the interaction can be evaluated as mutual information.

One of the relational expressions in information theory allows the calculation of mutual information I(X;Y) from the joint entropy H(X,Y) and the marginal entropies H(X) and H(Y) of two independent random variables X and Y[7]. Equation (4) shows the formula for calculating mutual information.

$$I(X;Y) = H(X) + H(Y) - H(X,Y) \tag{4}$$

The mutual information I(X;Y) is calculated by subtracting the true combined uncertainty H(X,Y) from the simple sum of the two entropies H(X) + H(Y). In other words, if two random variables are not independent, simply adding their respective uncertainties results in double-counting the information they share; this double-counted region is the mutual information. Thus, because mutual information represents the magnitude of the mutual influence between two pieces of information, a larger value indicates a greater mutual influence.

For the input images targeted in this paper, if "component 1 only" and "component 2 only" is considered as X and Y, respectively, the "composite of component 1 and component 2" is a composite of X and Y. This can be interpreted as the marginal entropy H(X), marginal entropy H(Y), and joint entropy H(X,Y), obtained without distinguishing between the components. Therefore, by performing multifractal analysis on each input image and using D1, which corresponds to entropy, it is possible to calculate and evaluate the mutual information using Equation (3).

Experiments of Mutual Information Using Simulation

To calculate the mutual information, images are generated through simulations and evaluated the changes in the multifractal analysis results. Using a simulation method usually used for the quantitative evaluation of self-organized structures via multifractal analysis, a two-component simulation was constructed [8, 9]. The simulation models the Picon method, which is known for its ability to preserve the self-organized structure of each functional component. In the simulation, the number of layers was sequentially increased (e.g., 2, 4, 8, and 16), with each layer containing alternating components. Simultaneously, to account for field-of-view shifts inherent in the SEM imaging process, the initial position of each layer was systematically varied. The total number of pixels for each component was fixed to achieve concentrations of 5% and 10%. In this step, the sizes of the aggregate structures were changed to 125, 250, 500, 750, and 1,000. This methodology generates a comprehensive set of simulated images by treating the number of layers, the size of the aggregate structures, and their starting positions as variable parameters. Each simulation pattern was repeated ten times. To mimic the behavior of actual SEM images, where the backscattered electron intensity varies with the atomic number of the filler material, different grayscale values were assigned to the first and second components in the simulation. Subsequently, multifractal analysis was performed on three sets of data: the first component only, the second component only, and a combination of both components. An example of an image generated by the simulation is shown in Figure 1. The component separation results for the simulation images shown in Figures 1(c) and 1(d) are presented in Figure 2.

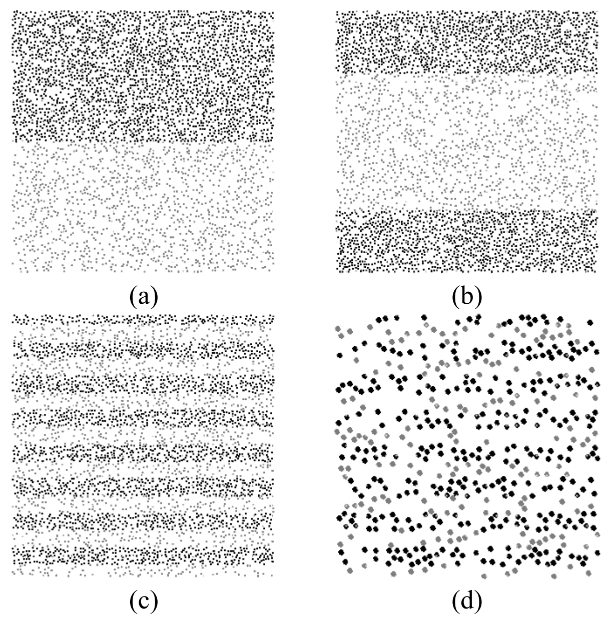

Figure 1. *Examples of images generated by simulation. Top row: examples of layer misalignment at layer number 2, (a) and (b). Bottom row: examples of aggregate structure size changes at layer number 16 (c) 125, and (d) 1,000)*

