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Circular Fast Fourier Transform Application: A Useful Script for Fast Fourier Transform Data Analysis of High-resolution Transmission Electron Microscopy Image

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Transmission electron microscope (TEM) is an excellent tool for studying the structure and properties of nanostructured materials. As the development of C_s-corrected TEM, the direct analysis of atomic structures of nanostructured materials can be performed in the high-resolution transmission electron microscopy (HRTEM). Especially, fast Fourier transform (FFT) technique in image processing is very useful way to determine the crystal structure of HRTEM images in reciprocal space. To apply FFT technique in HRTEM analysis in more reasonable and friendly manner, we made a new circular region of interest (C-ROI) FFT script and tested it for several HRTEM analysis. Consequentially, it was proved that the new FFT application shows more quantitative and clearer results than conventional FFT script by removing the streaky artifacts in FFT pattern images. Finally, it is expected that the new FFT script gives great advantages for quantitative interpretation of HRTEM images of many nanostructured materials.

Key Words: Fourier transformation, Circular region of interest, High-resolution transmission electron microscopy, Electron crystallography, Image processing

INTRODUCTION

Transmission electron microscope (TEM) is an excellent analytical tool for studying the microstructures and properties of nanostructured materials. As the development of C_s-corrected TEM, which has a sub-Å spatial resolution, high-resolution transmission electron microscopy (HRTEM) imaging is able to analyze directly the atomic structure of nanostructured materials (Sato et al., 2009). Especially, a fast Fourier transform (FFT) technique in the image processing of HRTEM micrographs is one of the most fruitful methods for determining the crystal structures because it can be applied to the band-pass filtering, masking filtering and noise filtering in reciprocal space (Nihoul, 1992; Kim et al., 2006; Kogure et al., 2008). However, in the FFT technique, a region of interest (ROI) tool which is used to select the specific area is very important to carry out the quantitative image interpretation, as an example such as interface of grain boundary, atomically defected area, and well-aligned area with atomic arrangement (Yehliu et al., 2011). There are several useful and commercial programs for this technique such as CRISP, DigitalMicrograph™ (DM), EM-MENU, and iTEM (Zou et al., 1996; EM-MUNU 4.0 BASIC-Advanced TEM image processing package, 2005; Galicia et al., 2013; iTEM solutions, 2014). Among these programs, DM is the most user friendly program and has an advantage of huge community for developing useful scripts and database (Mitchell & Schaffer, 2005). However, the FFT analysis of HRTEM images can be used only for a rectangular ROI (R-ROI) in DM program. This R-ROI operation always produces vertical and

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horizontal streak lines around periodic reflection spots which have the structural information of HRTEM images. These streak lines are displayed due to the intrinsic feature of R-ROI. This problem could be solved by applying the circular ROI (C-ROI) which could be used for the improvement of the image processing and the analysis of the HRTEM images of nanostructured materials.
In this study, we developed and reported a new useful script for effective application of the FFT analysis in DM program.

MATERIALS AND METHODS

Fourier Transformation Method

The two-dimensional (2D) Fourier transform F(u,v) of a 2D function f(x,y) in the spatial domain (x,y) is defined as follows:

$$F(u,v) = \iint_{-\infty}^{\infty} f(x,y)e^{-j2\pi(ux+vy)}dxdy,$$

where u and v are spatial frequencies in x and y directions, respectively.
To apply the above equation to 2D data, we need 1) discretization of the above equation and 2) confinement of the spatial domain in finite region. For the discretization, we can use the well-known FFT. For practical calculation, we use 2D finite data in the spatial domain, which implies the multiplication of a certain type of a region function to confine the integral range for the Fourier transform. This confinement arises some artifacts in the Fourier domain owing to Fourier response of the region function. One of simple region functions is a 2D rectangular function which is defined as:

