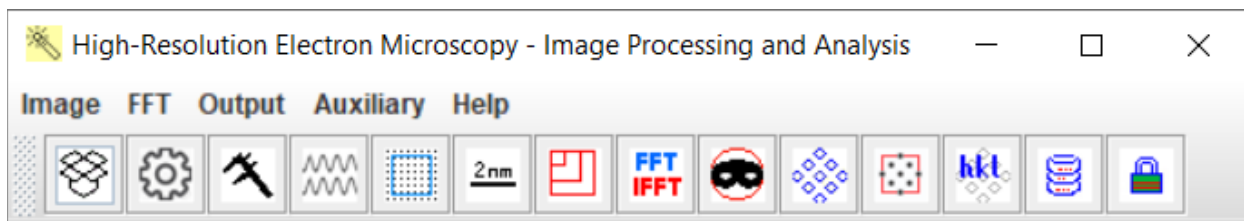


***LANDYNE<sup>+</sup>***

# **User Manual**

*High-Resolution Electron Microscopy  
Image Processing and Analysis  
Part I: General Application*

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## Highlights

- Convenient tool for selecting area, resizing, and rotation of experimental images.
- Measure the scale bar and transfer to selected image, FFT pattern or IFFT image.
- A series of intensity profiles on HREM images can be retrieved and compared.
- Square and Inscribed circle of an arbitrary length for FFT.
- Varies of masks are available for inversed FFT images.
- Histogram equivalent contrast algorithms for enhancement of the IFFT image.
- Tool for adding a scale bar and indices for FFT pattern.

## 1. Introduction

### 1.1 Landyne suite

Landyne suite is a software package developed by Dr. X.-Z. Li for electron diffraction simulation and crystallography analysis since 2010. The software package can be used as a research tool as well as a teaching aid. The current version includes fifteen stand-alone software components [1-13]. Each of them was designed for one topic of application in simulation, analysis, or data processing. A launcher is available for the software suite, a tool to conveniently access all software components. The executable codes, user manuals, and a set of crystal structural data are available on the author's webpage <https://landyne.com> and <https://www.unl.edu/ncmn-enif/xzli/computer-programs>. Table 1 shows the components in the Landyne software suites and its extension Landyne<sup>+</sup> for transmission electron microscopy.

Table 1. The components in the Landyne and Landyne<sup>+</sup> software suites

Software	Description of components in the Landyne suite	Reference
PTELS	Periodic table of the elements for the Landyne suite	[2]
SVAT	Structural viewer and analytical tool including atom cluster and layer.	[3]
SPICA	Stereographic projection for interactive crystallographic analysis.	[4]
SAED	Simulation and analysis of electron diffraction (spot) patterns.	[5]
PCED	Simulation of PCED (ring) patterns and phase identification.	[6]
QSAED	Processing, quantification, and analysis of SAED (spot) patterns.	[7]
QPCED	Processing, quantification, and analysis of SAED (ring) patterns.	[8]
HOLZ	Simulation of HOLZ pattern including dynamical correction.	[9]
SMART	Simulation and measurement of rocking curve for crystal thickness.	[10]
SAKI	Simulation and analysis of Kikuchi lines and double diffraction effect.	[11]
TEMUC	Lattice determination of unknown structure in TEM/ED experiments.	[12]
ESPOT <sup>+</sup>	Electrostatic potential maps derived from electron diffraction patterns.	[10]
CTFscope <sup>+</sup>	CTF simulation and visualization for conventional and AC-TEM.	[13]
EMIPA <sup>+</sup>	HREM image processing and analysis: a general application.	[10]
EMCIP <sup>+</sup>	HREM image processing and analysis: crystallographic image processing.	[10]

### 1.2 Image processing and analysis

Electron microscope image processing and analysis is divided into two parts, one for general purposes and the other focusing on crystallographic image processing. The core of image processing is the Fast Fourier Transform (FFT) technique.

An FFT is an algorithm that computes the discrete Fourier transform (DFT) of a sequence or its inverse (IDFT). James Cooley and John Tukey independently rediscovered these earlier algorithms. They published a more general FFT in 1965 that is applicable when  $N$  is composite and not necessarily a power of 2, as well as analyzing the  $O(N \log N)$  scaling. Bluestein's FFT algorithm (1968), commonly called the chirp-z algorithm (1969), is a fast Fourier transform (FFT) algorithm that computes the discrete Fourier transform (DFT) of arbitrary sizes (including prime sizes) by re-expressing the DFT as a linear convolution. Bluestein's FFT algorithm was adopted for DFT in the electron microscope image processing and analysis.

In EMIPA, the experimental image can be resized and rotated image. Part of the image can be selected and saved with a new scale bar. A series of linear profiles can be retrieved. Typical filters are available for FFT and IFFT processing. The indices can be added for the FFT pattern with an auxiliary tool. Histogram of the IFFT image can be optimized.

In EMCIP, the experimental image can be enhanced with crystallographic image processing. A contrast transfer function is included for correcting the crystallographic phase in the FFT data. Experimental electron diffraction intensities can be used to replace diffraction intensities in the FFT data. The image can be processed using pre-built the 17 plane symmetry groups and displayed in the pseudo-color image and contour map.

