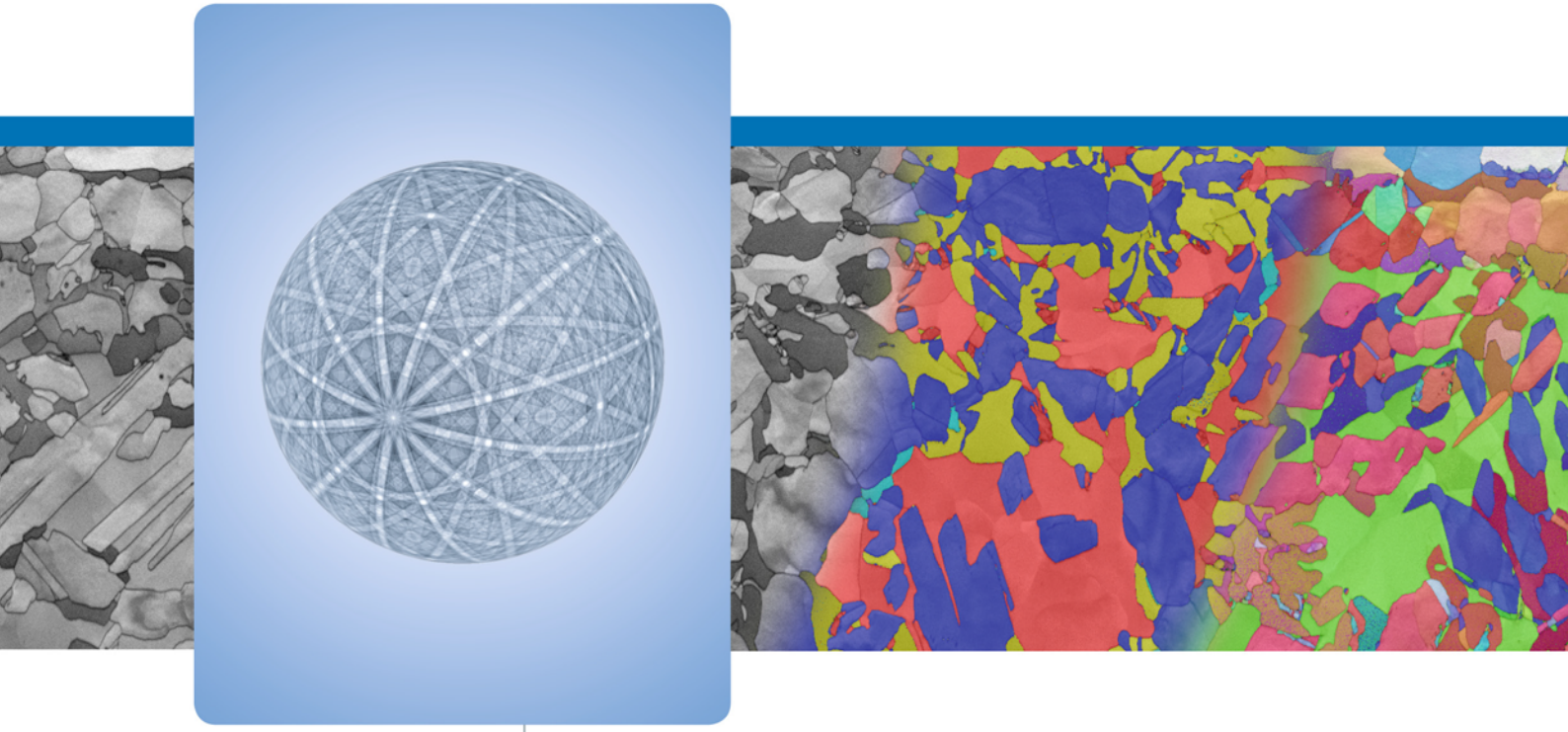

QUANTAX EBSD

Fully-integrated high-performance EBSD analysis system

User Manual

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We have checked the contents of this manual for agreement with the hardware and software described. Since deviations cannot be precluded entirely, we cannot guarantee full agreement. However, the data in this manual are reviewed regularly and any necessary corrections are included in subsequent editions. Suggestions for improvement are welcome.

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Contents

1 Introduction

QUANTAX is the ideal all-purpose microanalysis system for industry, research and education. Different system levels and various options are provided for scaling and tuning of QUANTAX to a broad range of analysis tasks and application environments. QUANTAX microanalysis systems are suitable for scanning electron microscopes, transmission electron microscopes, electron beam microprobes, dual beam devices, as well as other X-ray spectrometry applications.

The QUANTAX EBSD analysis system for scanning electron microscopes is an easy-to-use yet fully functional tool for Electron Backscatter Diffraction measurement and evaluation. QUANTAX EBSD offers full versatility and flexibility for the investigation of all kinds of crystalline materials, whether standalone or in conjunction with the QUANTAX EDS system for simultaneous EBSD and EDS analysis.

An intuitive user interface, the flexible project management package, as well as various options for quick and comprehensive report generation complement the analysis toolboxes. The software tools are tailored to meet both the needs of the novice as well as the experienced user. All QUANTAX systems' ESPRIT software includes an online help system.

This manual provides a general software overview and a practical step-by-step description of the most common measurement and evaluation procedures that can be performed with the QUANTAX EBSD system. For a complete description of the QUANTAX EBSD system, please refer to the QUANTAX EBSD User Manual. The integrated assistants and the online help of the ESPRIT software provide additional support. Details on the individual software and hardware parts and additional technical data are contained in separate manuals. The individual device manuals can also contain further references regarding operational safety. Please follow all safety instructions closely to avoid hazards to personal safety and equipment. In case of necessary maintenance, reinstallation, severe computer breakdown, hardware changes, etc. the Bruker customer support or your local supplier have to be contacted for further assistance and instructions.

According to the modular structure of QUANTAX not all parts of this manual may apply in detail to a given installation nor should they be taken literally in all cases. For instance, if the general term "electron microscope" is used this applies to the whole class of electron-beam or dual-beam systems; SEM also includes STEM, microprobes, or other scanning devices.

The ESPRIT software layout may vary according to the modules actually installed on your system and therefore may differ slightly from what is shown in the illustrations and figures.

2 Safety Information

The operation of the QUANTAX EBSD system is restricted to trained personnel familiar with the system as well as the product documentation, general safety precautions, and laboratory rules. A briefing on safety issues is given at the time of installation or during user training.

Local, state, or federal regulations have to be taken into account additionally to the safety instructions given here. Additional instructions for specific parts of the QUANTAX EBSD system - e.g. EBSD detectors, TKD sample holder - may be contained in the according manuals.

The QUANTAX EBSD system may only be used in combination with electron microscopes or similar devices. Any other use beyond that is considered non-intended usage. The operator, not the manufacturer, assumes sole liability for all personal injury and material damage arising from non-intended usage.

2.1 Radiation Safety

⚠ DANGER

Changes to the original detector installation are strictly prohibited. Radiation safety may be impaired by improper installation or de-installation.

The normal electron sample interaction that takes place in the electron microscope generates X-radiation. Microscopes are generally designed to shield this type of radiation sufficiently.

The e-Flash detector is installed according to the applicable radiation safety regulations. Changes to the original installation and equipment, including flanges, vacuum sealing, support, etc. are strictly prohibited.

In case the e-Flash detector has to be uninstalled, make sure that the **original blind flange** of the electron microscope vendor is used to seal the sample chamber port. In case the original flange is not available contact the microscope vendor for support.

2.2 Electrical Safety

⚠ DANGER

High voltage inside. Do not remove covers.

All parts have been designed according to the safety requirements for electrical equipment for measurement, control and laboratory use, or the European Low Voltage Directive, respectively. The system must be correctly installed and used only for the purposes it is designed for. Especially grounding of the system or system parts - as performed during installation - must not be changed for any reason. In case of any supplements or replacement parts being installed, supply voltage settings must be checked and adjusted to the local mains voltage.

Certain parts of the system may contain dangerous voltages. No covers need to be removed during regular operation; maintenance should only be carried out by trained and certified personnel.

2.3 Electromagnetic Compatibility

Due to its physical construction, the EBSD detector may not fully comply with common standards regarding electromagnetic immunity of general electronic equipment. This is not a disadvantage under normal circumstances because the QUANTAX EBSD system works under the same conditions as electron microscopes and the laboratory environment is designed to meet the requirements of these instruments.

Bruker devices fulfill all requirements regarding active electromagnetic compatibility (emission rules).

3 The QUANTAX EBSD System

3.1 Hardware System Components

Typical QUANTAX EBSD system parts

- Electron BackScatter Diffraction detector
- Pattern streaming interface
- SEM control interface
- QUANTAX server computer
- Optional client advanced workstations
- ESPRIT 2 software packages

System components of QUANTAX EBSD comprise the EBSD detector and interface hardware, one or more computers, and several software modules. All parts are selected for performance and trouble free interaction. Exchanging any part of the QUANTAX EBSD system with non-approved items (e.g. user defined computers) may affect its functionality and/or its capabilities. Different software options determine the system level.

3.1.1 EBSD Detectors

EBSD detector – functional principle. The most important components of an EBSD detector are the phosphor screen, the optics system, the CCD camera and the guiding system. The phosphor screen is used to transform the backscattered electron signal produced by the interaction between the sample and the electron beam into a photon signal. The light produced by the phoshor screen will then be focused by the optics system onto a CCD chip. Images of the phosphor screen (Kikuchi patterns) will be recorded by the CCD chip and transferred (pattern streaming) to the computer. The guiding system is used to insert/retract the phosphor screen/ optics system/ CCD camera assembly close to/away from the sample.

Fig. 3.1-1 Bruker *e*⁻Flash EBSD detector

Bruker *e*⁻Flash EBSD detectors. The *e*⁻Flash 1000 EBSD detector is designed for fast data acquisition while the *e*⁻Flash HR is intended for applications requiring high quality and high pixel resolution patterns.

e⁻Flash detectors are maintenance-free, durable, completely vibration free and do not require any consumables.

