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DELIVERABLE D23

Workpackage WP5

Software for automation of TEM/CBED methodology for strain determination

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Abstract

This report which is the final deliverable (DM23) of work package 5 aims to summarize the work and explains the software for TEM/CBED image analysis and automatic strain determination.

With the CBED module running under analySIS[®] by Soft Imaging System, convergent beam diffraction TEM images of Si (130), (230) and (150) acquired at 100keV and 200keV can be analyzed. The automatic algorithm detects the lines precisely and the results can be obtained within a few minutes. The software calculates the effective voltage and the strain tensor and its trace by simply clicking on a button. Using this software means that a series of images of a semiconductor structure can be analyzed within a fraction of the time otherwise needed when using the traditional manual method.

A complete remote control setup has been implemented to drive the LEO 912 and LEO 922 TEM microscopes for an automatic CBED image series acquisition.

The software is commercially available at the end of the STREAM project, i.e. end of March. (or: short after the end of STREAM, namely end of April). To speed up the last measurement campaign the software has already been passed over to some partners (LAMEL, ST, and USFD) of the consortium for analysing series of CBED images.

1. Introduction

This software includes the following tasks:

- Automated acquisition of TEM/CBED patterns via a procedure which can be routinely used by the microelectronics industry. A set of points along ROIs (regions of interest) in the cross-sectioned structure can be chosen and the electron probe will be sequentially located in each of them for the CBED pattern acquisition without requiring the operator's control.
- Camera automation procedures, e.g. specific functions such as shading correction to suppress dark current offset in cameras and gain correction to compensate for inhomogeneous sensitivity due to CCD sensor deficiencies and fibre optical coupling.
- Image and data archiving in a database for later research and higher productivity. A template for the database which contains selected images and all associated significant data necessary for storing images.
- Image Processing and filtering in such a manner that individual lines diffraction patterns may be automatically detected and mathematically represented. This includes computation of HOLZ pattern models to identify the relevant HOLZ lines.
- Computation of the effective voltage in a TEM by comparison of simulated HOLZ patterns and experimentally achieved images on perfect silicon.
- Computation of the strain tensor and its trace for a given TEM/CBED image and a series of images acquired over an area of a semiconductor

TEM/CBED images are difficult in contrast depending on the quality of the microscope and the quality of the CCD camera. The HOLZ lines are not always clearly visible and sophisticated image pre-processing must be done in advance to detect the lines automatically.

2. Image Acquisition

The CCD camera control and the acquisition of TEM images can be subdivided into two different tasks.

2.1 Automated camera procedures and image acquisition

Camera automation procedures include specific pre-processing or post-processing functions. These functions are:

- shading correction to suppress dark current offset in the camera,
- gain correction to compensate for inhomogeneous sensitivity due to CCD sensor deficiencies and fibre optical coupling.

These functions are available under analySIS 3.2 while using the following cameras:

- KeenView (SIS)
- MegaView III (SIS)
- BioCam
- Proscan
 - Frame transfer (1K×1K)
 - Bottom mount (2K×2K)
- Orca (Hamamatsu)
- MegaPlus (Kodak)
- Sensicam (PCO)

Real time functionality to improve the image quality and TEM alignment are a FFT (Fast Fourier Transformation), bad pixel correction and real-time histogram calculation to capture optimal dynamic range of the signal.

Images taken with our TEM cameras, KeenView and MegaView III, and images taken with our frame grabber board GrabBit PCI and DigiBoard are automatically calibrated to real world units. This automatic calibration tool requires communication (remote control) between the software and the microscope. We have expanded the list of supported microscopes to make this tool available for many different TEM systems. In addition the images can be calibrated after acquisition so measurements are always correct.

2.2 Import functionality

Due to different camera manufactures and image acquisition systems the software must provide import filters. Depending on the access to the code of the file format to the Soft Imaging System GmbH the image import filter can automatically scale the images to the correct values. If the file format is not accessible to the Soft Imaging System GmbH the images have to be imported in a standard image file format and calibrated with the software.

A cooperation with FEI has started to import image series taken with the TIA system (Tecnai Image Acquisition) where the TEM is driven in a scanning mode and the user can take at each pixel a CBED pattern. These series will be imported into analysis and also the TEM specific settings will be automatically imported.

3. Microscope control and automated image acquisition

Within the STREAM project the remote functionality of analySIS[®] has been expanded and an automated acquisition of TEM/CBED patterns via a procedure which can be routinely used by the microelectronics industry was developed.

The acquisition of an image series is independent of the analysis of the images and consists of three major steps:

3.1 Correlation between the image coordinate system and the microscope system

In Figure 3-1 the dialog for calibration is displayed. It is important to correlate the pixels (image points on the monitor) and the real positions on the specimen (beam position). Therefore the two coordinate systems, display system and TEM system, must be linked together. The calibration is done by acquiring 3 images taken with a small spot (TEM in spot mode). Each of these images is taken with an offset (Step width). Automatic particle detection locates the spot position in each image and calculates the distance in nm between the spots. This gives the calibration data (x- and y-resolution) in nm/tic (nm per digital units on the microscope). The complete procedure is done automatically by pressing the *Calibrate* button. This behaviour is special for the LEO microscopes or microscopes working in “normal” image mode and spot mode. TEMs working in a STEM mode do not require this procedure.