$$\mathrm{rect}(x,y) = \begin{cases} 1, & for\ |x| \leq 1/2 \text{ and } |y| \leq 1/2 \\ 0, & otherwise \end{cases}$$

with its Fourier transform given as the 2D sinc function:

$$\mathrm{sinc}(u,v) = \frac{\sin(\pi u)\sin(\pi v)}{\pi^2 uv}$$

Fig. 1A and B show the 2D color level display of a rectangular function and its Fourier response. The Fourier response of 2D rectangular functions shows streaks toward x- and y-axis directions, i.e., ringing side lobes that are the intrinsic feature of sinc function. As mentioned above, this streaking feature affects the resulting Fourier transform of finite 2D data.
To reduce this streaking noise, circular region function can be

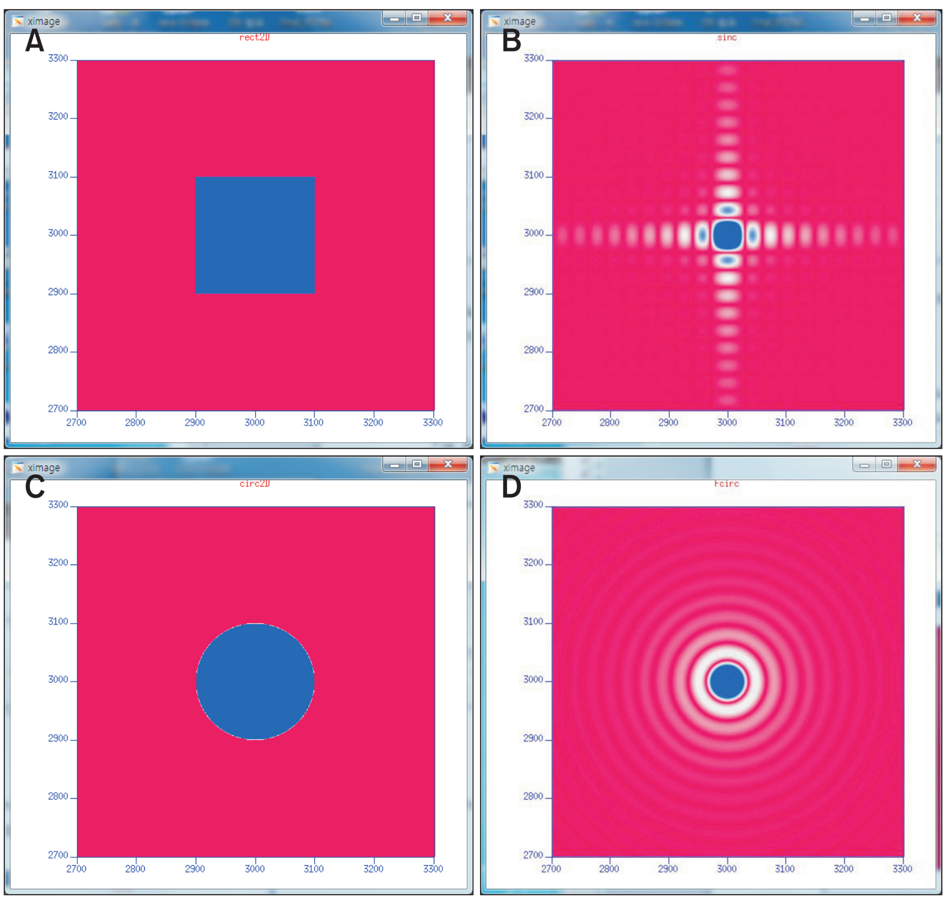

Fig. 1. Fig. 1A and B are the color level display of two-dimensional (2D) rectangular data and it's magnitude of fast Fourier transform (FFT). Fig. 1C and D are the color level display of the 2D circular data and it's magnitude of FFT.

used whose Fourier response is known to show no streaking events. The 2D circular region functions, i.e., a cylinder function, and its Fourier response are as follows:

$$\mathrm{circ}(x,y) = \begin{cases} 1, & for\ r \le 1 \\ 0, & otherwise \end{cases}, \qquad F(u,v) = J_1(2\pi\rho)/\rho\,,$$

where $r = \sqrt{x^2+y^2}$, $\rho = \sqrt{u^2+v^2}$, and J_1 is the first order Bessel function of the first kind.