3.1.2 Pattern Streaming Interface

The network (red) cable used to transfer the patterns from the EBSD detector to the QUANTAX server computer is plugged on the computer side into a dedicated high speed Ethernet network card. If the connection between the EBSD detector and the dedicated network card is incorrectly setup or modified, the EBSD detector will not be detected by the automatic search performed by the Bruker ESPRIT software.

3.1.3 SEM Control Interface

Data interface. The proprietary Bruker MegaLink high-speed data interface transfers the EDS spectrometer data in real time to the QUANTAX server. The PCI plug-in board Bruker IO-Scan can connect up to 4 spectrometers simultaneously. Bruker MegaLink is a serial interface protocol featuring full galvanic isolation for improved noise immunity at connection length of up to 30 m. For basic spectrometer functions that do not require real time spectrometry a standard computer interface (RS232) can be used as an alternative.

Fig. 3.1-2 PCI-plug in IO-Scan

QUANTAX scan system. The proprietary Bruker MegaLink high-speed data interface transfers the EDS spectrometer data in real time to the QUANTAX server. Additionally, the PCI plug-in board IO-Scan is used for controlling the x/y electron beam deflection as well as two separate digitizers for the image signals of the electron microscope (EM). Position tagged spectrometry data acquisition is provided for advanced EDS line scan and element mapping. Digital signal processing supports the server computer in time critical tasks. Control signals for hardware scan switching are provided as well.

Microscope data transfer. Microscope data transfer is based on different networking technologies according to the type of microscope. For older brands, serial connections (RS232) are also provided.

3.1.4 Advanced Workstation Computer

Client-server architecture. All QUANTAX systems feature client-server architecture. The server part controls the EBSD detector, the EDS spectrometer and microscope hardware and performs basic data evaluation; the client system is what is visible to the user and provides the graphical user interface (GUI). Client and server can share one computer or run on different computers. Multiple client workstations can connect to a QUANTAX server with network access.

☞ The client and/or server application may share computers with the SEM installation.

3.2 ESPRIT 2 Software

Server workstation. Based on the operating Windows® system, the QUANTAX server can be used as standalone unit or network component. The connections to the optional client workstations are accomplished either via a separate network or via the intranet of the company or lab. With appropriate upgrades it is also possible to connect to wide area networks. The QUANTAX server performs the measurements and primary mathematics. It also provides the public and private data areas of the QUANTAX user. With most installations, the first client application is also running on the server computer.

System requirements. QUANTAX requires Windows® 7 with a service pack level specified at time of installation. Operating system updates are to be approved by Bruker Nano. Only computers provided or approved by Bruker Nano may be used.

Windows® administrator rights are required for the installation of QUANTAX. Ask your system administrator for help.

Hardware drivers. All necessary drivers, e.g. for the IO-Scan card, for the CCD camera, etc. are installed on the Advanced Workstation computer delivered with the EBSD system. If for whatever the reason all or some of the the hardware drivers have to be reinstalled, all drivers can be found on the ESPRIT installation CDs delivered with the system.

License file. A user and system specific license file is contained on a separate CD. During the initial start of ESPRIT the user is prompted to provide this CD for registration.

The license file (Licence.pdf) is stored to the server computer; after completion the license CD should be kept in a safe location.

Software options. Licenses control general access to the ESPRIT software as well as installed options. Selected options or the complete license can be time-limited. Updated license files obtained from Bruker Nano can be read in the **System** workspace (see section 4.7). Changes will be enabled after restarting ESPRIT.

☞ Do not save the license with a pdf-reader. This procedure destroys the license.

The license is also provided as hard copy. The contents can be checked against the file, which can be opened by any pdf-reader or from the **System** / **System** workspace by clicking the Show button.

Hardware key. The system license is bound to a system specific hardware key coded into the QUANTAX server hardware. Client workstations can receive certification from a licensed server via the network. Standalone PCs (data stations) must be equipped with an optional USB dongle replacing the hardware coded key.

USB Dongle. The QUANTAX dongle for standalone systems (systems without access to a QUANTAX server) fits any USB-port on the regarding PC. A software driver for the dongle must be installed during system installation and can be found on the ESPRIT installation CD; the dongle must be present to use the data station.

Install the QUANTAX base system selecting option **Data Station (with dongle)**. Leave the ESPRIT install CD in the drive and plug in the dongle into a convenient USB-port.

Windows® will detect the new hardware automatically and display an installation wizard. Note that the dongle does not replace but only enables a valid QUANTAX license.

3.3 General Operating Instructions

3.3.1 Detector Maintenance

***e*-Flash detectors.** Bruker *e*-Flash detectors are maintenance-free. There is no additional wearout caused by permanently powering the EBSD detector; nonetheless it is recommended to switch the detector OFF if not in use for long periods of time.

Special care should be taken regarding the sensitivity of all signal-transmitting surfaces. At all costs, avoid any contact with the phosphor screen or the FSE/BSE detectors of ARGUS™.

Cleaning. Covers of electronic compartments must never be opened. Only dry cleaning (dusting) of the outer compartments is permissible. The phosphor screen must not be cleaned at all.

3.3.3 Software and Data Handling

Backing up data. Even state-of-art, complex and versatile software systems cannot be designed to completely exclude the possibility of damage or impairment by improper operation and/or misuse. The safety measures provided by the operating system can only moderate this. Additionally no existing computer system is actually immune against potential hardware or software errors. Appropriate backing-up of all relevant data is strongly recommended. No warranty claims can be accepted in case of data loss for whatsoever reasons.

Maintaining system integrity. The QUANTAX EBSD system is installed on special selected and configured computers. Any change of the system configuration, user status, access rights, or else can impair system integrity. Also new applications, especially multi-media, internet, and game software can interfere with QUANTAX. The internal client-server architecture of QUANTAX depends on Windows® communication services that may be adversely modified by subsequent installations.

Recovering from errors. In cases of program lockup due to improper operation or unexpected circumstances a restart of ESPRIT is normally sufficient. In more severe cases a restart of the personal computer and/or the QUANTAX server may be required. More severe system breakdowns - if any - should be handled by trained service personnel.

If by any chance dust should have collected on the screen surface, remove it with a gentle puff – air and gas blowers usually have too much pressure, and may destroy the phosphor surface; the same applies to compressed-gas containers commercially available for cleaning sample surfaces. Using a photographer's lens brush will definitely cause mechanical damage to the phosphor surface. In order to remove visible defects use the static background processing selectable in the Signal Assistant.

If you intend to take off the detector from the SEM for storage, make sure that the detector screen is protected; as a precaution, we recommend that you remove the screen from the holder in this case. If you have a fitted ARGUS™ detector, you should also remove the single detectors and store them in a safe place.

Keep the phosphor screens in a place that is as dry and dark as possible. The manufacturer recommends storage under vacuum.

For more details on detector maintenance please consult the *e*-Flash Reference Manual.

3.3.2 Electronic Units

Setup. Unauthorized changes to the electronic and electric installation are not permitted. Besides safety regulations (see chapter 2) also electromagnetic immunity and noise pick up issues were addressed during installation.

Note that electronic parts may have to be adapted to the local mains voltages, if this should change for whatsoever reason. Also replacement parts have to be checked for proper settings before being connected to the mains supply. Details are described in the according reference manual.

☞ The detectors are sensitive measurement devices, which can be impaired or destroyed by inappropriate use or harmful influences.

Electrostatic damage. All electronic components and computers require the typical operating precautions for electronic products. All usual preventive measures against electrostatic discharge (ESD) must be carried out. All components of the QUANTAX system are designed for laboratory use only.

4 The ESPRIT 2 Software

4.1 Start-up and Login

Fig. 4.1-1 ESPRIT Login screen

☞ System functions, especially concerning the measurement system (e.g. calibrations) will affect subsequent users. It is advised to exercise special caution here.

The ESPRIT software runs on the QUANTAX server and the client workstations. However the user only has to start the client application; the server software and communication drivers will start and log in automatically.

Startup. To start ESPRIT click the program icon on the Windows® desktop or in the Windows® Start menu. The ESPRIT login screen is displayed prompting user name and password.

Login. Enter user name and password and click the Login button. The password is stored on the local workstation, if the corresponding option is checked. The name of the last user is always retained.

Multi-user systems. On multi-user systems several users can access, manage, and evaluate private and shared data simultaneously. The unique user name and password will give access to the private data and settings. Select the server to log in from the pull down menu below after clicking on the arrow symbol of the Login button.

After logging in with a unique user name the current settings and data will be loaded from the private user profile volume on the QUANTAX server.

Remote login. With client-server installations (option LAN) it is possible to log in from any connected remote client workstation. The first user to start a measurement will gain access to the detector and imaging system. This user will be able to perform measurements from the remote workstation. The access to the acquisition hardware remains locked to others as long as this user is logged in.

4.2 User Administration

Fig. 4.2-1 QUANTAX communication server access

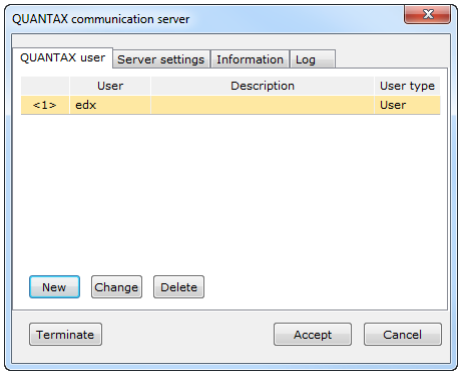


Fig. 4.2-2 QUANTAX user list

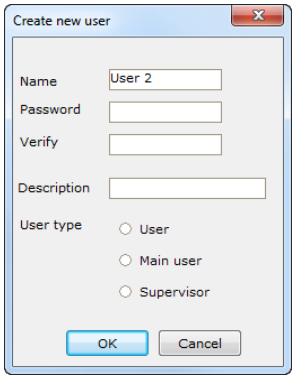


Fig. 4.2-3 Assigning a new user

The QUANTAX communication server controls the user assignments as well as the internal and external client-server communication. Service tools and information for troubleshooting are also provided. The communication server runs on the QUANTAX server computer. It is also present in single computer and standalone systems.

Clicking the Bruker icon in the Windows® system tray of the server computer opens the console of the communication server. With exception of the actions described below no changes to the communication server settings must be made. Unauthorized altering of settings can render the system useless and lead to severe data loss.