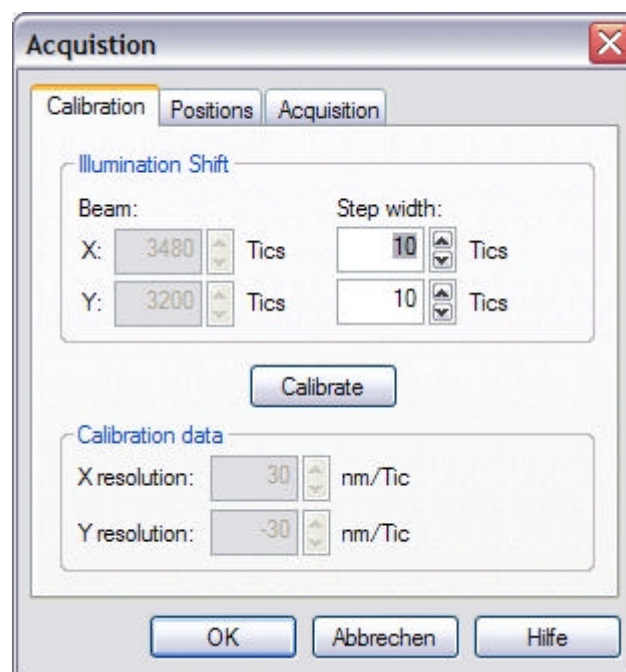


Figure 3-1: Calibration Dialog

3.2 Positioning of points in an overview image where CBED pattern should be acquired

A very important procedure is the exact positioning of points on the sample where CBED pattern should be acquired. The user has the choice to set single points, points along a polygon and inside a rectangular. The points are marked in the overview image for later identification. In Figure 3-2 the dialog for positioning of the points is displayed and in Figure 3-2 an overview image with red marks is displayed. The later positioning of the beam will be done by beam shift. The beam is controlled by the microscope in digital units thus this beam shift can be done in discrete steps (Tics). As a consequence not all positions in the overview image are possible to be located by the beam.

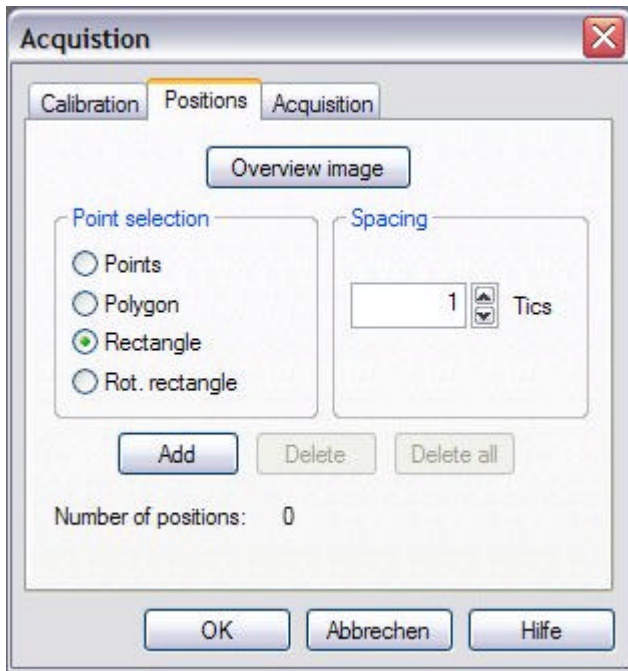


Figure 3-2: Position dialog

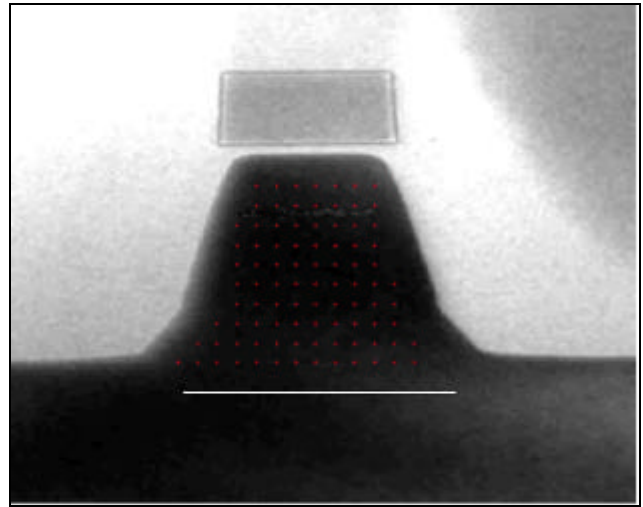


Figure 3-3: Overview image

3.3 Positioning of the electron beam (beam shift) on the sample, acquisition and save routine of the images in a database

After the points have been defined the electron probe will be sequentially located in each of them for the CBED pattern acquisition without requiring the operator's control. In the "Acquisition dialog", see Figure 3-4, the user can give the image series a prefix and he has the choice where the images should be saved, in a directory or in a database. We recommend saving the images in a database. In a database the images can easily be found even in a huge set and additional information can be attached to the images.