## 2. Design and features

### 2.1 Graphic design

EMIPA graphic user interface (GUI) was written in Java Swing. Figure 1 shows the main panel with a drop-down menu and a graphic toolbar menu. The menu includes i) Image (loading image, resizing\rotating image, a caliper, a tool for line profile and exit) and ii) FFT (FFT area, FFT process, Masks and Inverse FFT); iii) Output (ROI, FFT indices, scale bar); v) Option (display option and PPI parameter); vi) Auxiliary (hide the toolbar, look and feel); vii) Help (current drive-SN, version and updated info). The toolbar menu includes the most frequent operations for the dropdown menu.

### 2.2 Function features

EMIPA provides basic tools to prepare the EM images for presentation or publication,

- i) The image can be easily shifted, a selected spot locates the center of the panel by clicking the mouse right button and resizes and rotates while the image spot on the panel center is kept.
- ii) The scale bar in the original image can be measured, and the length of a new scale bar can be reset and repositioned to the selected area of the image. The image can be saved to a file in the JPG, PNG, and TIFF formats.
- iii) A series of intensity profiles can be generated from the selected lines on the image. The array of intensity peaks on the image can be retrieved.

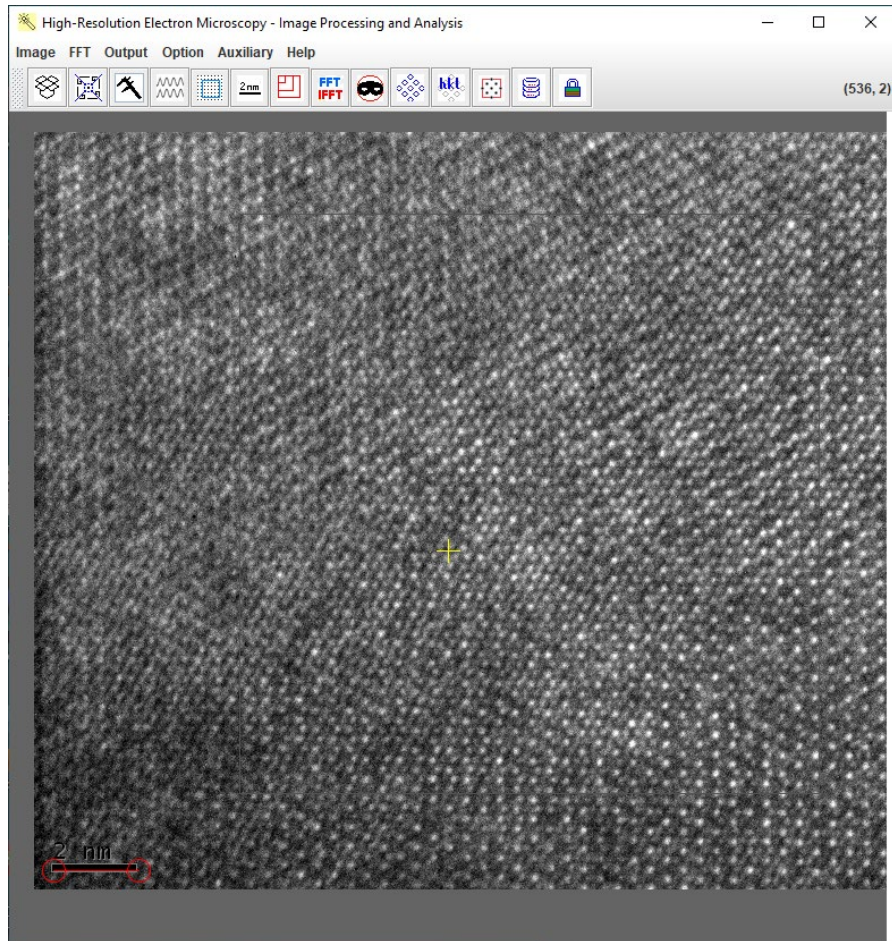


Figure 1. The GUI of EMIPA with a drop-down menu and a toolbar menu. The panel shows an electron microscopy image as an example.

EMIPA provides a general FFT/IFFT processing procedure to enhance the EM image,

- i) A square area with arbitrary (not bound to the power-of-2) lengths can be selected. A circular area inside the square area can be used to improve the FFT pattern, on which the streak lines with a square area will be dramatically reduced with a circular area. The circular areas for the FFT patterns are especially suitable for the electron microscopy images of the nanoparticles.
- ii) After calibrating the scale bar in the original image and the scale-bar can be added to the FFT patterns. *Indexing can be added on* with an auxiliary tool. The indices can be added to the FFT pattern with an auxiliary tool. The FFT patterns can be saved to a file in TIFF format.
- iii) Various filters are provided for inverted-FFT transformation. The filters include an aperture-like inside circle, an outside circle, a circular band, a strip passing the incident beam, a pair of disks in mirror symmetry, and an array of disks. The inverted-FFT image can be shown in pseudo-color and posted back to the original image.
- iv) The array-of-disks filter can be used for the two basic vectors of the FFT pattern, which is needed by adding indices on the FFT pattern, and a unit cell of the structure may be added on the inverted-FFT image. Figure 2 shows the FFT/ IFFT panel with an example pattern

- that overlays an aperture-like circular filter. Various dialogues are provided for input, output, and operations. We will illustrate the usage of these dialogues in the next section.
- v) A histogram tool can be used for contrast optimization of the IFFT image.

### 3. Instructions for use

A license is required for using EMIPA. For an unlicensed user, a license file dialogue will show in Figure 2. Click Explore for evaluation with a demo file or Volveré as “I will be back” in Spanish.

