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Classification of in-situ RHEED Images Using Principal Component Analysis

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Abstract

Reflection High-Energy Electron Diffraction (RHEED) method, which is an analysis method of surface structure through electron beam irradiation, was adopted in Molecular Beam Epitaxy (MBE) and is widely used as an in-situ observation method for crystal growth. In particular, the RHEED pattern is dynamically changed according to crystal growth conditions such as surface temperature and material supply, so it is also important for securing reproducibility of growth. This RHEED pattern has been classified and recognized by the experimenter experience. We previously proposed to classify/recognize RHEED patterns using deep neural network using a convolutional neural network (CNN). However, since this method requires labeling of the acquired image, this also includes the experimenter know-how.

In this study, we investigated classification of RHEED pattern datasets without labeling by using the principal component analysis (PCA) method that reduces the dimension of the image. The coefficients were plotted by the components corresponding to the pattern. As a result, similar pattern images formed clusters, demonstrating that unsupervised learning is possible for the classification/recognition problem of the RHEED patterns.

1. Introduction

Reflection High-Energy Electron Diffraction (RHEED) is widely used because it allows in-situ observation of sample surface behavior during molecular beam epitaxy (MBE) growth[1,2]. However, RHEED pattern analysis relies on the accumulated know-how of researchers, and there is also a time limit. We reported classification of RHEED patterns by deep learning using a convolutional neural network (CNN)[3]. However, a large number of labeled image data are required, and the labeling is limited to "supervised learning" based on the judgment of researchers. The principal component analysis can be clustered according to the principal component of each data, and each can be classified. There is also a feature that is "unsupervised learning" that can summarize the features of data without the need for prior information such as labels [4,5].

In this paper, we report successful classification of RHEED images during MBE growth of GaAs by using the principal component analysis (PCA). The result paves the way toward unsupervised learning for the efficient classification/recognition of the RHEED patterns.

2. Experimental Methods

Crystal Growth and RHEED Image Collection

RHEED images were collected during MBE growth of GaAs on n-type GaAs(001) substrate. (2×4) pattern images were taken at a substrate temperature of 580°C and c(4×4) pattern images at 480°C with a pyrometer. Images were obtained from [110], [11-0], [-1-10], and [-110] directions with one rotation while rotating the substrate at 12 rpm (72°/s). (see Figure 1) The collected images were 1024×1024 pixel uncompressed 14 bit grayscale images. Exposure time of all collected images was 23 ms.

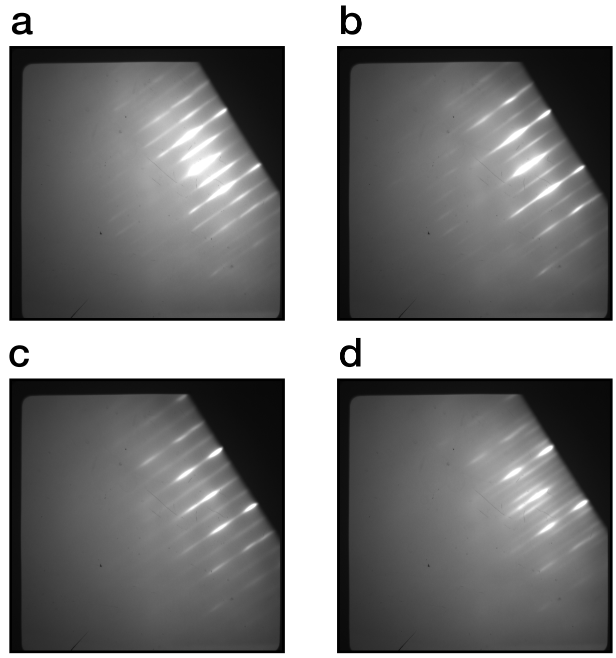

Fig. 1 RHEED image when electron beam incident direction were (a) [110] direction at 480 °C (×4 pattern), (b) [1-10] at 480 °C (×4 pattern), (c) [110] direction at 580 °C (×2 pattern), and (d) [1-10] at 580 °C (×4 pattern).