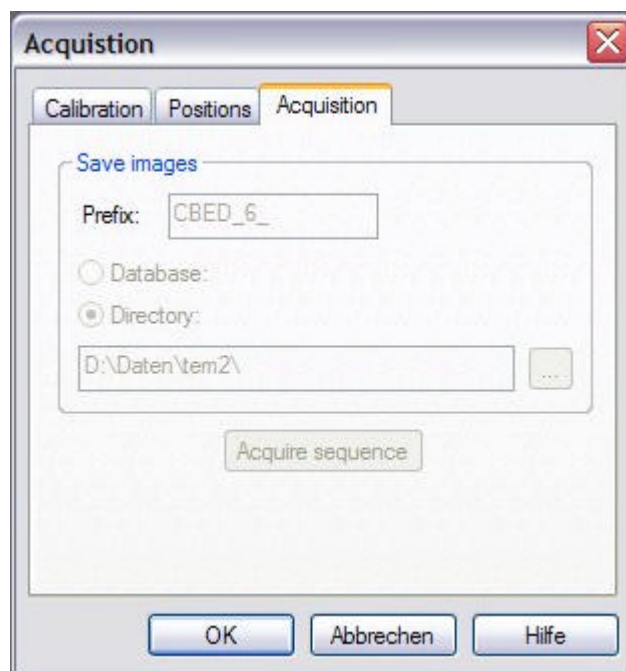


Figure 3-4: Acquisition dialog

4. Processing and Analysis

The treatment of TEM/CBED images can be difficult due to varying contrast, depending on the quality of the microscope and the quality of the CCD camera. The HOLZ lines are not always clearly visible and sophisticated image processing must be done in advance to detect the lines automatically. A new algorithm speeds up the computation time and the quality of the detection algorithm. The software will guide the user through the various steps of pre-processing and image analysis by a GUI (Graphical User Interface). The GUI has been set up in such a way that user effort is reduced to a minimum of parameters, which makes reproducibility of results much reliable.

The pattern simulation and fit routines are based on a code written by LAMEL (Roberto Balboni). This code was migrated from FORTRAN to the programming language C successfully for integration into our software *analySIS*[®]. In addition this new code was made more flexible and split into different tasks. The settings are stored in “ini” files, and with respect to this “ini” files the user can define new zone axes and new relevant reflections. Also new materials like GaAs are much easier to implement into the software due to the flexible design.

In the following it will be given a short description of the steps for a complete processing and analysis of CBED images including simulation and strain determination.

The software has been split into different tasks according to:

- (4.1) Basic properties and pattern simulation,
- (4.2) Image pre-processing,
- (4.3) Line detection,
- (4.4) Line selection,
- (4.5) Selection of fit algorithm, e.g. voltage fit and cell parameter fit.

4.1 Basic properties and pattern simulation

In the dialog box *Properties* (Figure 4-1) the user has to define three parameters: *Atomic Species* (e.g. Silicon), the used *Zone* axis and the initially used *Accelerating voltage* (setting in the microscope).

These settings have to be made once and can be left unchanged during analyzing a series of CBED images taken under the same conditions. For this project the material will be exclusively Silicon and our partner LAMEL has defined the best zone axis. In the past only the $\langle 130 \rangle$ zone axis was used, but now also the $\langle 230 \rangle$ and the $\langle 150 \rangle$ zone axis can be chosen. The $\langle 230 \rangle$ zone axis is as sensitive as the $\langle 130 \rangle$ for strain measurements and the tilt angle is much smaller. The different settings for these zone axes are stored in “ini” files called *si_1_3_0.ini*, *si_2_3_0.ini* and *si_150.ini*. Currently 16 lines must be chosen for strain measurements for $\langle 130 \rangle$ and 18 lines for $\langle 230 \rangle$.