Fig. 1C and D show the 2D color level display of the 2D circular region function and its Fourier response. The Fourier response of the 2D circular region shows no streaking events; however omnidirectional ringing side lobes are observed. These side lobes blur the image of the FFT of 2D finite data. Even though the quality of FFT result is degraded by this blurring, its omnidirectional features do not severely degrade the FFT image as the streaking events from the sinc function.

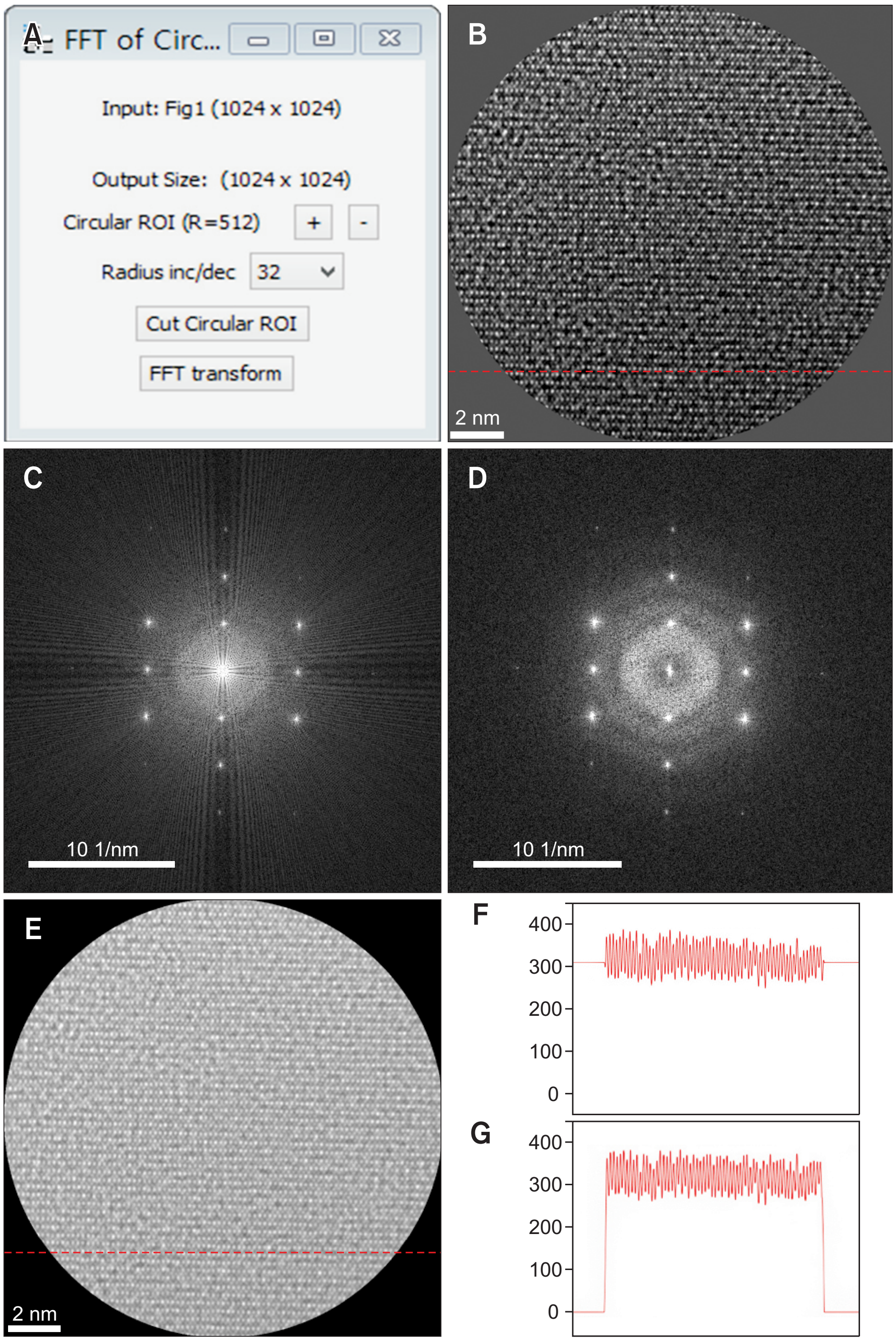

Fig. 2. Fig. 2A and B display the description of circular region of interest (C-ROI) tool for high-resolution transmission electron microscopy (HRTEM) image processing. Fig. 2C and D show correction of abnormal intensity distribution on fast Fourier transform (FFT) pattern extracted from HRTEM image by using C-ROI tool. Fig. 2C displays the abnormal fringe occurred due to zero intensity distribution outside ROI (E) and these abnormal fringe can be corrected applying the averaged intensity to the region (D). Fig. 2F and G show the intensity profile obtained from Fig. 2B and E, respectively.

Circular ROI Application

Fig. 2A and B show the main display of DM script tool for C-ROI FFT that we have developed. Firstly, this script reads an HRTEM image which will be assigned the C-ROI. Output size of C-ROI is set to default size (256×256). The size selection of specific C-ROI can be controlled by the click of the size controlling button after radius change step is determined as shown in Fig. 2A. For an FFT application, the ROI dimensions should be selected by integral power of two in the