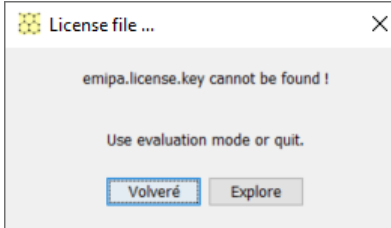


Figure 2. The license dialogue appears when the license file is missing. In this case, users may select the Explore button and load the emipa\_demo.tif for evaluation purpose.

#### 3.1 Load HREM images and basic processing

HREM images can be loaded by using the drag-drop method or the hierarchical file system. If the image is in the experiments folder, users may use the file system directly to load the image; otherwise, the drag-drop method is more convenient.

The loaded images can be adjusted image center to the panel center by clicking mouse right button, can be resized and rotated by using the Image Operation dialogue.

Figure 3 shows the image operation tools, (a) caliper, (b) adjustment, (c) scale bar, and (d) ROI. The scale bar of the image needs to be measured by the caliper so the length of the image is calibrated. The image adjustment dialogue for contrast inverse, shifting, resizing, and rotation of an image.

EMIPA can be used to prepare images for EMCIP from experimental HRTEM images. EMCIP focuses on crystallographic image processing but does not include these basic processing functions.

#### 3.2 Select a part of image for output of an image

The contrast of the image can be inverted, and a selected spot on the image can be easily shifted to the panel center by mouse pointer and right button click. The image spot in the panel center will keep when the image is resized and rotated.

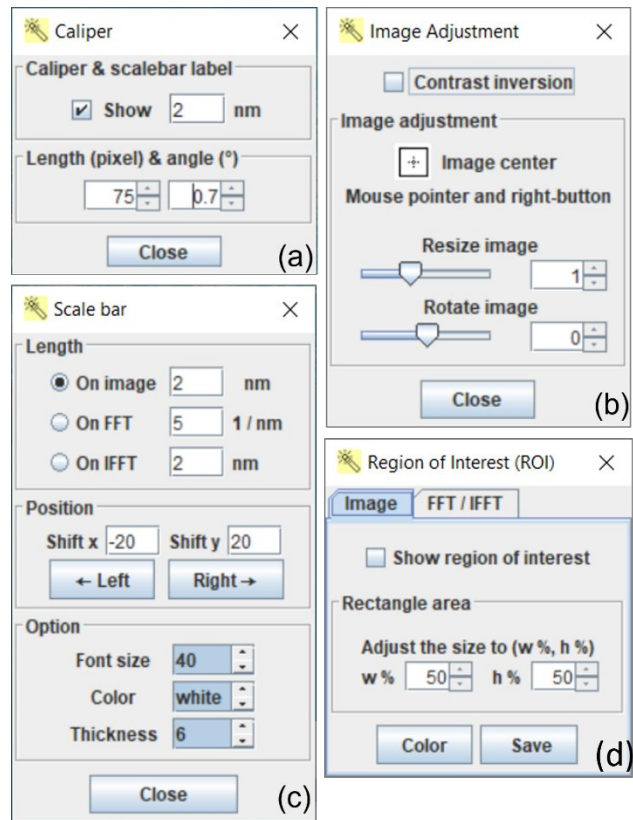


Figure 3. The image operation tools (a) caliper, (b) adjustment, (c) scale bar, and (d) ROI.

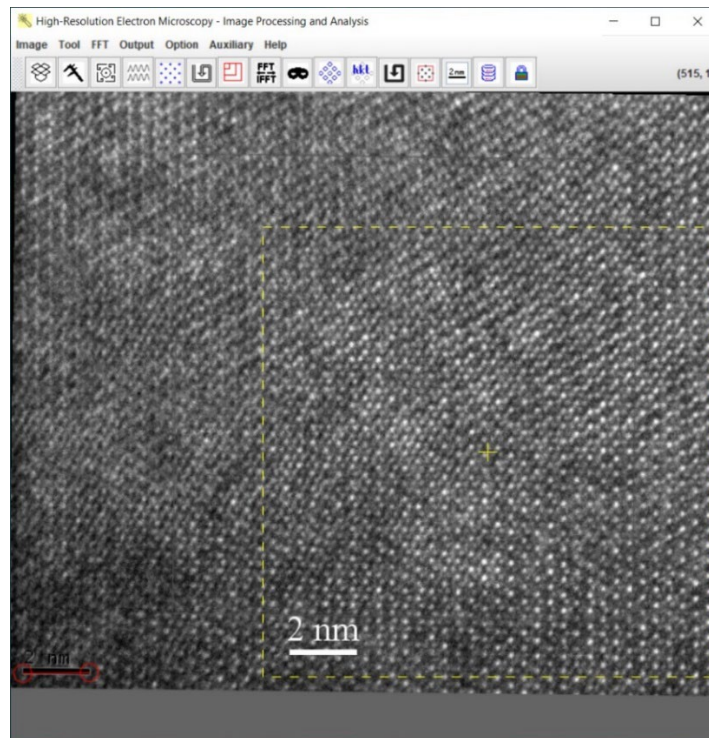


Figure 4. The image is slightly rotated for alignment and calibration on the scale bar. An area is selected and ready for output.