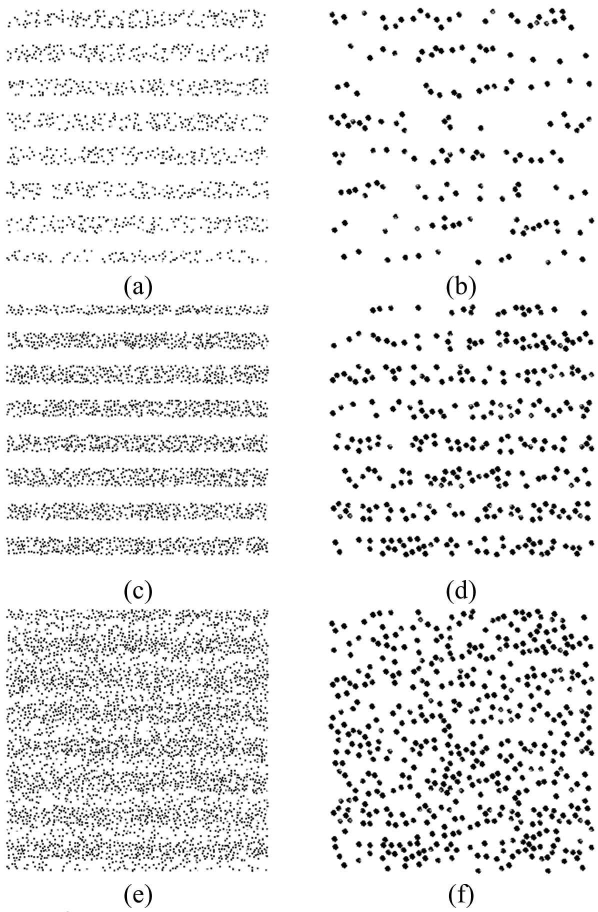

Figure 2. *Component-separated results. First row (a), (b): single component only (5%). Second row (c) and (d): two components (10%). Third row (e) and (f): composite result of the first and second components (15%).*

Results

A total of 3,300 simulation images comprising five aggregate sizes, six layer number patterns, and 11 layer shifts, with each combination repeated ten times, were subjected to multifractal analysis to obtain D_1 values. The resulting D_1 values are shown in Figure 3. Based on these D_1 values, the conditional entropy and mutual information were calculated using Equation (4); the results are shown in Figures 4 and 5. Each plot represents the average of 110 simulation images for the same aggregate size and number of layers. In Figure 3, the standard error is nearly zero and is not visible in the plots. In Figures 4 and 5, the standard errors are shown as error bars. Here, component 1 (5%) is denoted as X and component 2 (10%) is denoted as Y.

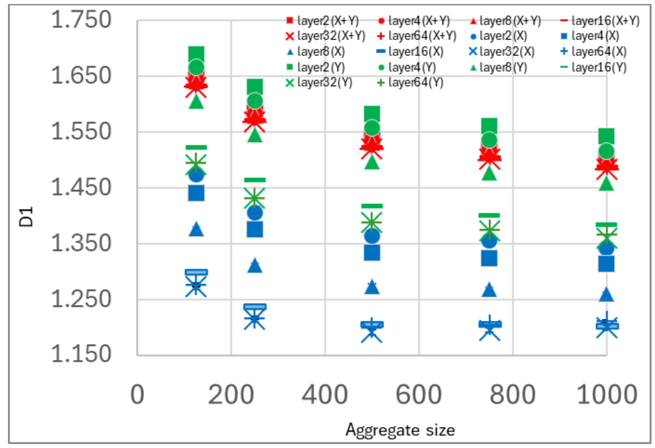

Figure 3. *D1 results averaged by aggregate size and layer count*

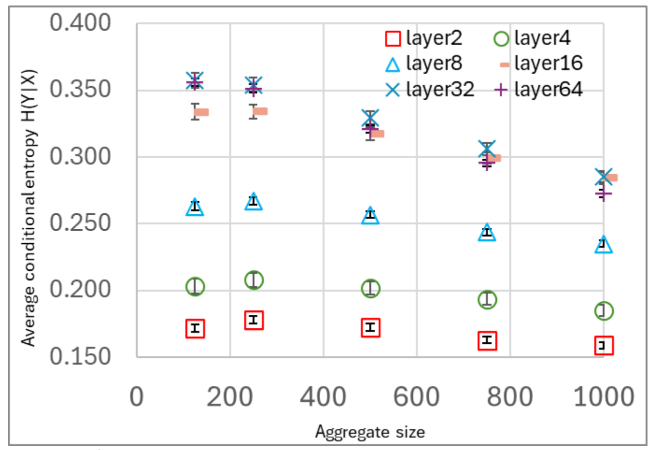

Figure 4. *Conditional entropy H(Y|X) averaged by aggregate size and layer number*

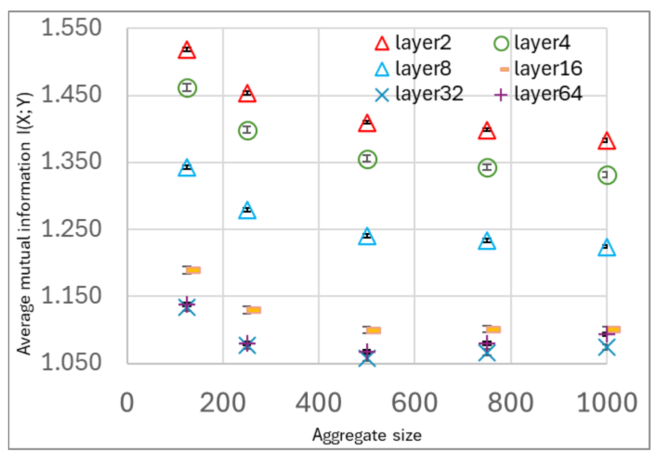

Figure 5. *Mutual information I(X;Y) averaged by aggregate size and layer number*

From Figures 3, 4, and 5, it is confirmed that the values of D_1, conditional probability, and mutual information for each pattern are sufficiently separate to distinguish between the patterns. The standard errors in the figures indicate that stable analysis values were obtained through the multifractal analysis, even with variations in the number of simulation trials and layer shifts.