Dataset Preprocessing and Principal Component Analysis

As a data set, 340 images of (2x4) pattern and 111 images of c(4x4) pattern were used. As the dataset pre-processing, image resizing and vectorization were applied. Each 1024×1024 pixel image was resized to 512×512 pixel size, and then converted to a 1×262144 matrix for principal component analysis.

Software

We used python 3 (3.7.4) and scikit-learn module (0.22) for this work.

3. Results and Discussion

Figure 2 shows the four principal components extracted by the principal component analysis method. The extracted PCA components are shown in false color. From these images, it can be seen that PCA extracts features of bright lines and bright points of the RHEED pattern. Each image consists of a linear combination of principal components, the degree of which is determined by the coefficients. Therefore, by scatter plotting the relationship of each component with the size of the coefficients, the characteristics of the features of each image can be obtained in a reduced dimension.

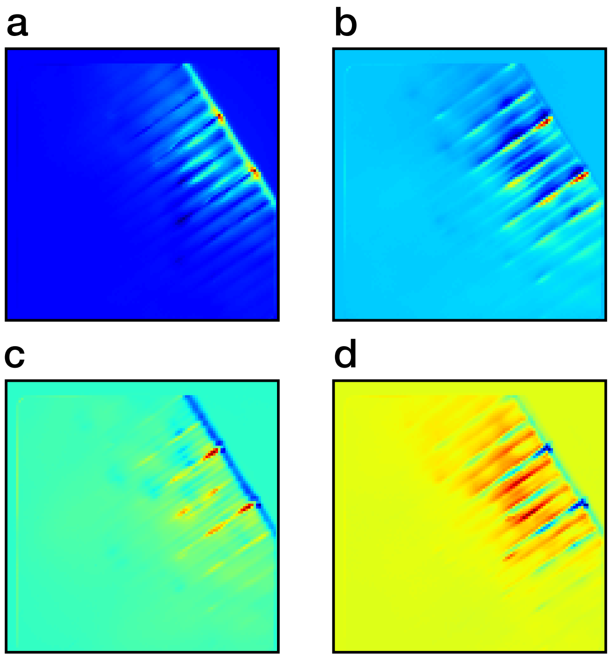

Fig. 2 Components of principal component analyzed RHEED images. (a) First component (component 1), (b) second component (component 2), (c) third component and, (d) fourth component.

Figure 3 is a scatter plot of the coefficients of the principal component 1 and that of the principal component 2. From this result, each RHEED image is divided by four domains. In the upper left part, there are RHEED images from the [110] direction of the c(4×4) pattern, and in the upper right part are RHEED images from the [1-10] direction of the c(4 ×4) pattern. In addition, there are RHEED images from the [110] direction of the (2×4) pattern in the lower left part, and RHEED images from the [1-10] direction of the (2×4) pattern in the lower right part. From these results, it can be seen that the PCA result of the image obtained when the substrate is rotated is (2×4) when formed on the bottom, and c(4×4) when formed on the top.

4. Conclusions

In this study, we performed the PCA on RHEED images when the GaAs surface restructure was (2 × 4) and c(4 × 4). The results indicated that the images successfully clustered according to the RHEED pattern without labeling. Although this model is still at a preliminary stage for application of PCA to RHEED images, it has the potential to introduce additional classification methods such as clustering classification and expand to more patterns. This study is also promising for the classification of the RHEED pattern based on the first “unsupervised learning”. The method developed here will be applied not only to classify simple GaAs plane patterns, but also to secure controllability of complex growth sequence such as quantum dot growth and GaAs growth on Si.

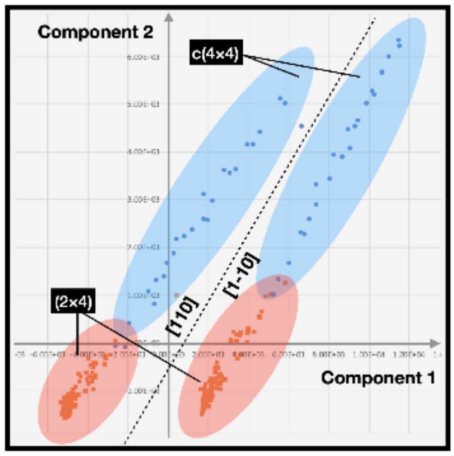

Fig. 3 Clustering of principal component analyzed RHEED patterns.

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