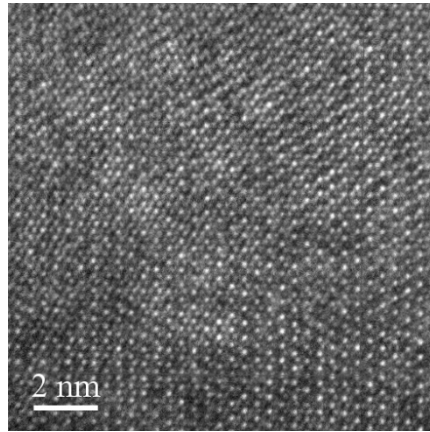


Figure 5. An area is retrieved from Figure 4 and saved as a TIFF image.

As an example, the image in Figure 1 is rotated to make the line image spots parallel to the vertical edge, and an area is marked with the RIO. The scale bar is measured for image length calibration, and a new scale bar is added to the ROI. The selected area is saved as a TIFF image, which is shown in Figure 5.

### 3.3 Retrieval of series of line profiles and position

HREM images in Figures 6 and 7 were taken in the  $Mn_2RuSn$  Heusler alloy [14]. A series of intensity profiles of an image can be compared or measured. The line profile dialog box is shown in Figure 6(a), three lines in blue, green, and red are marked on an image, and the corresponding line-scan profiles are in Figure 6 (b) and (c).

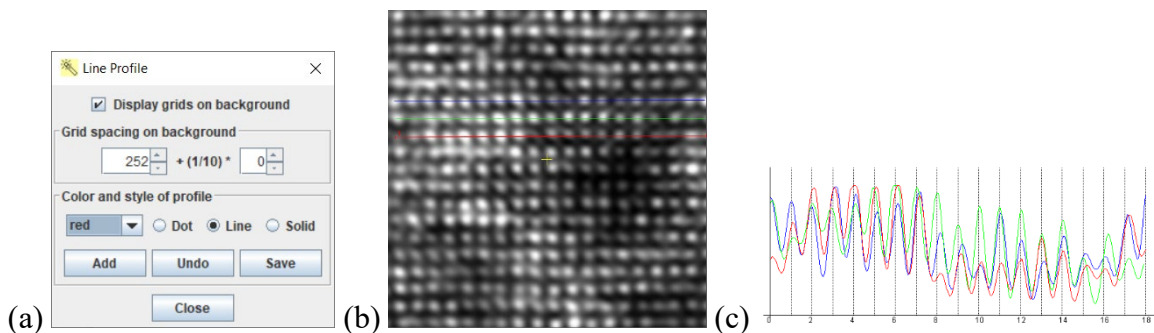


Figure 6. (a) The line profile analysis on an image and (b) the line-scan profile. HREM image was taken in the  $Mn_2RuSn$  Heusler alloy.

### 3.4 FFT and IFFT processing

The square area with its edge length in arbitrary length (not bound to the power of 2) will be used for FFT transformation. The length can be determined by holding the mouse's left button and dragging the mouse pointer. The location of the area can be replaced by clicking the mouse left button. A circular area within the square area is an option for FFT transformation. Compared with the square areas, the circular areas will reduce the FFT patterns' streak lines. The circular areas for



the FFT patterns are especially suitable for the electron microscopy images of the nanoparticles. Figure 7 shows the FFT area dialog box.

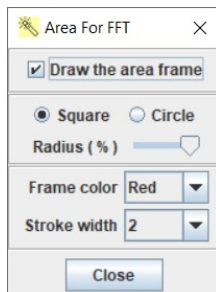


Figure 7. The FFT area selection dialogue.

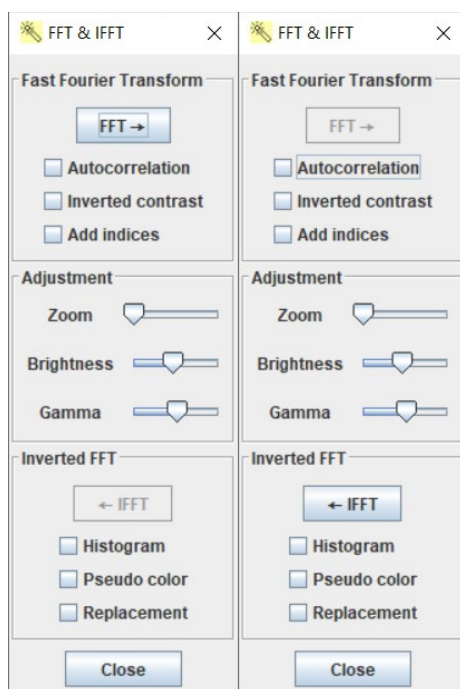


Figure 8. The FFT and IFFT dialogue. Adjustment operations are available.

Figure 8 shows the FFT and IFFT dialogue. The autocorrelation, inverted contrast, and indices are implemented on the FFT panel; the unit-cell display, pseudo-color, and replacement are implemented on the IFFT panel. The zoom, brightness, and gamma adjustment operations work on both the FFT and IFFT panels. It is obvious that the FFT operation must be carried out before the IFFT operation. The FFT operation can also be re-executed after the IFFT operation has been executed. The selected area is on the area in the original HREM image. Figure 9 is an FFT pattern obtained from the HREM image in Figure 1 and a circular mask on the FFT pattern.