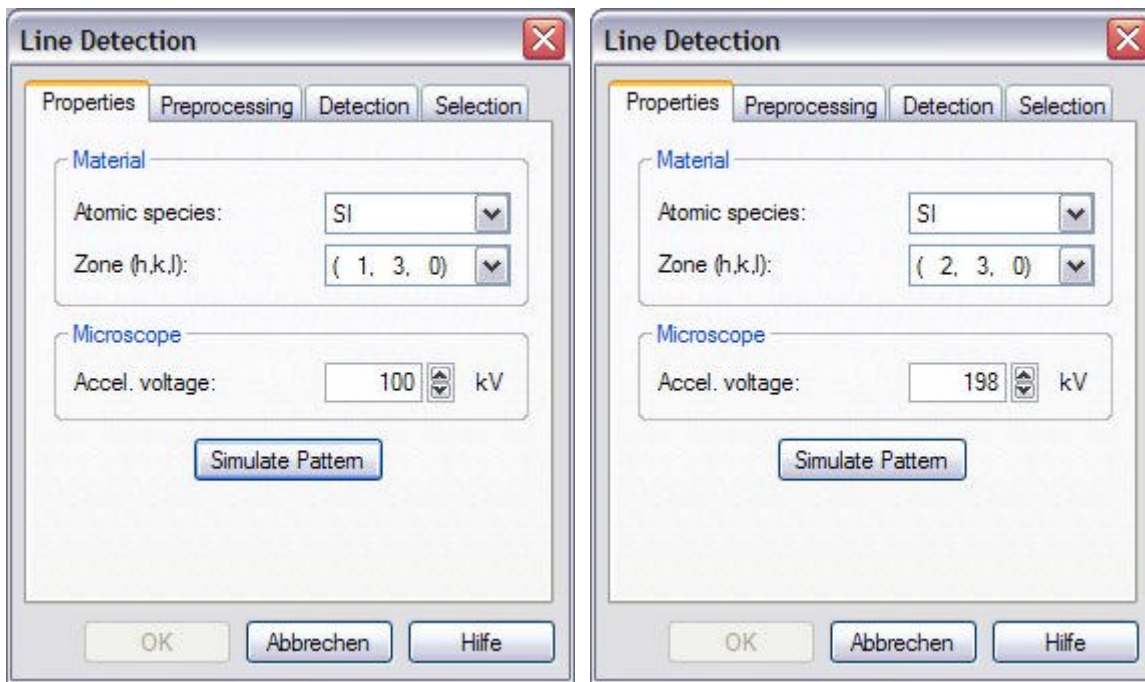


Figure 4-1: Properties – basic settings and pattern simulation

The button at the bottom, *Simulate Pattern*, will generate a HOLZ line pattern according to the selected material, zone axis and accelerating voltage. The experimental and the simulated images can be seen in Figure 4-2. This feature is meant to help the user to identify the lines for detection. It is possible to rotate, scale and shift the simulated pattern to resemble the experimental pattern. Once the orientation and the scaling of the simulated pattern are equal to the experimental one, the user can easily recognise the relevant lines which are necessary for strain measurement.

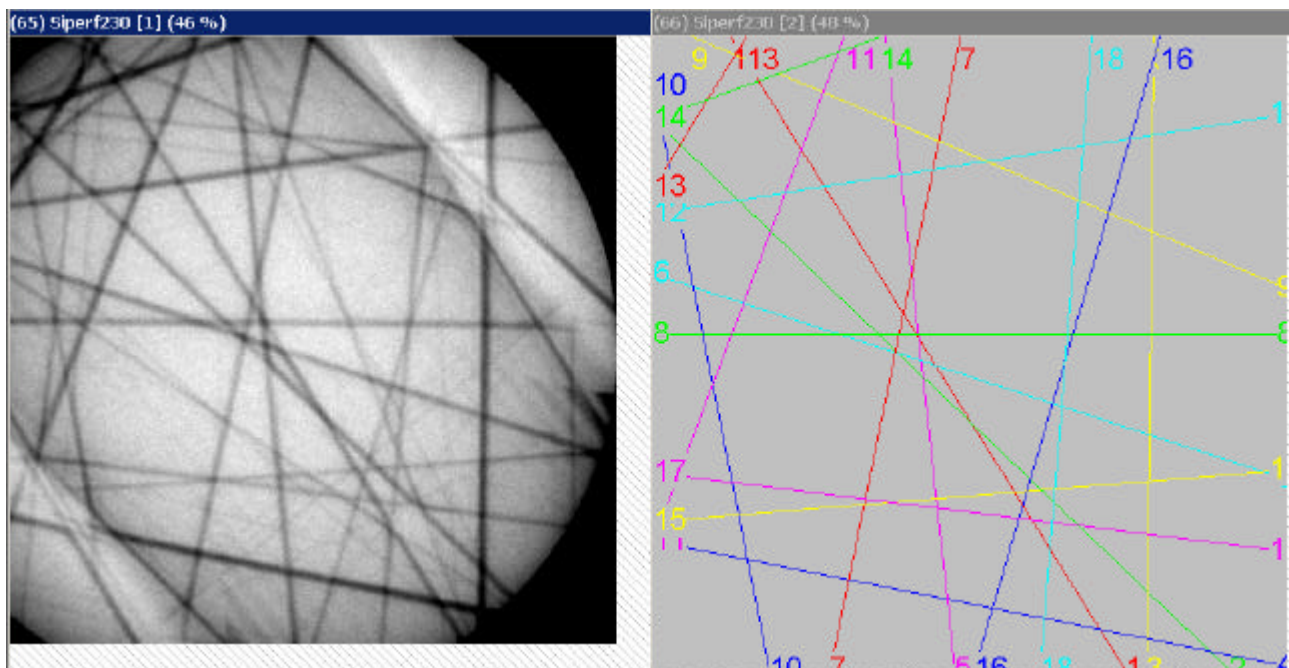


Figure 4-2: CBED/TEM image and simulated HOLZ pattern

4.2 Image pre-processing

As already described, CBED/TEM images are difficult in contrast, and the HOLZ lines are not always clearly visible. This requires a sophisticated image pre-processing for later line detection. The mayor steps in pre-processing of the images are:

- (4.2.1) Automatic shading correction,
- (4.2.2) Inverting the contrast of the image,
- (4.2.3) Selecting a ROI (region of interest),
- (4.2.4) Sampling rate setting.

4.2.1 Automatic shading correction

The background contrast in TEM images is not homogeneous, and an automated shading correction is necessary. This shading correction must have specific setting. An $N \times N$ average matrix filter has to be applied to the image and the original image will be divided by this filtered image. Using an offset while dividing these two images, the resulting image will have a very narrow grey value histogram distribution of the background values. Since the line detection should occur automatically the mean grey value of the lines should differ sufficiently from the mean grey value of the background.