Discussion

Mutual information (Figure 5), the focus of this study, was found to converge at approximately 1.100 as the number of layers increased. A larger value of mutual information $I(X;Y)$ reflects greater interaction between the two components. The conditional positional entropy $H(Y|X)$ indicates the degree of influence on one structure when another structure is determined. In this experiment, because $I(X;Y)$ is larger than $H(Y|X)$ and the overall arrangement of the structures composed of X and Y shows strong correlation and interaction, the individual structures of X and Y are not significantly affected by the other components.

As the number of layers increases, $I(X;Y)$ decreases, whereas $H(Y|X)$ increases. This occurs because adding more layers creates additional boundaries where the structures of different components meet. Near these boundaries, the arrangement of each component' structure is influenced by that of the other component; even if one structure can be identified, the uncertainty of the other structure increases, likely causing the increase in the value of $H(Y|X)$. This increased uncertainty means that the entropy of each component approaches independence, which is thought to result in a decrease in $I(X;Y)$.

Next, as the size of the aggregate structures constituting each component increased, both $I(X;Y)$ and $H(Y|X)$ decreased. In this simulation, the total number of colored pixels was fixed at 5% for the first component and 10% for the second component, relative to the entire image. Therefore, increasing the size of the aggregate structures that form the structure reduces the number of aggregated structures. In this case, positional entropy commonly decreases because there are fewer free structures that can be placed. This principle is similar, and it is believed that the overall entropy in the simulation image decreases as the number of aggregate structures decreases, resulting in lower values for both $I(X;Y)$ and $H(Y|X)$.

Thus, it was confirmed that multifractal analysis can accurately evaluate the interactions and state changes of structures with two or more components. Therefore, it is possible to quantitatively evaluate the mutual information of structures within an image using multifractal analysis.

In this study, simulation patterns were simplified to clarify the calculation and correspondence of mutual information using multifractal analysis. However, in naturally occurring structures with two or more components, the shapes of the individual structures of the first and second components are expected to differ significantly. In the future, we will increase the number of simulation patterns to further evaluate the mutual information.

Conclusion

Conventional multifractal analysis only evaluates the entire structure contained within an image. In this paper, we propose a simulation-based method to evaluate interactions when there are two or more constituent elements of a structure that self-organize through mutual interaction. The results of the simulation experiment demonstrate that the mutual information between the two components can be analyzed. Although this discussion is limited to D_1, there is scope for future consideration of other moment orders.

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Author Biography

Yoshihiro Sato received his Ph.D degree in computer science from Tokyo City University, Tokyo Japan, in 2022. Since 2023, he has been a lecturer with the Department of Design and Data Science at Tokyo City University. His current research areas include 3D data processing, 3D vision, and texture structure analysis.

Taito Ogiya received his M.E. degree in applied chemistry from Tokyo City University and is currently a doctoral student in advanced ceramics at Nagoya Institute of Technology. His research focuses on powder processing and analytical methodologies, particularly in particle-dispersed polymer composite systems.

Fumio Munakata is an emeritus professor at Tokyo City University. His research focuses on developing new materials and substances through a crystallochemical approach based on materials science perspectives, as well as constructing interfaces and microstructures for new material.

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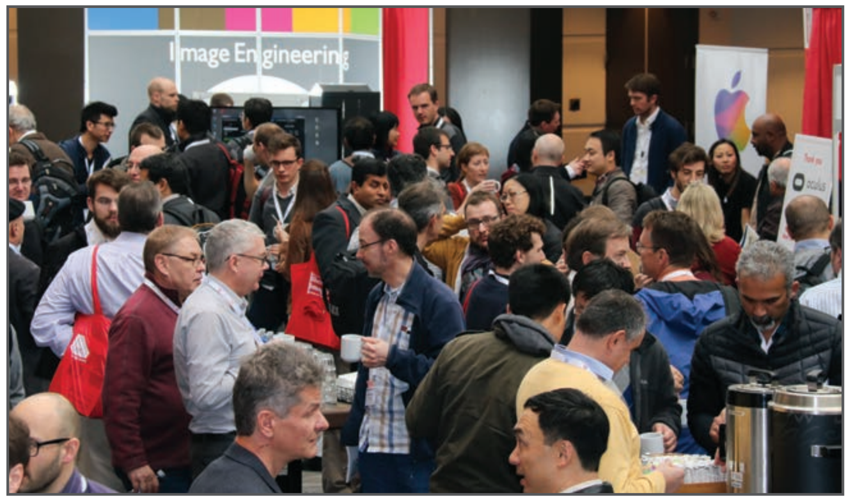

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