previous version of DM program, whereas the upper version of 2.0.0 allows to select the ROI region for non-integral power of two. Therefore, C-ROI can be also adjusted with detailed range. Finally, the desired C-ROI can be formed by pressing the cut C-ROI button. Additionally, Fig. 2C and D show two different FFT patterns extracted from HRTEM image (Fig. 2B). Fig. 2C shows that abnormal fringes are included in FFT pattern. These abnormal fringes are produced due to the consideration of inappropriate direct current (DC) term, in FFT calculation. The DC term is the 0 Hz term and is equivalent to the average of input signals. The common FFT calculates the input signal as the sum of sinusoidal functions except the DC term. So, the inappropriate DC term may cause a severe distortion in the Fourier domain. Fig. 2E shows the signal windowed simply by the circular region; the intensity outside C-ROI was zeroed, whereas Fig. 2B shows the one windowed considering the DC term; the intensity outside of C-ROI was replaced the average of inside C-ROI. Fig. 2F and G show the intensity profiles along straight lines (red dashed in Fig. 2B and E). As shown in the diagonal intensity profiles, the zero level in Fig. 2B is consistent with sinusoidal functions due to a proper DC term. In contrast, the zero level in Fig. 2D is severely biased and inconsistent with the sinusoidal functions due to an improper DC term, which is expect to cause the low frequency distortion in Fourier domain. Therefore, the intensity outside of C-ROI are set automatically to the average of inside C-ROI data and applied onto FFT calculation (Fig. 2C).