4.2.2 Inverting the contrast of the image

The second step is to invert the image so the lines are always bright. Depending on the acquisition system this function can be disabled.

4.2.3 Selecting a ROI (region of interest)

During the evaluation of the software it has been found that the selection of the ROI is a critical point regarding the reproducibility of the results. Especially in the $\langle 230 \rangle$ zone axis the region of interest must be set accurate, and a “normal” rectangular ROI is not sufficient. The presence of intense lines at the periphery of the pattern in the $\langle 230 \rangle$ zone axis (which interact dynamically with HOLZ lines) are very critical. Due to this behaviour we now have implemented a more flexible setting. The region of interest used (ROI) for the automatic line detection consists of 4 different styles and can be selected under mouse control:

- Ellipse,
- Polygon,
- Rectangle,
- Rot. Rectangle.

The important areas can be separated, whereby a high reproducibility can be achieved. Selecting only part of the image will also speed up the detection algorithm, and unwanted artefacts occurring at the edge of the image are eliminated.

4.2.4 Sampling rate setting

Finally, the user selects a sampling rate that corresponds to the resolution of the detection. A ratio of 1:1 means that every pixel is taken into account for detection and a ratio of 1:2 means only every

second pixel is used. Lines crossing under a very narrow angle can only be detected if all pixels are used for the calculation (sampling rate = 1:1).

The GUI corresponding to the Pre-processing functions is displayed in Figure 4-3.

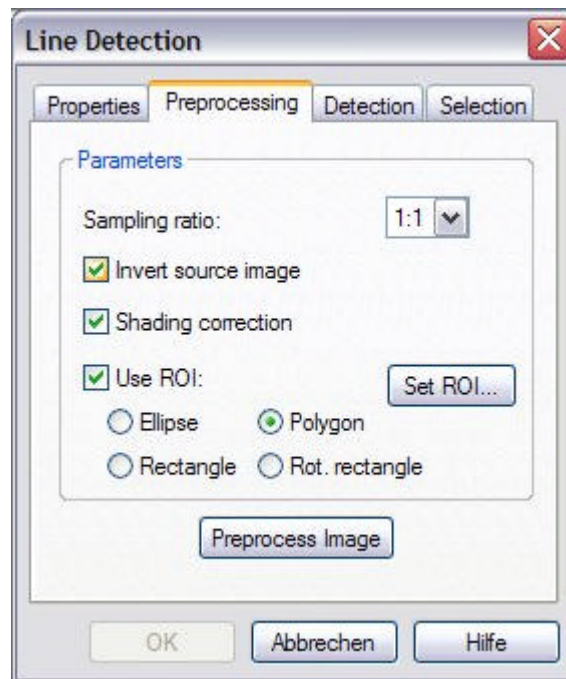


Figure 4-3: Line detection -- pre-processing interface

The button *Preprocess Image* will execute the steps as describes above and will generate a transformation of the image. This transformation “scans” the image at each data point (depending on the sampling ration) for lines. The mathematical approach is given by the “Hessesche Normalform”:

$$x \cos \alpha + y \sin \alpha - p = 0$$

x, y the Coordinates in the image,
 α the angle,
 p the distance between the line and the origin.

4.3 Line detection

The line *Detection* dialog, see Figure 4-4, has 3 changeable fields for

- (4.3.1) *Noise reduction*,
- (4.3.2) *Threshold* setting,
- (4.3.3) *Tolerance*.

4.3.1 Noise reduction

The noise in TEM images mainly contains high frequencies and therefore a low-pass filter should be applied. This additional filtering was implemented to improve the line-detection automation and to reduce artefacts during lines detection.

4.3.2 Threshold setting

For every line a mean grey value is calculated, and with the adjustment of the *Threshold* lines with different contrast are accepted. This feature separates the lines from the background, see chapter 4.2.1.

4.3.3 Tolerance

The Tolerance parameter is a combined setting of radial and angular resolution (see chapter 4.2.4) between neighbouring lines. If the tolerance is set to 0 (auto mode) the centre of gravity of the peak in the transformed image is used for calculation of the line. If very close (narrow angle) lines are present the tolerance can be set to values different of 0. In that case a different algorithm is used to separate the lines and the user has to find the best setting.