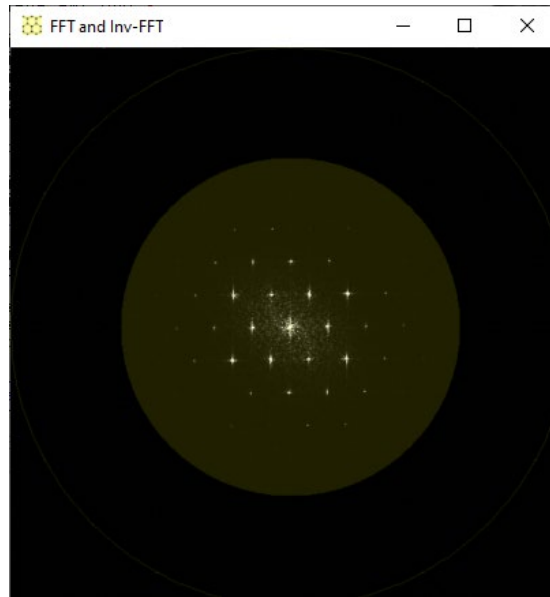


Figure 9. The FFT pattern from the HREM image in Figure 1 and a circular mask.

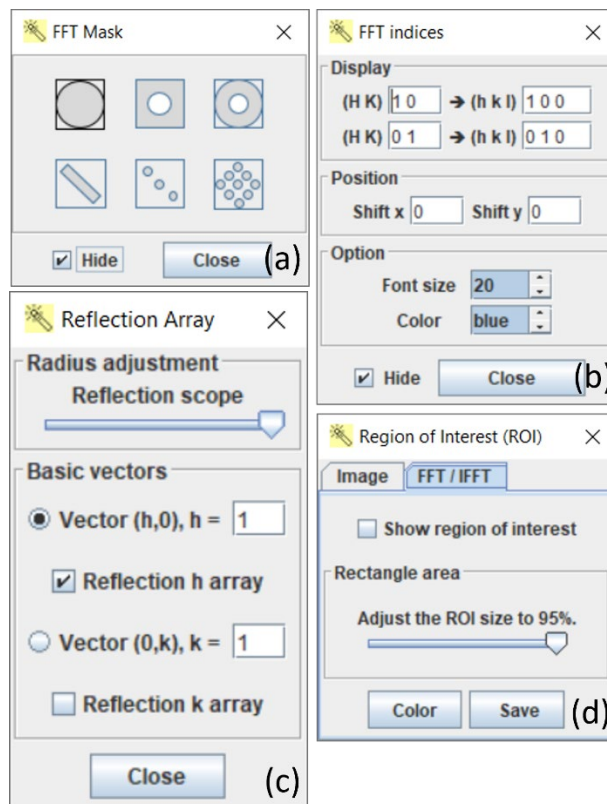


Figure 10. (a) Various FFT masks for the IFFT operation and two basic vectors, (b) Indices of the FFT pattern, (c) construction of the 2-dimensional reflection mask, and (d) The Region of Interest dialogues for image and FFT/IFFT panels.

The IFFT operation needs an FFT mask after the FFT operation. Six FFT masks are shown in Figure 10(a). The sizes can be adjusted with the mouse wheel or the arrow keys, and the positions

of the marks can be defined with the mouse pointer. The default choice is the first one – a circular aperture. The last one - an array mask can be chosen as a 2-dimensional array defined by two basic vectors, as shown in Figure 10(c).

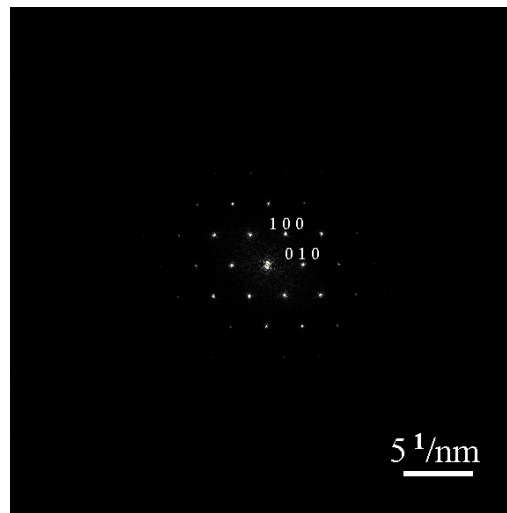


Figure 11. The output of the FFT pattern with two basic indices and a scale bar.

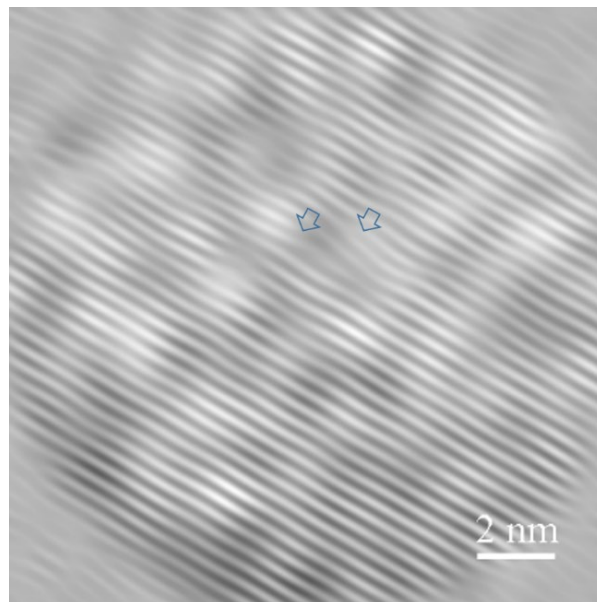


Figure 12. The IFFT pattern by using a mask with a pair of reflections. Two dislocations cores are pointed out by arrowheads.

### *3.5 Indices and a scaling bar on FFT pattern and a scaling bar on IFFT image*

The two basic vectors can be more accurately defined by enlarging the FFT panel and using the reflections' positions with higher indexes. They also provide that base for the positions of the indices in Figure 10(b).