New users are to be assigned from the QUANTAX communication server. Double clicking the Bruker icon in the Windows® system tray opens the console of the communication server.

The tab **QUANTAX user** lists the current assigned users. A new user can be added after clicking the New button. A password can be entered (leaving the field empty is permitted) and an optional user description can be added. As user type **User**, **Main user**, and **Supervisor** can be selected.

User has limited access to the ESPRIT **System** workspace. This user level only allows access to the **Appearance** tab and can review the connected instruments and license.

The **Main user** has limited access to the ESPRIT **System** workspace. This user level has full access to the tabs **System**, **Appearance** and can calibrate the connected EDS detectors as well as the imaging system. The **Main user** has no access to the service settings of the WDS detector and the electron microscope driver.

The **Supervisor** has full access to all tabs in the ESPRIT **System** workspace.

Each new user is automatically assigned a folder structure in a private volume of the server. Default methods, a predefined user profile, and demo data are copied to the user folders.

Altering user name and password can be done at any time from the QUANTAX communication server (icon in the Windows® task bar) by clicking Change in **QUANTAX user** tab.

The user data and profile are automatically copied to the new user data structures. Backups of important data, which are always recommended, are especially advisable when changing user names.

Normally there is no need to delete assigned users. If users have to be deleted, it has to be made sure that all user data to be retained are copied to public volumes.

To delete a user, highlight the user name in the list provided in the **QUANTAX user** tab of the QUANTAX communication server. After clicking Delete the deletion of the user data has to be confirmed separately. Caution, once confirmed, the deletion cannot be revoked! If deletion of the data is not confirmed, the data are retained invisibly; a new user with the same name as a previously deleted will be assigned to the idle data.

The number of assigned measure client ports determines how many users can log in simultaneously to the server computer. Per default only one port is assigned, so that only one user at a time can log in to the server computer. Even when multiple ports are present, the hardware can only be controlled by one user at a time.

Fig. 4.2-4 Access to QUANTAX server settings

Select a new port number in the field **Measure client ports** and click Add >. Usually, the number following the last assigned port in natural order is adequate. Ask your system administrator for help.

Note: The communication server port in the top box must not be altered; it must always match the settings on the client workstations.

The **connection setting** for a client workstation is accessed from the ESPRIT login screen. Select the entry **Configuration** from the **Server** dropdown list. The **QUANTAX SERVER SETTINGS** dialog will open.

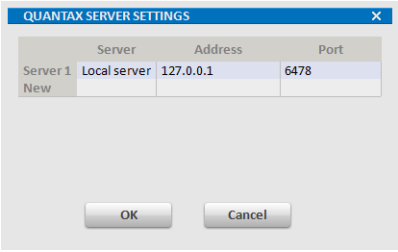


Fig. 4.2-5 Assigned measure client ports

A random name can be given to a connection. If the client workstation also runs a server, select "Local server" for a name and input network address 127.0.0.1. The port number must match the setting of the communication server (see section above); default is 6478. Ask your system administrator for help with network addresses and port numbers.

4.3 Workspaces

Workspaces are ESPRIT screen areas in which images and data are displayed, the analysis is performed and the results are processed. A workspace can be selected by clicking on the corresponding workspace icon. The active workspace icon is highlighted.

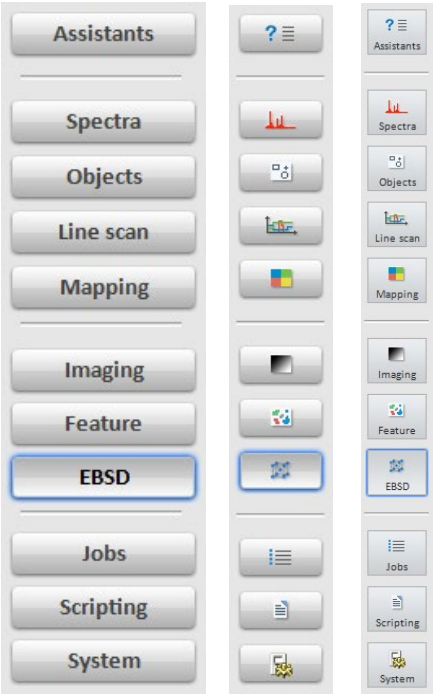


Fig. 4.3-1 ESPRIT workspace list in normal, fullscreen and large style buttons mode

Assistants
gives access to a step-by-step guide for common analysis procedures.

Spectra
allows spectrum acquisition and analysis of (saved) X-ray spectra.

Objects
permits point, multipoint and area EDS analysis.

Line scan
is used to perform qualitative and quantitative line scan EDS analysis.

Mapping
allows the acquisition of maps: intensity maps and HyperMaps (Bruker's position-tagged spectrometry tool (spectral imaging)). Mapping also includes the chemical phase analysis tool **AutoPhase.**

Imaging
allows capturing and processing saved electron microscope images.

☞ The name of each workspace is displayed on the icon, if the **Large style buttons** checkbox under **System** / **Appearance** is activated.

☞ When changing the workspace during an active measurement, a confirmation dialog box pops up and after clicking OK the current measurement will be terminated.

Feature
is used to perform particle analysis and chemical classification. Refer to the ESPRIT Feature User manual for details.

EBSD
gives access to the fully integrated EBSD (electron backscattered diffraction) analysis package. Refer to the QUANTAX EBSD User Manual for more details.

Jobs
is the workspace for configuring ESPRIT's powerful analysis automation tool and running unattended fully automatic data acquisition tasks.

Scripting
permits writing and running user defined scripts.

System
is used to adjust global settings and different calibration parameters of existing detectors. Additional functions: display settings (language, font size); license management; communication with electron microscope and motorized sample stage.

⚠ DANGER

Take special care when changing any parameters in the **System** workspace. Not only do these changes affect all QUANTAX user profiles, they may influence measurement results. Using the system with wrong **Microscope** and **Stage** parameters may damage the electron microscope.

4.4 Display Control

Program window and title bar. The title bar at the top of the ESPRIT program window contains the general control buttons common to the Windows® applications.

The complete ESPRIT window can be resized by dragging and pulling the handle on the bottom right-hand corner or on one of the border lines. To switch to full screen display, click the icon in the title bar; switch back by clicking the icon. The icon minimizes the program window. The icon activates the program help system. Please note that the icon closes ESPRIT completely, not just the active workspace.

To scale individual parts the striplines between different screen areas on the ESPRIT interface can be dragged (a changing mouse cursor indicates availability of this option).

Full screen / dual screen mode. An image or a diagram chart can be decoupled from the ESPRIT window and switched to full screen by clicking the full screen symbol on the upper right-hand corner of the corresponding screen area. If a second monitor is attached, the decoupled window can be dragged and pulled to the second monitor and ESPRIT can be used in extended display mode. Revert from full screen mode by pressing the ESC key or clicking the full screen symbol again.

Configurator bar. The configurator bar compiles all attached hardware parts as well as information about the sample and standards, the scan settings and the report and project editor. All parts of the configurator bar are described in detail in section 4.5.

Image capture chart. The workspaces **EBSD, Objects, Line scan, Mapping** and **Imaging** have a dedicated chart for controlling the electron image capture. Analysis spots, objects, scan lines, and mapping areas can be defined on the captured image. Image capture is controlled directly from the current workspace.

One or two of the imaging detectors (typically SE and ARGUS, when available) can be connected to the QUANTAX hardware and selected for image capture.

Icons and buttons. A number of icons and buttons associated to the different workspaces and display charts are provided. All icons can be displayed in normal or large style button mode. The mode can be changed by activating/ deactivating the corresponding checkbox in the **System/ Appearance** workspace.

Using the triangles at the control buttons opens drop-down menus to enter acquisition and analysis options.

Diagram axis labels and column titles can be selected with .

Data lists and thumbnail images will be highlighted by clicking onto them. Multiple items can be selected by using the SHIFT or CTRL key to perform batch processing.

4.5 Configurator Bar

Fig. 4.5-1 Configurator bar (extended)

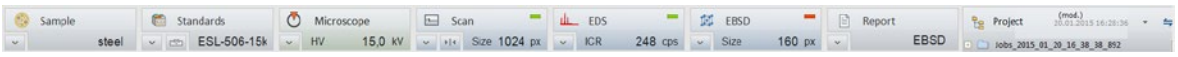


Fig. 4.5-2 Configurator bar (small)

The configurator bar consists of a horizontal row of buttons (configurators) in the upper part of the ESPRIT window that mostly allow the configuration of the hardware components available in the QUANTAX system. The number of configurators that actually appear on the screen depends on the license and may differ from the images shown in this manual.

The individual configurators display relevant adjustable parameters of sample, standard libraries, X-ray excitation sources, scan unit, spectrometers, EBSD and other detectors, as well as the report and project tools. They will be explained in detail in the next sections.

The configurator bar is resizable by moving the lower stripline. The configurator bar can be minimized by pulling the stripline upwards. When minimized, the individual configurators show only one parameter.

The parameter to be displayed can be set by the user by clicking with the right mouse key on the displayed value in the configurator and selecting the desired parameter in the **Select entry** menu.

Use the downward-facing arrow in the left bottom corner of a configurator (or icon, depending on the display mode) to access the corresponding configuration dialog.

4.5.1 Sample Configuration

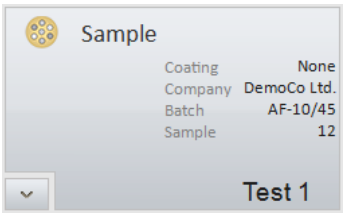


Fig. 4.5-3 Sample configurator

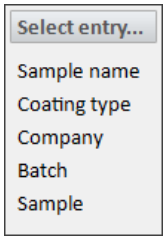


Fig. 4.5-4 Sample configurator select entry menu

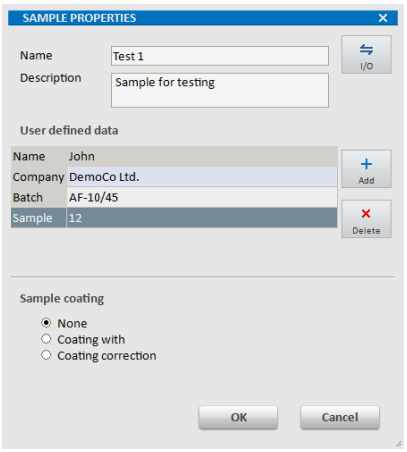


Fig. 4.5-5 Sample properties dialog

The **Sample configurator** is used to display and manage information about the sample. The information displayed is divided into the following parameters:

- Sample type
- Coating type
- Company
- Batch
- Sample

The parameter to be displayed can be set by the user by clicking with the right mouse key on the displayed value in the configurator and selecting the desired parameter in the **Select entry** menu.