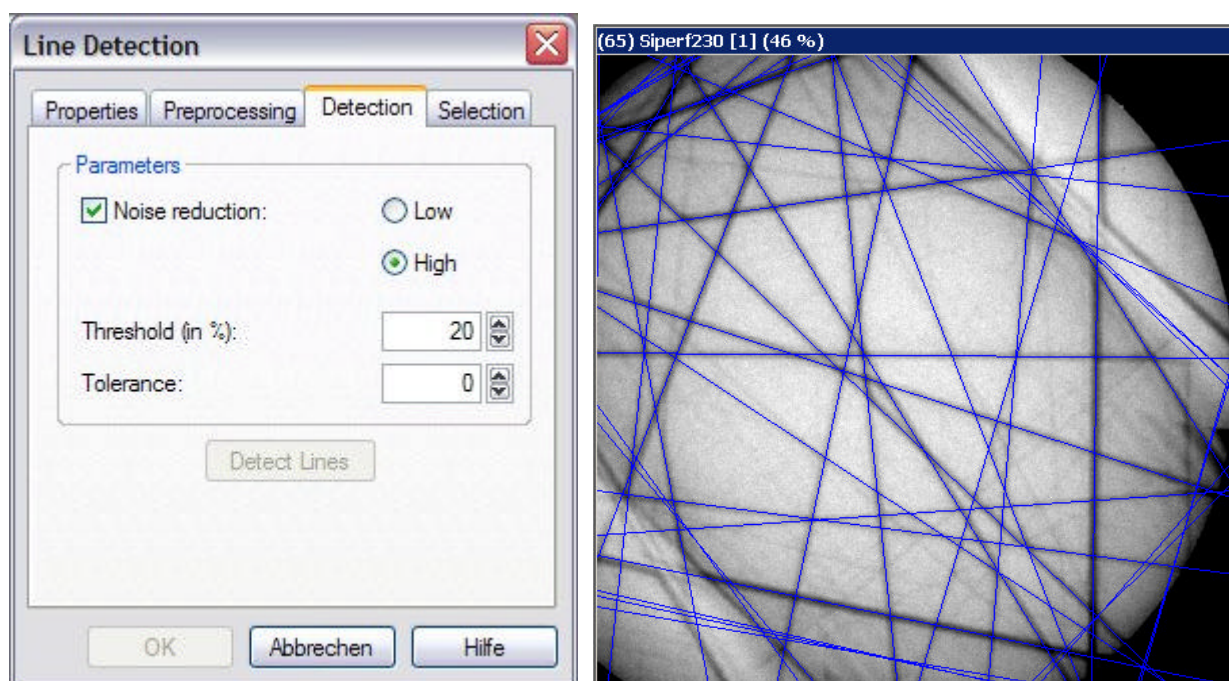


Figure 4-4: Detection – line detection parameters

Figure 4-4 shows the user interface for line detection. The detected lines will be marked with a colour and drawn in the overlay of the image. The quantity of detected lines (blue lines) depends on the settings of *Threshold* and *Tolerance*. The user should check and compare with the simulated image whether all relevant lines are marked.

4.4 Line selection

In the dialog *Selection* the user has to select the relevant HOLZ lines. The lines are labelled by their Miller (h,k,l) indices taken from a pull down menu. This predefined list can be changed by a corresponding “ini” file. This “ini” file can be changed to the best set of lines for strain calculation. Currently we are working with a set of 16 lines for <130> and 18 lines for <230> defined by LAMEL (Dr. Balboni).

Pushing the SET button the user has to mark the lines with a sequential numbering according to the list. In some cases it is difficult to distinguish between lines crossing under narrow angles. For this

reason the sensitivity of the mouse (capture region) can be changed by the user. It is also possible to zoom in the image to verify the selection the user has done.

Once the user has marked all relevant lines the distances between the crossing points will be calculated by pushing the *Calculate Distance* button. The dialog for the line selection is shown in Figure 4-5. The output of the calculated distance will be automatically attached to the image if the user has used an image database. Otherwise the output file will be saved into the same directory where the images have been loaded.

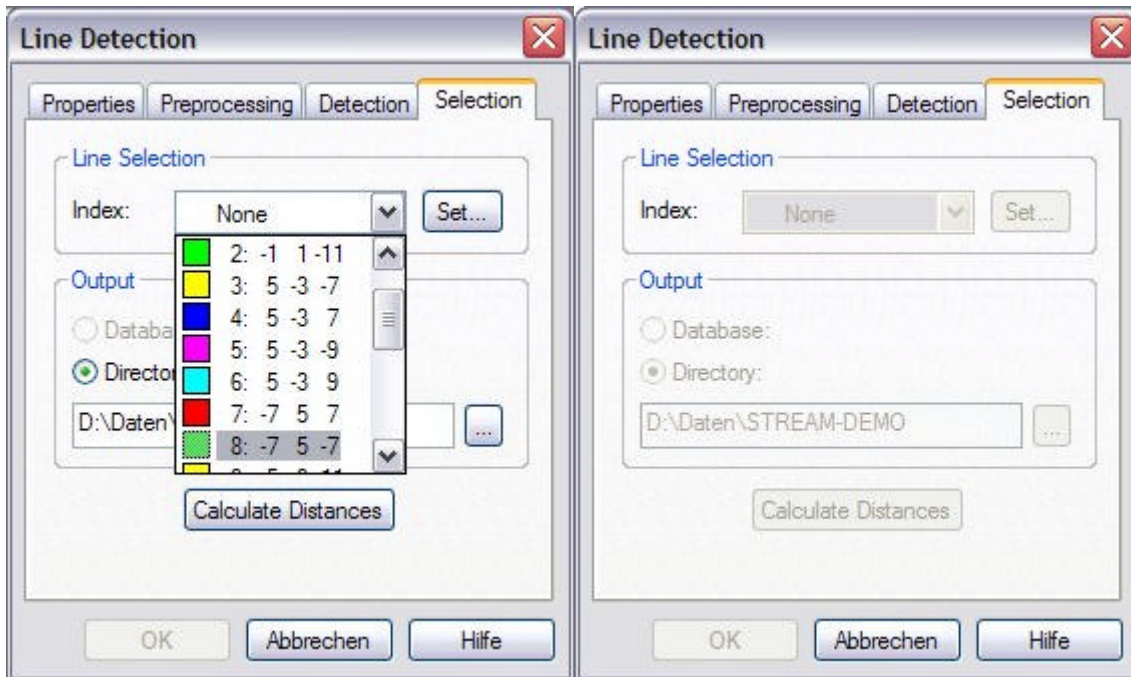


Figure 4-5: LineDetect -- selection

4.5 Selection of fit algorithm, e.g. voltage fit and cell parameter fit

The analysis and fit procedure of the software is divided up in three parts:

- (4.5.1) CBED Selection,
- (4.5.2) CBED Voltage Fit,
- (4.5.3) CBED Cell Parameter Fit.