RESULTS AND DISCUSSION

To evaluate the usefulness of the new C-ROI tool, a few of experimental HRTEM images were examined and processed. First application result for HRTEM image of GaN thin film grown on sapphire substrate was shown in Fig. 3. Fig. 3A displays the HRTEM image for the interface region of GaN (upper layer) and Al_2O_3 (lower layer). Fig. 3B and C are the FFT patterns extracted by C-ROI and R-ROI tool, respectively. It is demonstrated that the the peak positions in each patterns are more easily found in the FFT pattern extracted by C-ROI tool. Especially, two reflections of $(006)_{Al_2O_3}$ and $(002)_{GaN}$ are more clearly distinguished in the FFT pattern extracted by C-ROI tool than those by R-ROI tool. It can be considered that this useful effect occurrs by removing the streaking formed by R-ROI. Therefore, the FFT patterns extracted by C-ROI tool look much better for publication of research paper. Second test result for HRTEM image of a $Cu(In_xGa_{X-1})Se_2$ (CIGS) solar cell structure was shown in Fig. 4. It displays the interface region of CIGS layer (left side, ①), CdS layer (right side, ②), and their interface region (③). Fig. 4B-D are FFT patterns extracted by R-ROI tool from CIGS layer, CdS layer, and interface region, respectively. Fig. 4E is FFT pattern extracted by C-ROI tool from interface region. As shown in Fig. 4B and C, the FFT patterns from two layer structures are very similar because the d-spacing values of all reflections in $[110]_{CIGS}$ and $[0001]_{CdS}$ are very closed within about 1.4%. There are several streaking related to some defect in Fig. 4C. These streaking also need to be analyzed in interface region of two layer structure. However, it seems to be included more streaking patterns in Fig. 4D (red arrow) which is converted

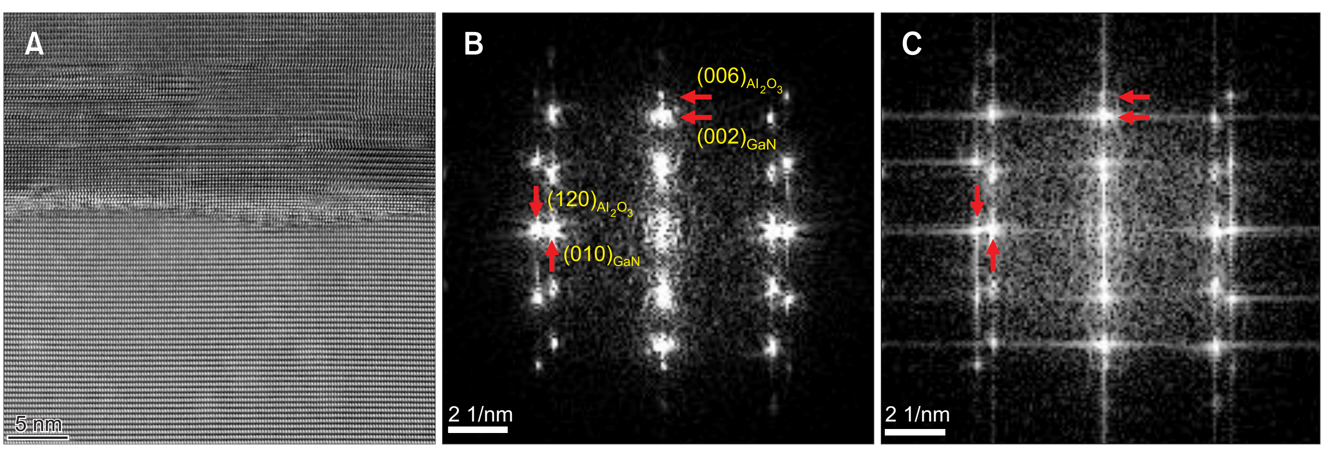

Fig. 3. Application example of circular region of interest (C-ROI) tool. (A) High-resolution transmission electron microscopy image of GaN grown on Al_2O_3 substrate. (B) Fast Fourier transform (FFT) pattern extracted from Fig. 3A by applying the C-ROI. (C) FFT pattern extracted from Fig. 3A by applying the rectangular ROI (R-ROI).