An example of the FFT output with indices and a scale bar is shown in Figure 11. An example of the IFFT image using a pair of reflections is shown in Figure 12. Two dislocations are revealed clearly and marked with arrowheads in the output.

### 3.6 Crystalline phase identification with HRTEM image

Supposed an HRTEM image was taken from a crystalline phase which is a one of several possible phases. 1. calibration the scale bar with the Caliper tool; 2. Selected an area for FFT and obtain the FFT pattern; 3. add the scale bar on the FFT pattern; 4. Use SAED6 to find the zone axis and the crystalline phase.

### 3.7 Histogram and contrast adjustment

A histogram tool is available to process the IFFT image. Contrast adjustment can be done using equalization algorithm. Figure 13 shows the interface of the histogram tool. Figure 14 shows the IFFT image and processed image with contract enhancement.

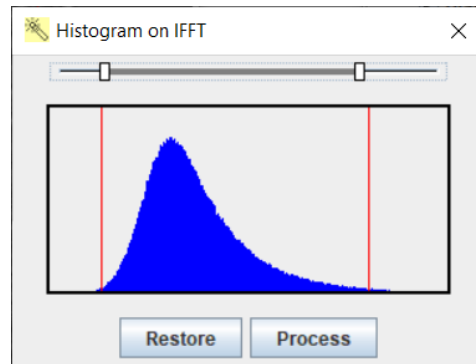


Figure 13. Histogram of the IFFT image and contrast adjustment with equalization algorithm.

### 3.8 Output of FFT pattern and IFFT images

The dialog boxes of region-of-interest (ROI) are shown in Figure 3(d) and Figure 10(d). Users may define the size and location of the ROI on the original image, the FFT pattern, and the IFFT image. The scale bar can be put up when the ROI is selected. Before adding the renewed scale bar on the image or the FFT pattern for output, the original image's scale bar must be calibrated using the Caliper. The image or FFT pattern within ROI can be saved in TIFF, PNG, JPEG, and GIF format.

## 4. Examples

### 4.1 HREM of $Fe_5CoTi$ alloy [15]

A TEM study has been carried out on crystal structures in the rare-earth-free intermetallic alloys,  $Fe_{3+x}Co_{3-x}Ti_2$  ( $x = 0, 1, 2, 3$ ). These alloys have been demonstrated to have potentially high magnetic anisotropy. In these alloys, the main intermetallic compound was recently reported as a new hexagonal phase with a space group of P-6m2. The present study reveals that the main compound belongs to Laves C14 variant surrounded by  $\alpha$ -Fe type crystal as the secondary phase

in the  $\text{Fe}_{3+x}\text{Co}_{3-x}\text{Ti}_2$  ( $x = 0, 1, 2, 3$ ) alloys, in agreement with the Fe-Ti and Fe-Co-Ti phase diagrams. The SAED, EDS, HRTEM, and XRD techniques have been carried out to characterize the intermetallic compounds in the  $\text{Fe}_{3+x}\text{Co}_{3-x}\text{Ti}_2$  ( $x = 0, 1, 2, 3$ ) alloys.

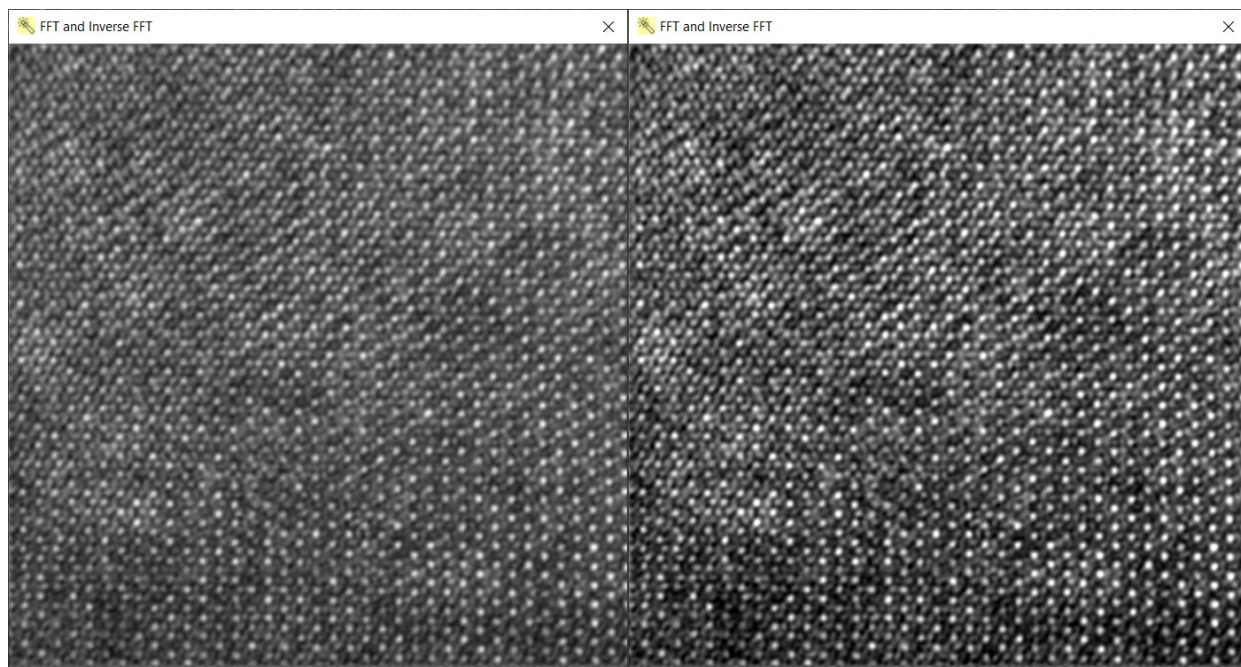


Figure 14. IFFT image and processed image with contrast enhancement.