Figure 4-6 shows the user dialog for selecting the different fit algorithms.

4.5.1 CBED Selection

The settings under the point *Material* will automatically be updated depending on the settings in the *Properties* dialog (see Figure 4-1). The Microscope settings (voltage settings) will also be updated automatically.

Depending on the selection in the field *Algorithm* in Figure 4-6 the user will be guided to one of two dialog boxes: CBED – Voltage Fit (Figure 4-7) or CBED – Cell Parameter Fit (Figure 4-8).

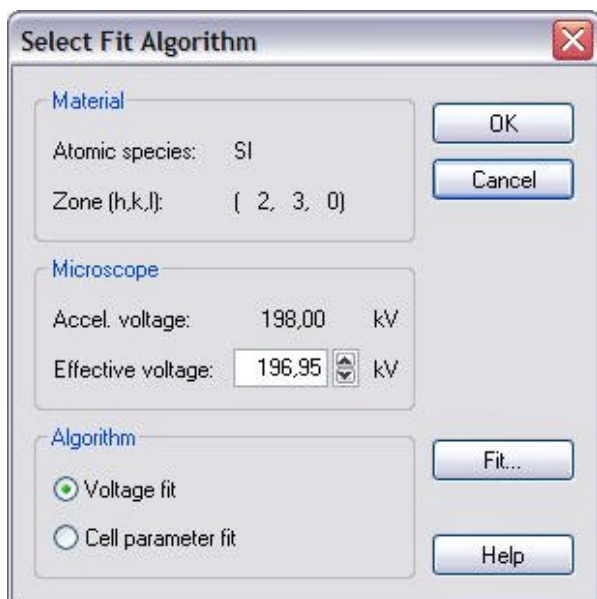


Figure 4-6 CBED Selection – basic settings



Figure 4-7: CBED -Voltage Fit

4.5.2 CBED – Voltage Fit

A precise calculation of the strain can only be achieved if the accelerating voltage is correct. As explained in Deliverable D2, the nominal accelerating voltage of the microscope cannot be included into the strain calculation, rather an ‘Effective voltage’ value must be determined. The first step in the experimental procedure is to take a reference image at an unstrained area. The effective voltage is calculated from this unstrained image. In Figure 4-7 the different input fields for the voltage fit are displayed. In the first section (*Accelerating Voltage*) the voltage interval and the step size of the fit must be specified. The *Lattice Parameters* for the undisturbed Silicon are well known and are included in the fields automatically. These values can be edited in the “Si.ini” file, and due to lattice changes at different temperatures the user can correct these settings manually.

The effective voltage will then be calculated by fitting the experimental pattern with patterns simulated in the specified voltage interval. The resulted *Effective Voltage* will be updated automatically in the corresponding field. The quality of the fit can be examined by analyzing the c^2 results in an output file. All information will automatically stored in the image information, and the system will “remember” that the image has been already examined. The voltage fit must only be done for perfect silicon.

4.5.3 Cell Parameter Fit

If the user has done the voltage fit the next step is to calculate the strain with the help of a cell parameter fit. Figure 4-8 shows the dialog box for the *Cell Parameter Fit*. Whereas for the *Voltage Fit* procedure the user has to define the range of accelerating voltages, fixing the cell parameters, now he has to define the range of lattice variations in the *Lattice Parameter* section, assuming the previously determined effective voltage. He can also fix different base vectors (e.g. $a=b$) or angle

dependencies (e.g. $\beta = 180 - \alpha$) by the *Equality* flag. These equality flags are very important and taking into account the symmetry of the lattice. Also the assumption that the angle γ is not independent (plain strain approximation) is very important and is necessary to achieve reliable results.

Pressing the *Execute* button the program will calculate the new lattice parameters, the strain tensor and its trace. This is done by a best fit routine which compares the various simulated patterns with the experimental pattern. The goodness of the fit can be controlled by the χ^2 value which is logged in an output file. Again, all information will be stored in the image information and saved with the image in the database.

Cell Parameter Fit

Lattice Parameters

	Minimum:	Maximum:	Step:	Equality:
a:	5,423	5,435	0,001	A*
b:	5,405	5,475	0,001	A* = a
c:	5,423	5,435	0,001	A* None
alpha:	89,8	90,02	0,01	*
beta:	89,98	90	0,01	* = 180-alpha
gamma:	89,98	90,02	0,01	* Planar strain

Execute

Results

Lattice parameters:		Strain tensor:		
a:	A*			
b:	A*			
c:	A*			
alpha:	*	Trace:		
beta:	*			
gamma:	*			

Back to selection

Figure 4-8: CBED – Cell Parameter Fit

5. Conclusion

This new software has completely replaced the procedure used by our partners in the past. The development of the software for line detection is finished, and Dr. Balboni (LAMEL) has already crosschecked the results achieved with both methods (“traditional manual” and “automatically software controlled” method). With the new software reliable results can be achieved with a minimum knowledge of the complex theory of strain determination by TEM/CBED images.