When clicking on the  icon in the bottom left corner of the **Sample** configurator, the **SAMPLE PROPERTIES** dialog pops up.

Before measurement, general properties of the sample can be entered in this dialog. All subsequently collected data (EBSD map, spectrum, image, line scan, map) will contain these parameters. Default input parameters are name and description. Additional user defined data can be added e.g. coating type, batch, etc. Additional user-defined data can be added clicking the  icon.

4.5.2 Microscope Configuration

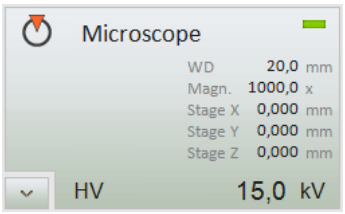


Fig. 4.5-6 Microscope configurator

The **Microscope configurator** displays the main parameters of the electron microscope.

- Magnification: Image magnification set on the electron microscope.
- High voltage: Acceleration voltage set on the electron microscope.
- WD (working distance): Sample – pole piece distance [mm].
- Stage X, Y, Z: Microscope stage position coordinates are displayed, if available

The parameter to be displayed can be set by the user by clicking with the right mouse key on the displayed value in the configurator and selecting the desired

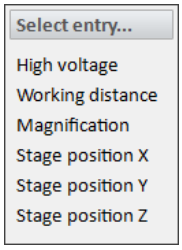


Fig. 4.5-7 Microscope configurator select entry menu

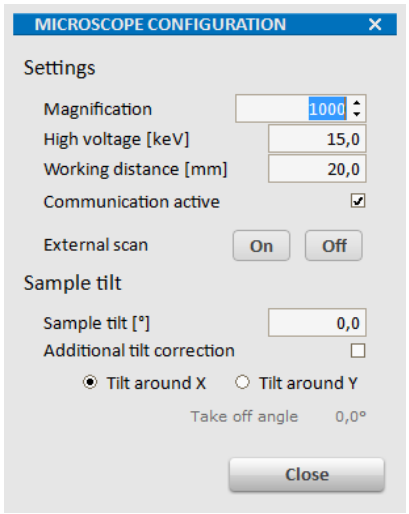


Fig. 4.5-8 Microscope configuration dialog

☞ Because sample tilt affects the take-off angle and hence the Bremsstrahlung background, its value affects the quantification results.

4.5.3 Scan Configuration

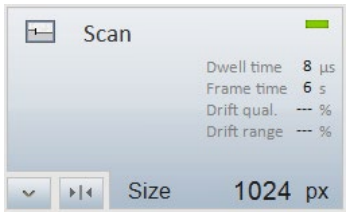


Fig. 4.5-9 Scan configurator

parameter in the **Select entry** menu.

When clicking on the  icon in the bottom left corner of the **Microscope** configurator, the **MICROSCOPE CONFIGURATION** dialog pops up. If the data communication between microscope and ESPRIT is active, the microscope parameters **Magnification**, **High voltage** and **Working distance** will be automatically transferred from the microscope to ESPRIT and displayed in this dialog.

Communication active. This option should be checked to maintain communication between the microscope and the ESPRIT software, otherwise relevant microscope parameters will not be transferred to ESPRIT. The communication is set up during installation and automatically enabled after starting ESPRIT.

If the communication is disturbed or not available with the current type of microscope, the microscope data has to be entered manually. To disable automatic data transfer intentionally, uncheck the control box **Communication active**.

Sample tilt [°]. When switching between different analysis modes, imaging at no tilt to TKD (-10**°** to -15**°** tilt) or to EBSD (70° tilt) the value of the sample tilt (in degrees) has to be entered in this field manually.

Additional tilt correction. Check this option, if the sample is tilted and the microscope has no image tilt correction capability. This is recommended when performing EBSD or TKD analysis in order to correct the tilt related distortions in images, element or orientation maps.

The **Scan configurator** displays the scanning parameters:

- Image resolution: Image size in pixels
- Dwell time: Signal collection time of a single pixel during image acquisition
- Frame time

The parameter to be displayed can be set by the user by clicking with the right mouse key on the displayed value in the configurator and selecting the desired parameter in the **Select entry** menu.

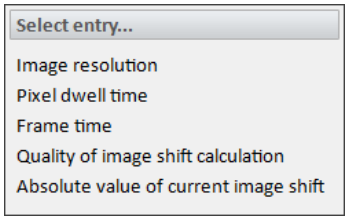


Fig. 4.5-10 Scan configurator select entry menu

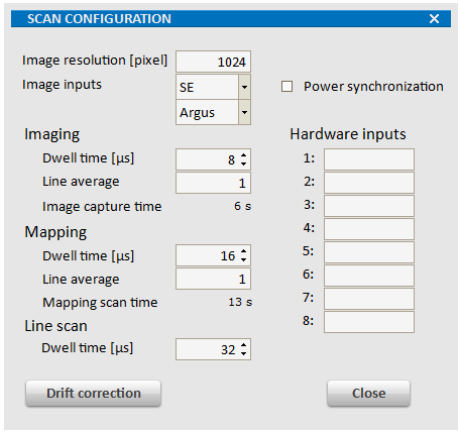


Fig. 4.5-11 Scan configuration

☞ When using the imaging system it is recommended to use dwell times of at least 8 µs.

☞ The dwell time can only be set in increments of numbers which are a power of two. Direct input of arbitrary numbers is not possible. Use the arrows in the input field.

☞ The line average factor can also be set from the dialog that opens after clicking the icon next to the image chart.

When clicking on the icon in the bottom left corner of the **Scan** configurator, the **SCAN CONFIGURATION** dialog pops up.

Image resolution. The entered value applies to the image width. Since the image aspect ratio is defined by the microscope and set during installation, the image height value is set automatically and is not displayed here.

Image inputs. If more than one image detector is connected to the QUANTAX scan system, e.g SE. BSE, ARGUS™, the desired detector can be selected here. For each channel only one image detector can be selected at a time.

Imaging. The **Dwell time** is the time the electron beam stays on a point while capturing an image. Select expanded dwell times to allow filtering and averaging of the image signal and obtain less noisy images. The **Line average** factor controls the number of times a horizontal line is scanned in the slow scan direction and averaged before proceeding to the next line. Increasing this factor provides noise reduction and expanded dwell times. Line averaging limits the increasing strain on the sample by maintaining a high scan speed. The line average factor will multiply the total image acquisition time. The total **Image capture time** is calculated and displayed.

Drift correction. When clicking on this button, the **Image drift correction** dialog pops up. It is described in detail in the QUANTAX EDS User Manual.

Power synchronization. When the according control box is checked, the scan process is synchronized to the cycles of the AC mains voltage. Power synchronization substantially reduces blurring of vertical lines caused by electromagnetic interference (at the expense of the scan speed). It is applicable for capturing any image or map. However, it is normally only useful in connection with very high magnification of the microscope. A special AC/AC adapter to be connected to the QUANTAX server is provided.

Hardware inputs. The IO scan card provides 8 counter inputs for TTL impulse signals. Detailed information is given in the IO scan reference manual.

4.5.4 EBSD Configuration

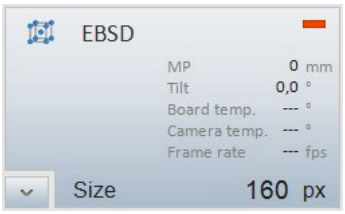


Fig. 4.5-12 EBSD configurator

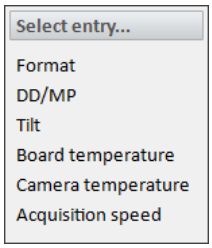


Fig. 4.5-13 EBSD configurator select entry menu

☞ If a too short DD value is used accidentally the detector will be stopped automatically once the end-stop is reached.

☞ Please note that by switching the camera **OFF** the communication with ESPRIT software will be interrupted. To reinitialize the communication it is recommended to restart the ESPRIT software after switching the camera back **ON**.

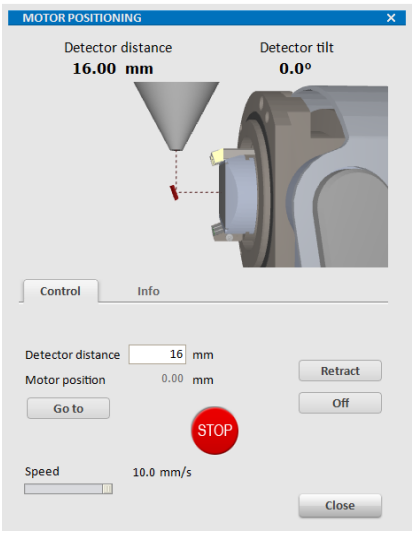


Fig. 4.5-14 Motor control interface

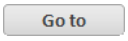
The **EBSD configurator** displays different parameters characterizing the current EBSD hardware status and geometry setup.

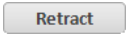
- DD (sample to Detector Distance)/ MP (motor position)
- Detector tilt from horizontal
- Frame rate (camera speed)
- Board temperature
- Camera temperature

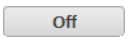
The parameter to be displayed can be set by the user by clicking with the right mouse key on the displayed value in the configurator and selecting the desired parameter in the **Select entry** menu.

The rectangle in the upper right corner of the **EBSD** configurator indicates the status of the instrument. A green rectangle means that the detector is activated and ready to use, a red rectangle indicates that the detector is idle. Toggling between activated and deactivated states can be achieved by clicking on the EBSD configurator.