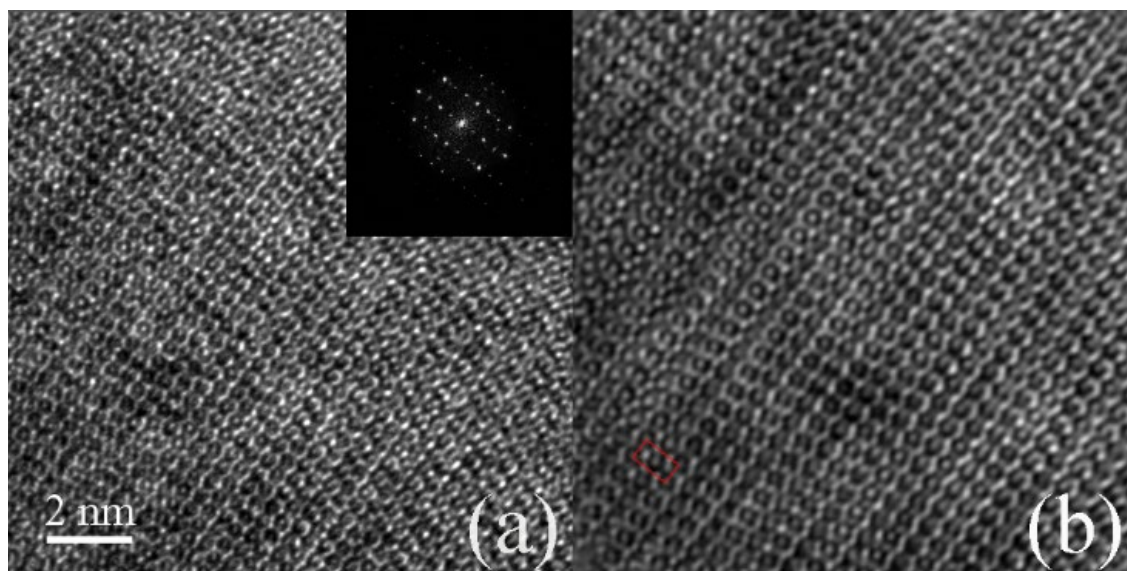


Figure 15. (a) HREM image and (b) the IFFT processing image of the main compound in the  $\text{Fe}_3\text{Co}_3\text{Ti}_2$  alloy

Figure 15 shows (a) the experimental HREM image of the main compound in the  $\text{Fe}_3\text{Co}_3\text{Ti}_2$  alloy, an FFT pattern is given as inset, and (b) the inverse FFT processing image, in which a unit cell is outlined. The relation between an HREM image and the projected crystal potential can be quite complex if the crystal is thick. In order to obtain an image which can be directly interpreted in

terms of projected potential, the crystals should be well aligned, thin enough to be close to weak-phase-objects and the defocus value for the objective lens should be optimal, *i.e.*, at the Scherzer defocus. The HREM image in Figure 15(b) can be directly interpreted with the structural projection and the electrostatic potential map of the Laves C14 variant.

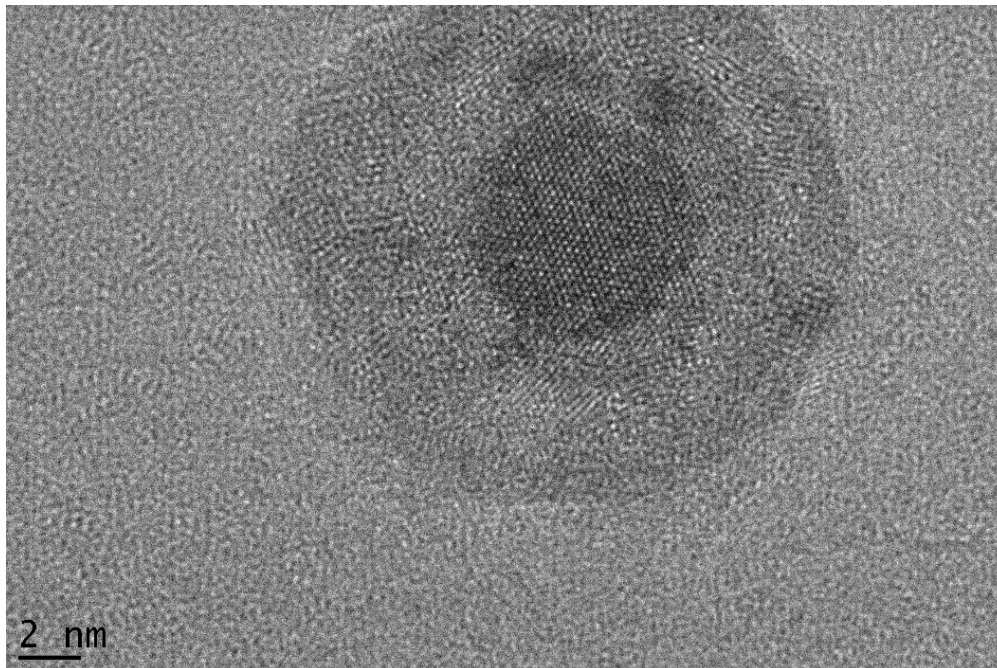


Figure 16. A high-resolution electron microscopy image of a CoSi particle. The crystal is nearly hexagonal, and the size of the crystal is about 10 nm.