Also the STREAM partners ST Microelectronics and USFD have measurements with the new software. To speed up the last measurement campaign the software is available for the STREAM partners in ST, LAMEL, University of Modena and USFD.

For the calculation of the strain field distribution over an interesting area in the semiconductor structure a series of tens of images have to be analysed at least. Using the automatic acquisition procedure described in Sect.3 for TEM, or even easier with a STEM, series of images consisting of several hundreds of images are obtainable. This makes the “manual method” not feasible for the user, and an automatic procedure essential.

As an example for the automatic line-detection algorithm two images are displayed in Figure 5-1. The images are provided by LAMEL and show a CBED image of the $\langle 130 \rangle$ zone axis. The left image was analysed by hand, the relevant lines are drawn into the image by hand. This procedure has taken a couple of hours. Within a few minutes the lines in the right image has been detected accurately by the software. Extracting the input values (distances of crossing points) for the fit routines (voltage fit or cell parameter fit) requires only a “click” on a button. Series of images of a semiconductor structure can be analysed within a fraction of time compared with the time needed with the “old method”.

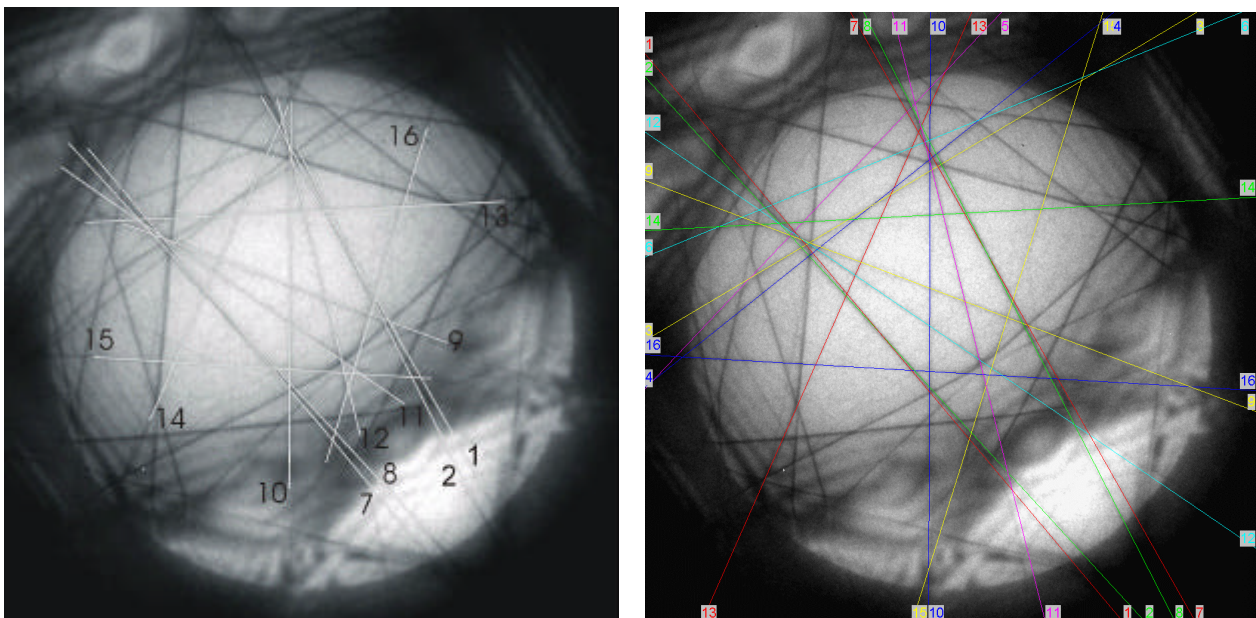


Figure 5-1: “old” line detection method and new method

An additional report concerning the software is given by Dr. Pavia of ST Microelectronics who summarises the usability of the software in Deliverable D18. And more examples concerning the usability and application to the different zone axis can be found in D20

5.1 Future perspectives

In deep sub-micron electronic devices, the $\langle 230 \rangle$ zone axis is more convenient than the $\langle 130 \rangle$ one, due to the smaller tilt angle required; LAMEL has demonstrated the good strain sensitivity of this zone axis. However, within the software the user has the choice between the $\langle 130 \rangle$ and the $\langle 230 \rangle$ zone axis. In D20 , Appendix I, it is described that also the $\langle 150 \rangle$ zone axis is suitable for CBED strain measurements. With new “ini” files also this zone axis can be used with the software.

Also the implementation of new materials like GaAs can be easily done. LAMEL has started successfully to investigate GaAs and to determine the strain. First results are presented in D20 Appendix II. This progress and the work of LAMEL is essential to make the new software module attractive and flexible enough for the industrial market.

The Soft Imaging System GmbH has planned to continue the good cooperation, which started with the STREAM project, with LAMEL even though the project has been finished.