When clicking on the  icon in the bottom left corner of the **EBSD** configurator, the **MOTOR CONTROL** dialog pops up. The following parameters can be set:

Detector Distance (DD). This box allows the user to type-in the distance at which the phosphor screen should be automatically positioned by the motor. When the  button is pressed the screen will start being inserted in the SEM chamber. The insertion speed can be changed using the **Speed** slide bar either before or during the screen insertion procedure.

Automatic detector retraction. The detector (phosphor screen) is automatically retracted to park position, i.e. 1mm insertion distance when the  button is pressed.

Camera can be **switched off** either manually by using the  button in the motor positioning interface or automatically at the end of a measurement (see section 5.5).

Emergency STOP. The insertion or retraction can be stopped at any moment by pressing the **STOP** button.

4.5.5 Additional Configurators

If additional detectors or X-ray sources are attached, their configurators are displayed in the configurator bar.

EDS detector(s). If one or more EDS detectors are used, the parameters of each individual detector can be set in the individual configurators. For details see the QUANTAX EDS User Manual and the XFlash® Reference Manual.

WDS detector. If a WDS detector is attached to the system, it can be configured under the WDS detector configurator. For details see the QUANTAX WDS User Manual and the XSense Reference Manual.

X-ray source. If an X-ray tube is connected, it can be configured under the X-ray source configurator. For details see the QUANTAX Micro-XRF User Manual and the XTrace Reference Manual.

4.5.6 Report

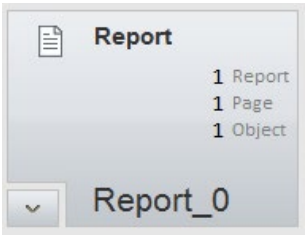


Fig. 4.5-15 Report preview

The **Report configurator** shows the number of opened reports, the number of pages, objects and the name of the selected report.

Clicking on the icon in the bottom left corner of the **Report** configurator opens the report editor. Further details on how to use the report function are described in section 5.8.

4.6 Loading and Saving Data and Results

Loading and saving data or moving to project or report can be done in two different ways: using the Import/ Export function (icon) or with a right mouse click into the data field.

A local, chart-relevant menu pops up providing the options:

- Load
- Open
- Add to project
- Add to report

- Save
- Copy
- I/O
- Print
- Export
- Properties.

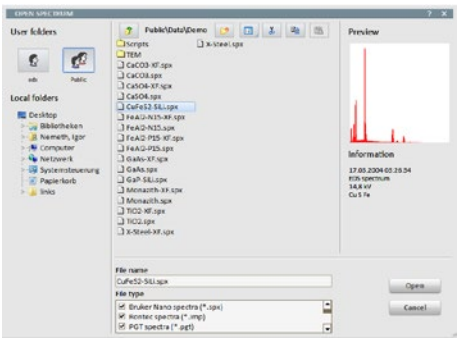


Fig. 4.6-1 File browser

Loading data. Data files can be loaded or imported into the current project, into an ESPRIT report or directly into the workspace. To open the file browser for loading data into the workspace, open the according Import/Export menu (I/O icon) and click **Load**.

Enter a filename or select a file in the list. A preview image and an info box will be displayed, if applicable.

☞ In client-server installations, local and network drives refer to the client computer. Access rights are defined by the local settings and network administration.

Note that different logical volumes are provided for general data, projects, reports, templates, and methods on the QUANTAX server.

The private data volume on the QUANTAX server is selected via the topmost icon labeled with the user name. To open the shared server folder or access the local or network drives, click the button labeled **Public** or a drive letter in the list below.

Any volume can contain an unrestricted number of folders and subfolders. To go one level up click the icon in the headline or use the Backspace button.

A list of file types selects multiple files for browsing. Only file types selected under **File type** are shown in the browser.

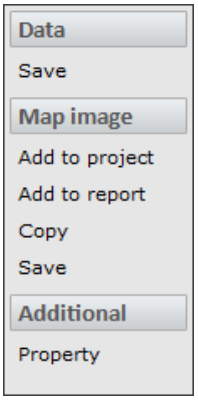


Fig. 4.6-2 Import/Export menu (e.g. EBSD map workspace)

Saving data to files. To save ESPRIT items (maps, images, etc.) open the Import/Export menu by clicking the I/O icon. Decide whether a graphic representation or data file is appropriate and click **Save** below the corresponding headline. A browser for saving files will open. The same selection of volumes and folders is provided as for loading data.

In the file browser enter or edit the file name and check the desired data format.

☞ The file browsers for loading and saving files also allow the control of the folder structure, copying and moving files between private, public, and local volumes, and performing other common file actions.

Graphic data output. Graphic export is possible using common graphical file types or the Windows® clipboard. To export graphical data to files use the option **Save** under the I/O menu subsections **EBSD map** or **EBSD profiles**. To exchange graphics via the Windows® clipboard, click **Copy** in the according subsection of the Import/Export menu or in the local menu after a right mouse click into the corresponding window area.

4.7 System Functions

Attention!
Any changes in the system settings will influence the global ESPRIT software. The user must proceed with caution when altering the system settings!

Clicking the System button in the main menu gives access to the **System** workspace. This workspace is divided into seven sections (tabs): **System**, **Appearance**, **Spectrometer**, **Imaging**, **WDS, Microscope** and **Stage**.

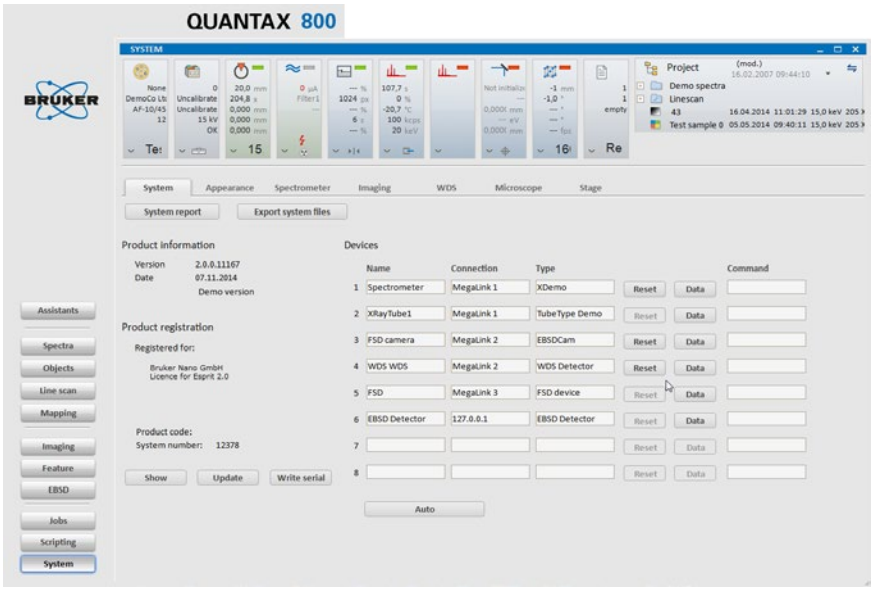


Fig. 4.7-1 Workspace System

4.7.1 System

The section **System** provides product information, user license administration, and control of the spectrometer settings. All items in this section are generally only of interest to Bruker service personnel. Unless explicitly requested, please do not alter any parameters within the system assignments.

System report. This area lists all relevant system settings. The report is valuable for troubleshooting and service. If requested by Bruker service personnel, the report can be exported via the 

icon.

Export system files. This dialog allows for export all system relevant setting files as a .zip file.

Product information. The current version of the ESPRIT software is displayed here. Please relay this information to Bruker Service upon service enquiry.

☞ The product registration is only valid for the specified system number. The system number of the current hardware is also listed in the product registration area.

Product registration. The product registration area shows the owner's registration information. Further details can be accessed by clicking on the Show button. This will launch the PDF reader to show the current product license. If a new license file is issued, the file in the ESPRIT software can be updated by clicking the Update button. A copy of the license file is stored to the QUANTAX server's profile folder. The license will be checked automatically by every time the ESPRIT software is started.

Devices. The assignment and setup of the X-ray spectrometer(s) is normally only performed during system installation.

The assignment is completely automatic. Each detector to be assigned must be connected to either the Bruker MegaLink port, a RS232 port, an USB port or via Ethernet of the QUANTAX server and powered on when the Auto button is clicked. All available ports are automatically scanned for valid connections. Once the spectrometer is located, the ESPRIT software must be restarted in order to register the newly found device.

After the restart of the ESPRIT software the available detectors are listed within the **Configurator bar** (refer to section 4.5).

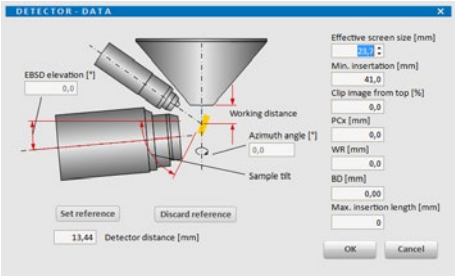


Fig. 4.7-2 EBSD detector data dialog

Clicking the Data button opens a dialog for setting parameters. The most important parameters in this dialog are the **Detector distance** which is used to define the sample-detector geometry used in the motor control dialog and the **Max. insertion length** which is a software END-stop. The latter will define the maximum distance the motor is allowed to insert the phosphor screen inside the SEM chamber. No values in this dialog should be modified by an untrained user unless specifically directed by a Bruker employee.

4.7.2 Appearance

The Appearance tab allows the user to configure settings related to the display of the ESPRIT software.

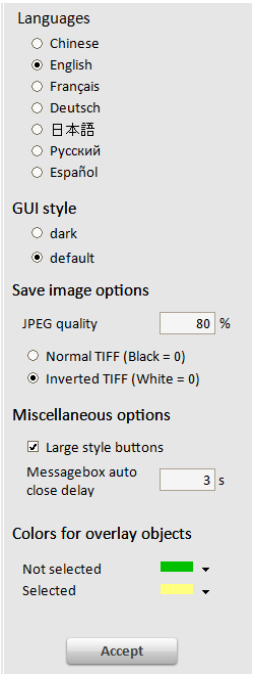


Fig. 4.7-3 Options in the Appearance tab

The subsection **Languages** allows the user to change the display language. Select a language and confirm by clicking Accept.