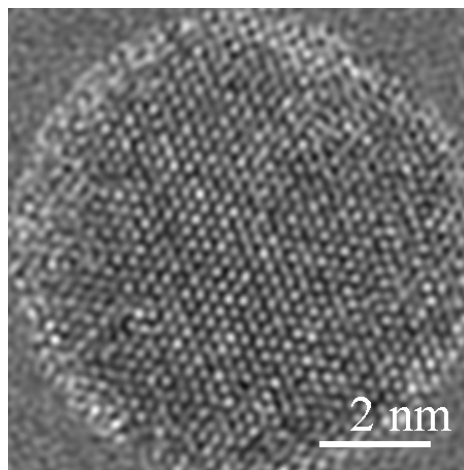


Figure 17. IFFT image of a CoSi particle. The crystal is nearly hexagonal, and the size of the crystal is about 10 nm.

#### 4.2 FFT pattern of nanoparticles

The nanoparticles were prepared by the cluster deposition method in Prof. Sellmyer's group at the University of Nebraska, Lincoln. An atomic CoSi vapor produced using direct-current plasma sputtering is condensed in a cooled inert-gas atmosphere to form nanoparticles in the gas-

aggregation chamber. Carbon-coated Cu grids with low nanoparticle coverage were used for TEM measurements. Figure 16 shows an HREM image of a CoSi particle. The crystal is nearly hexagonal, and the size of the crystal is about 10 nm. The HREM image was enhanced in the IFFT image with a mask with an array of reflections by using EMIPA, as shown in Figure 17.

#### 4.3 Study of carbon fiber

Carbon fiber, the strongest commercially available structural material today, is a lightweight reinforcement used to strengthen polymer composites. Scientists seek to strengthen advanced, high-performance fibers using exceptionally strong and fatigue-resistant carbon nanotubes, sheets of one-atom-thick carbon molecules shaped into hollow cylinders.

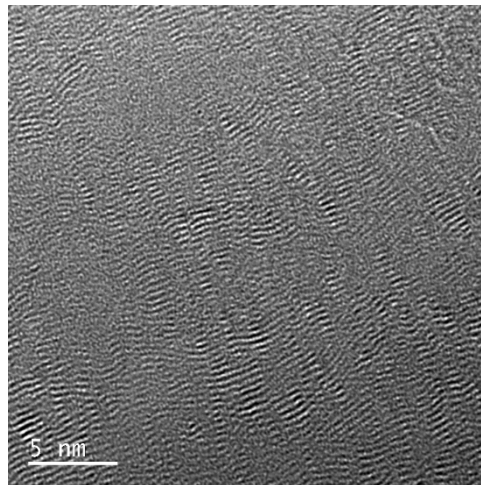


Figure 18. The cross-sectional image of a carbon fiber along its long side.

Figure 18 shows the cross-sectional image of carbon fiber along its long side, fabricated by Prof. Dzenis' group at the University of Nebraska, Lincoln. The distribution of the graphite sheets was studied by using EMIPA. The spacing of the graphite sheets in the carbon fiber is determined to be 0.387 nm on average. Figure 18 shows an FFT pattern and an IFFT image of the experimental image in Figure 17.

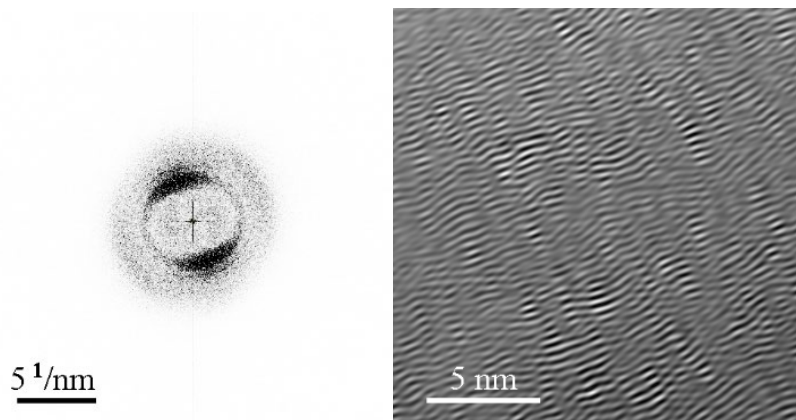


Figure 19. An FFT pattern and an IFFT image of the experimental image in Figure 18.

## 5. Installation

### 5.1 Computer requirement

Java virtual machine, i.e., J2RE, must be installed for running Landyne5, including EMIPA. Java Advance Image is needed for the TIFF file; copy `jai_codec.jar` and `jai_core.jar` to, e.g., `java\jre\lib\ext\` folder.

### 5.2 Software installation and licenses

The executable bytecodes, together with the data files for testing and the user manual, are available in compressed form (`landyne5.zip`) <https://www.unl.edu/ncmn-enif/xzli/computer-programs> and <https://landyne.com>. Both short-term and perpetual licenses are available at LANDYNE ([jlandyne@gmail.com](mailto:jlandyne@gmail.com)). Suggestions and comments are welcome.

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