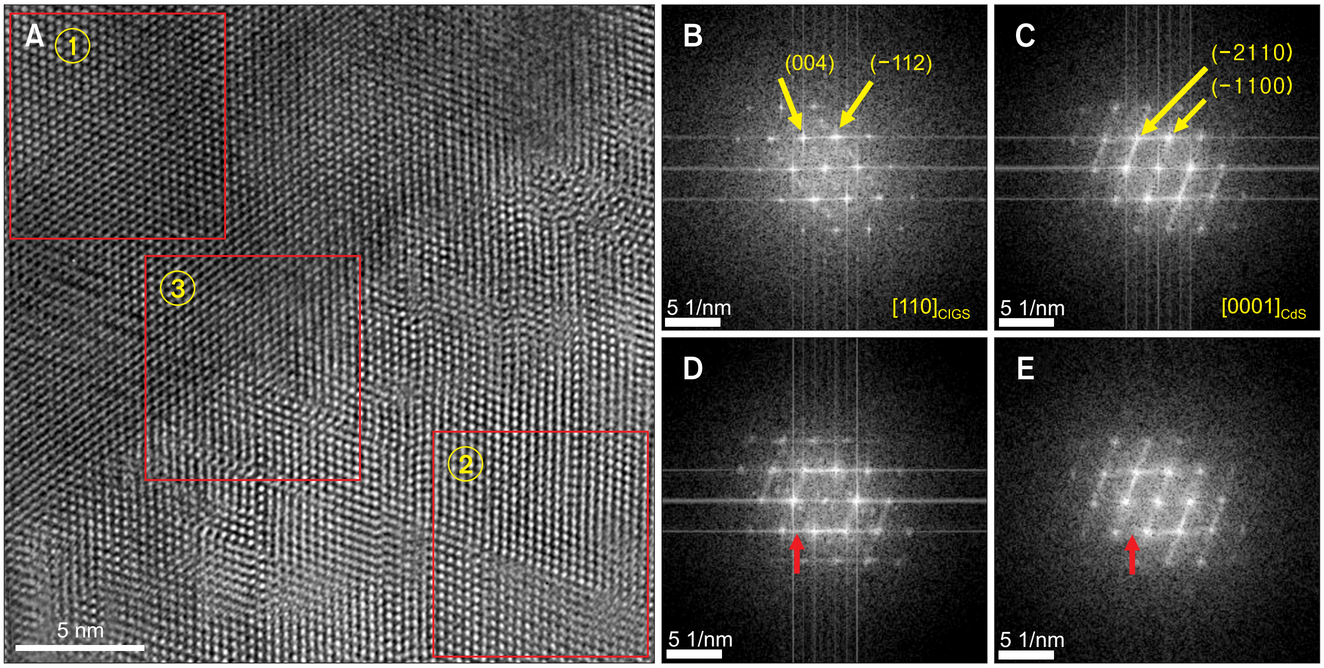

Fig. 4. (A) Application example of circular region of interest (C-ROI) tool for $Cu(In_xGa_{x-1})Se_2$ (CIGS) solar cell structure. Fig. 4B-D indicate the fast Fourier transform (FFT) patterns extracted from three areas of high-resolution transmission electron microscopy image by applying the rectangular ROI (R-ROI). Fig. E is the FFT pattern extracted by applying the C-ROI.

by R-ROI tool. This confusion can be solved by using C-ROI tool as shown in Fig. 4E.

From above investigation, the C-ROI tool can be useful for determining the crystal structure and analyzing the defect structure exactly. Moreover, its FFT patterns can be helpful for readers to understand the paper.

CONCLUSIONS

In this technical note, the usefulness of the C-ROI script for structure analysis of HRTEM images was addressed through a few simple image processing experiments. This script allows us to display the correct reciprocal space without unnecessary streaking lines and to extract the fine structural information using additional image processing steps. Therefore, it is expected that this script can be very useful tool for the analysis of many defect and interface of nanostructured materials in atomic scale. This script can be obtained by contacting corresponding author (Kim J. -G., jjintta@kbsi.re.kr) after the final modification.

CONFLICT OF INTEREST

No potential conflict of interest relevant to this article was reported.

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