The **GUI style** allows user to change the ESPRIT interface to the dark color scheme for use in low light conditions (e.g. in TEM rooms).

The subsection **Save image options** permits the user to reduce the quality of the images saved in jpeg format, in order to keep to the file size low. For images saved in TIFF format. Two types of gray palettes can be selected: **Normal** TIFF assigns black to 0, and **Inverted** TIFF assigns white to 0.

In the subsection **Miscellaneous options** the user can activate/ deactivate the **Large style buttons** mode. If the checkbox is activated, the name of the workspace or function is shown on the icon, e.g. / Options. The **Auto close delay** option defines the time the mouse-over hint messages of the icons are displayed.

The **Colors for overlay objects** in different workspaces can be selected in this subsection. Overlay objects are objects (points, lines, rectangles, …) to e.g. extract and display spectral information from the mapping data cube.

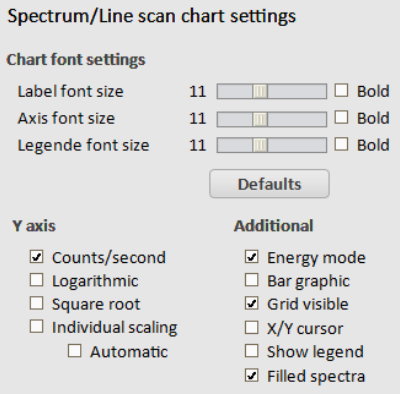


Fig. 4.7-4 Spectrum/ Line scan settings

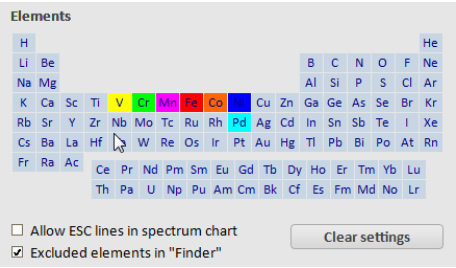


Fig. 4.7-5 Periodic table

In the **Chart settings** tab, font sizes and properties of the spectrum chart can be modified.

To use a fixed color setting for a particular chemical element, click on the element symbol on the periodic table to change the elements properties. If no specific color is defined, a random color is assigned.

The option **Excluded elements in 'Finder'** should be checked by default. This allows to see all possible elements when using the finder, even those that are excluded for the Auto ID (the Auto ID works best especially for noisy spectra, if the user excludes some elements that are not expected in the sample). The box should only be unchecked, if the excluded elements should not be shown in the Finder.

In the **Table settings** tab, the user can specify the default settings for the export of tables.

In the **Spectrum tables** tab, it is possible for the user to select the type of information the quantification table should display post quantification.

4.7.3 Spectrometer

This section applies only to EDS detectors. For details please refer to the QUANTAX EDS User Manual.

4.7.4 Imaging

The Imaging tab gives access to image and SEM stage calibration.

Image input. The image input links the communications between ESPRIT software and the SEM. The settings here are SEM dependent and should only be modified by Bruker service personnel.

Image calibration. The image calibration is performed to calibrate the pixel values within the ESPRIT software. It is possible to calibrate based on the SEM scale bars, but user should ensure that the pixel values on the microscope is up to date before performing image and stage calibration in the ESPRIT software.

A SEM standard calibration grid or any specimen that has features of known geometry can be used for image calibration. After capturing a SEM image, locate the features of the image by the green overlay line. To adjust the line, click on the line once to show the sizing handles, then drag the handles to fine tune the position of the end points of the line.

Once confirmed, enter the correct/certified values of the line length in µm. Click the Accept button to store the according calibration value.

Stage calibration. This option calibrates the stage movement alongside the SEM image for montage purposes. Before stage calibration, user must ensure that the line length (pixel calibration) is properly calibrated.

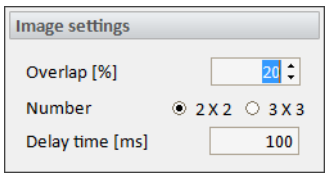


Fig. 4.7-6 Stage calibration setup

To start calibration, capture a SEM image, then open the acquisition settings by clicking on the ▽ icon in the Acquire button. The settings that can be changed here include the percentage of overlap (it is advised to use the same overlap value for actual montage acquisition in other modes), 2 x 2 or 3 x 3 images. Click on the ▽ icon again to confirm the settings.

For best results, it is recommended to switch off the scan rotation on the SEM to ensure that the stage movement matches the scan direction. Click the Acquire button to start image acquisition. A progress bar will show the progress of the image acquisition.

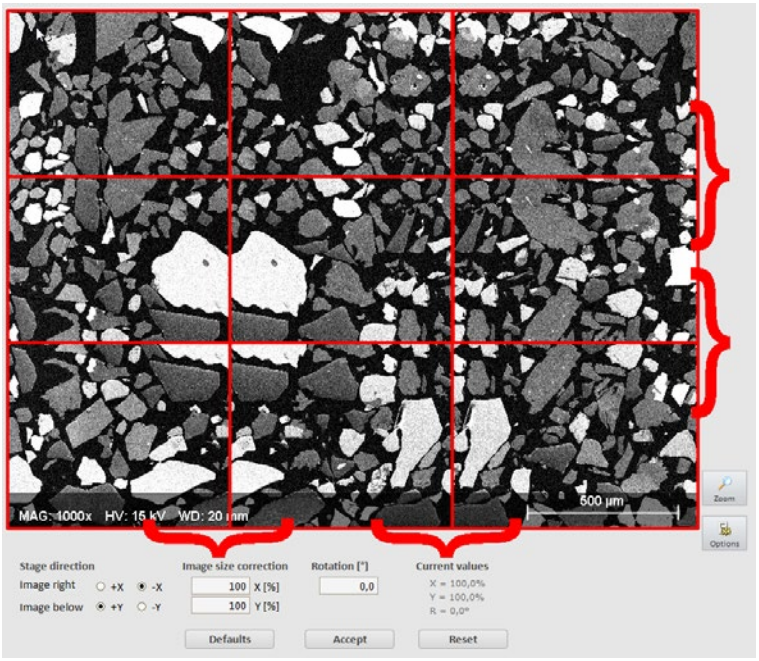


Fig. 4.7-7 Stage calibration

Once all images have been acquired, fine tune the overlap in the XY directions or the rotation and press ENTER on the keyboard. The correction in X will only change the overlap in the X direction, the same applies to Y. The rotation will change the relative rotation between adjacent fields. In the image, the red curly brackets highlight the misaligned overlaps. Adjust the overlaps and rotation in small steps. Care should be taken to focus not on the corners of the image overlaps but at the straight edges (in the corners the image distortion is at its worst).

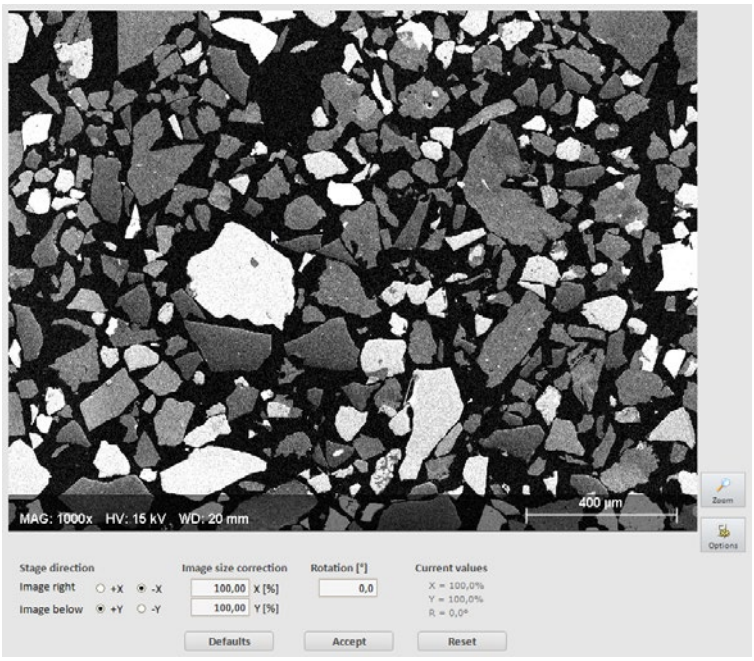


Fig. 4.7-8 Best fit of stage calibration

☞ It will not always be possible to get a perfect fit, especially with the first frame (top left) as the image may be affected by stage backlash.

Once the user has determined the best fit after adjustment, the settings can be confirmed by pressing the Accept button. The **Current values** will then be updated.

4.7.5 WDS

For details refer to the QUANTAX WDS User Manual.

4.7.6 Microscope

☞ Microscope data is also controlled via the **MICROSCOPE CONFIGURATION** dialog. To enable the microscope data transfer, the **Communication active** checkbox must be ticked.

The microscope communication settings are fixed during installation of the QUANTAX system. Image channel names are set to "Ch 1" and "Ch 2" by default. These names can be changed here to EM-specific channels (e.g., SE, BSE, HAADF,…). It is not advised for users to modify the other settings in this section unless explicitly told by Bruker Service personnel.

4.7.7 Stage

☞ The limits must not be changed without informing Bruker Service personnel.

To verify the stage limits, select the Stage tab. The stage limits for the SEM are set during installation of the QUANTAX system.

4.8 The Help System

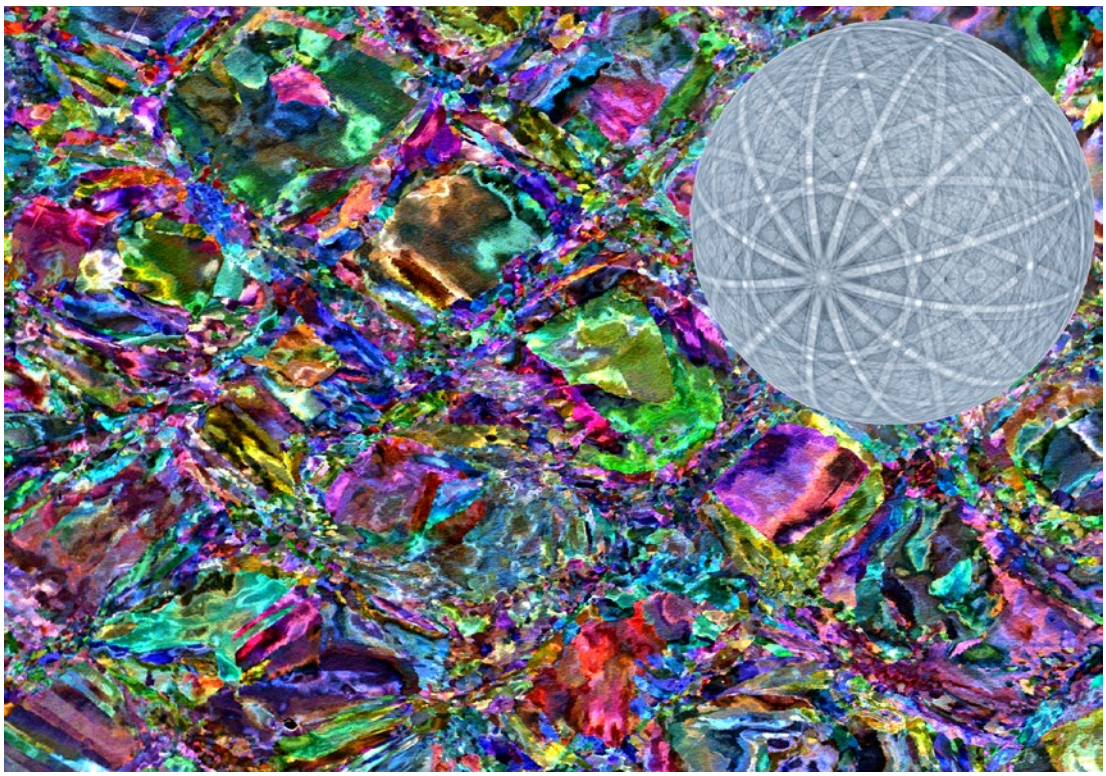
Help system. ESPRIT features a multi-level help system. Descriptions are provided for all major control elements. Dialog boxes pop up, if manual interaction is required. To prevent performing undesired actions warnings are displayed to the user.

Program help. The linked user manual can be accessed from the program window using the ? icon.

Context sensitive help. The mouse cursor is context sensitive. When moving the mouse over objects, e.g. buttons and icons, labels containing short explanations are displayed.

Assistants. Interactive assistants provide step-by-step instructions for common analytical tasks.

5 Data Acquisition and Analysis Short Reference



This chapter gives the analyst a quick overview of the most important tools of ESPRIT software, permitting a quick start to perform analyses with the QUANTAX EBSD system. In-depth discussion of specific functions and settings is left to the QUANTAX EBSD User Manual. For ease and comfort of use the relevant sections of these manuals are referenced wherever necessary.

The procedures described here assume standard (default) ESPRIT settings. They also refer to the use of a scanning electron microscope (SEM) or similar. Differences in the analysis of bulk samples and electron transparent samples are pointed out.

5.1 Preparatory Steps

This section describes the actions needed prior to starting the analytical work with the QUANTAX EBSD system.

SEM setup

	Step	Example/hints
1	Select a sample prepared for EBSD analysis. For TKD analysis refer to the TKD Quick User Manual.	*Use a conductive sample with no topography and polished surface. Stainless steel is a good example.*
2	Set the electron microscope into operation and adjust high voltage, magnification, and working distance designated for EBSD analysis.	*High voltage 20 kV* *Magnification 1000x* *WD 15-20 mm (sample size dependent)*
3	Correct the beam alignment, astigmatism, and hysteresis. If necessary, set the scan rotation.	***Required probe current might vary depending on the detector used and the desired acquisition speed. The setting of the scan rotation is required when the default beam scan direction is not parallel with the tilt axis.***
4	Use dynamic focus and image tilt correction (70 °), if available.	***Sample tilt: 70°***
5	Start ESPRIT and log in.	*Refer to section 4.1.*
6	Click the EBSD or EBSD button to select the EBSD workspace.	

Insert the EBSD detector

	Step	Example/hints
1	Switch on the IR chamber scope.	*It is highly recommended to move the detector under careful observation using a chamber scope (not only during the insertion but also for vertical shift of the screen using the tilt capability of the e-Flash detectors).*
2	Place the sample in EBSD position, i.e. at 70° tilt and under the beam.	

3 Click the icon in the bottom left corner of the **EBSD** configurator to open the **MOTOR POSITIONING** dialog.	*Insert the detector only after placing the sample in EBSD position. Always use the **MOTOR POSITIONING** dialog (refer to section 4.5.4). Using the manual interface on the detector will force the motor into losing its reference position. Any subsequent use of the Motor positioning dialog will automatically activate the retraction to reference position.*
4 Set the desired **Detector distance** (DD) in mm by entering a **Motor position** value (MP).	*It is recommended to insert the detector in two steps: first to a DD of ~25mm (good distance for FSE imaging) and then to the typical **EBSD distance** of 16mm ±1mm. It is always a good habit to observe the chamber scope image while inserting the EBSD detector.*
5 Click the Go to button to confirm the detector movement.	

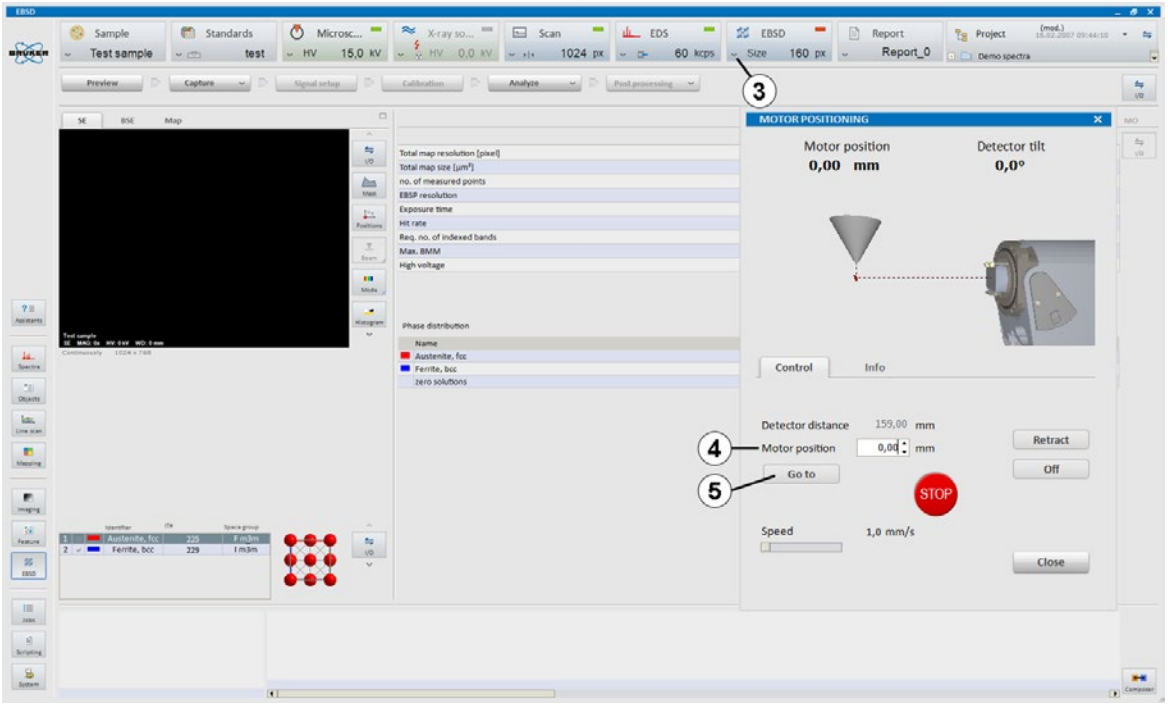


Fig. 5.1-1 Insert the EBSD detector

Image capture

Step	Example/hints
1 Use the icon in the bottom left corner of the **Scan** configurator to open the **SCAN CONFIGURATION** dialog.	
2 Define the size in pixels of the image to be acquired from the current field of view.	

3 Select which signals to be acquired, e.g. SE, ARGUS™.

4 Click ⌄ on the Capture button to open the **Capture parameters** menu.

5 Select **Continuous** image capture mode.

6 Left click outside the menu to close it and click Capture to start the image acquisition.

Switch between tabs on top of the image to see the different images, e.g. SE, ARGUS™, etc. While the image is being acquired click Capture *to stop the acquisition at the end of the frame. Click* Capture *twice to stop the image acquisition immediately. The pixel size is calculated automatically based on the magnification and the image size. Current pixel size will be displayed in the legend bar together with other details once the image capturing is complete.*

7 To change the **pixel size** to a specific value open the **Capture parameters** menu again, type in the value and confirm it by pressing the <Enter> key on the keyboard.

*To preserve the current field of view please check the **Preserve image size** box; otherwise the magnificantion will be changed to obtain the new pixel size.*

8 Capture a new image with the desired step size.

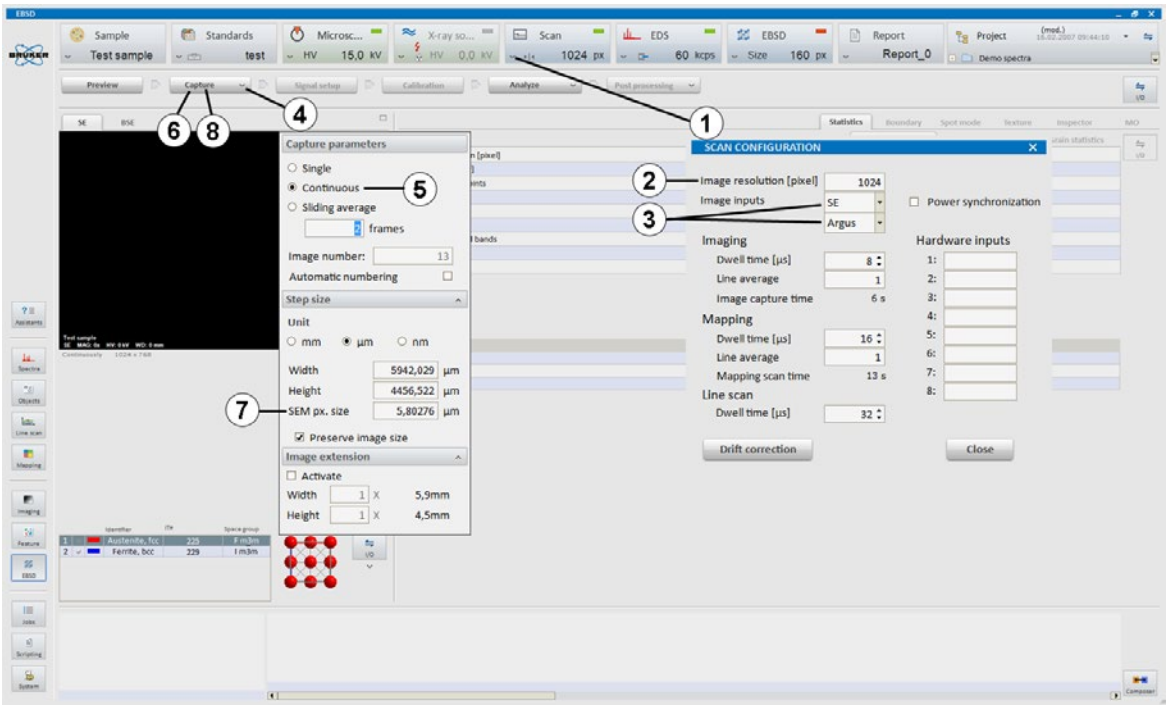


Fig. 5.1-2 Image capturing

5.2 EBSD Signal Setup

This section describes the steps required for optimizing the EBSD signal.

	Step	Example/hints
1	Click Signal setup to access the workspace where signal settings can be changed.	
2	Choose the EBSP resolution.	*160x120 pixels is an EBSP resolution that exists on both detector types and is a good start to get accustomed with how the system works.*
3	Select the Raw tab to see the live image of the phosphor screen.	*If the raw image is too dark increase one or more of the following parameters: **Exposure time** and **Gain** in the software, Probe current and kV on the SEM side. In case of image saturation decrease the values of one or more parameters listed above.*
4	Use the detector tilt hardware feature to optimize the sample-detector geometry.	*The sample-detector geometry is optimal if the brightness maximum in the "Raw" image/pattern is positioned just below the middle horizontal line. If a geometry optimization is required refer to section 4.4 in the QUANTAX EBSD User Manual.*
5	Go to the Processed tab.	
6	Check the **Dynamic background** option.	
7	Use contrast values of 0.5% to 1%.	
8	Check the **EBSP quality meter** bar to have an idea of the achievable pattern quality.	*Good values for pattern quality would be higher than 7. For more details on optimizing the EBSD signal refer to section 4.4 in QUANTAX EBSD User Manual.*
9	Click Accept once a satisfactory signal is reached.	

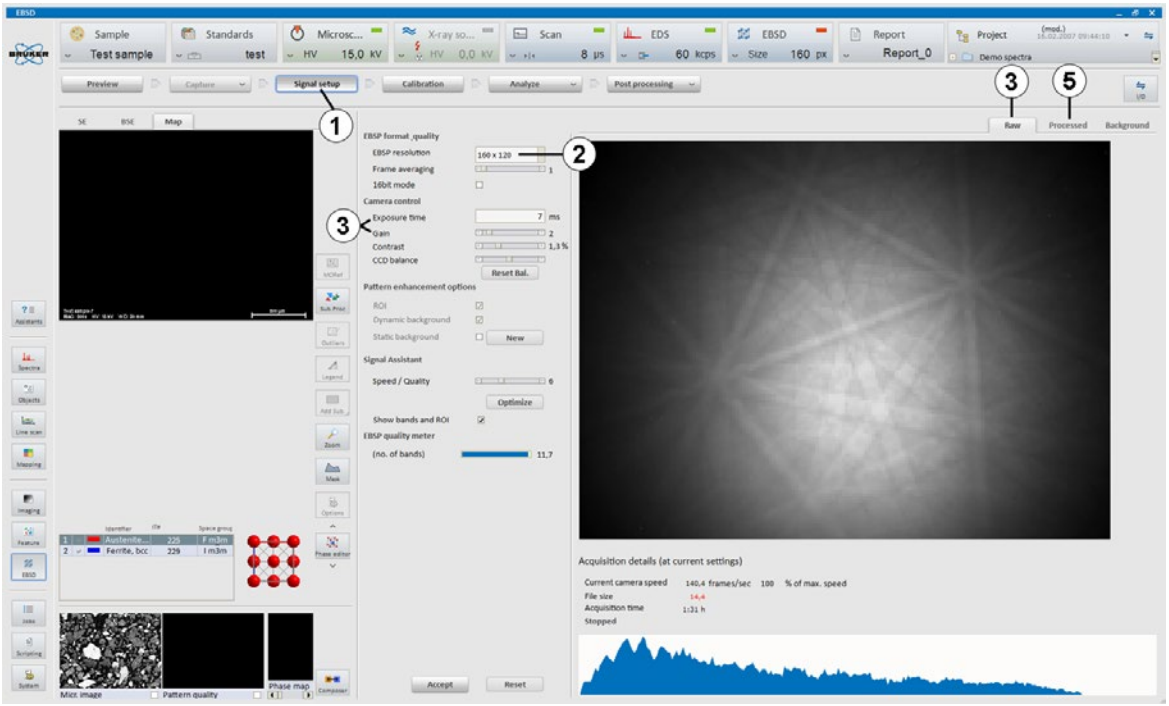


Fig. 5.2-1 EBSD Signal setup – Part 1

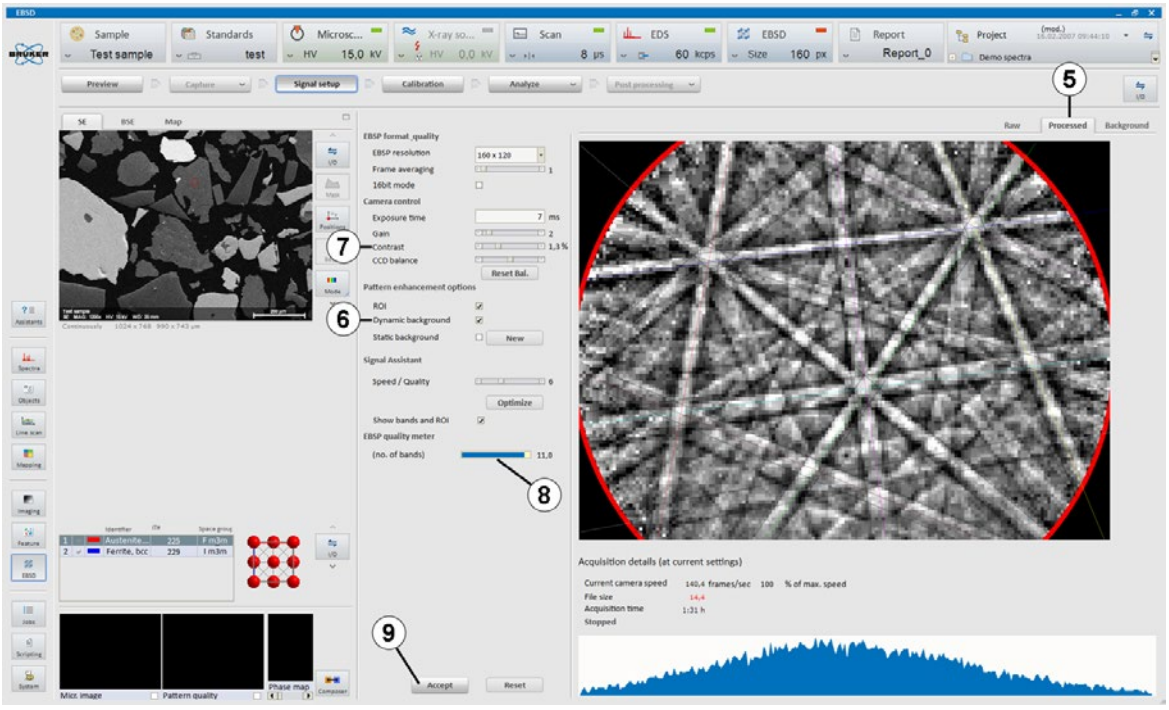


Fig. 5.2-2 EBSD Signal setup – Part 2

5.3 Pattern Center Calibration

The calibration procedure determines the screen position with respect to the sample within the SEM chamber. For this procedure the ESPRIT software requires the crystallographic details as input, i.e. phase file of at least one phase present in the sample. The calibration can be done on the sample to analyze, i.e. a standard sample is not required.

	Step	Example/hints
1	Capture an image.	*Use a relatively high magnification >1000x*
2	Click Calibration to access the pattern center calibration workspace.	
3	Click Phase list or in the phase list workspace to open the **Phase list** dialog.	*This dialog enables a search within commercial, free as well as user defined databases.*
4	Use the icon to open the periodic table and choose chemical element(s) by clicking on it.	*Alternatively, type in the element(s) symbol(s) in the box next to the Search button.*
5	Click on the Search button to start the search for candidate phase(s) that is/are present in the sample.	*A list with candidate phases appears on the left-hand side of the dialog.*
6	Select the phase to be used for calibration and indexing from the candidate list by clicking it	
7	Click the Add button.	*The candidate phase will be added to the phase list on the right-hand side of the dialog.*
8	Press the OK button to close the **Phase list** dialog.	*All changes will be accepted.*
9	Click Calibrate to start the automatic pattern center calibration.	*At the end of the calibration procedure a **Certainty** index will be given. If its value is larger than 90% press Accept to complete the calibration procedure. If the **Certainty** index is lower than 90% refer to section 4.5 in the QUANTAX EBSD User Manual for more details on how to improve the results.*
10	Click Accept to complete the calibration.	*The Calibration workspace will be automatically closed.*

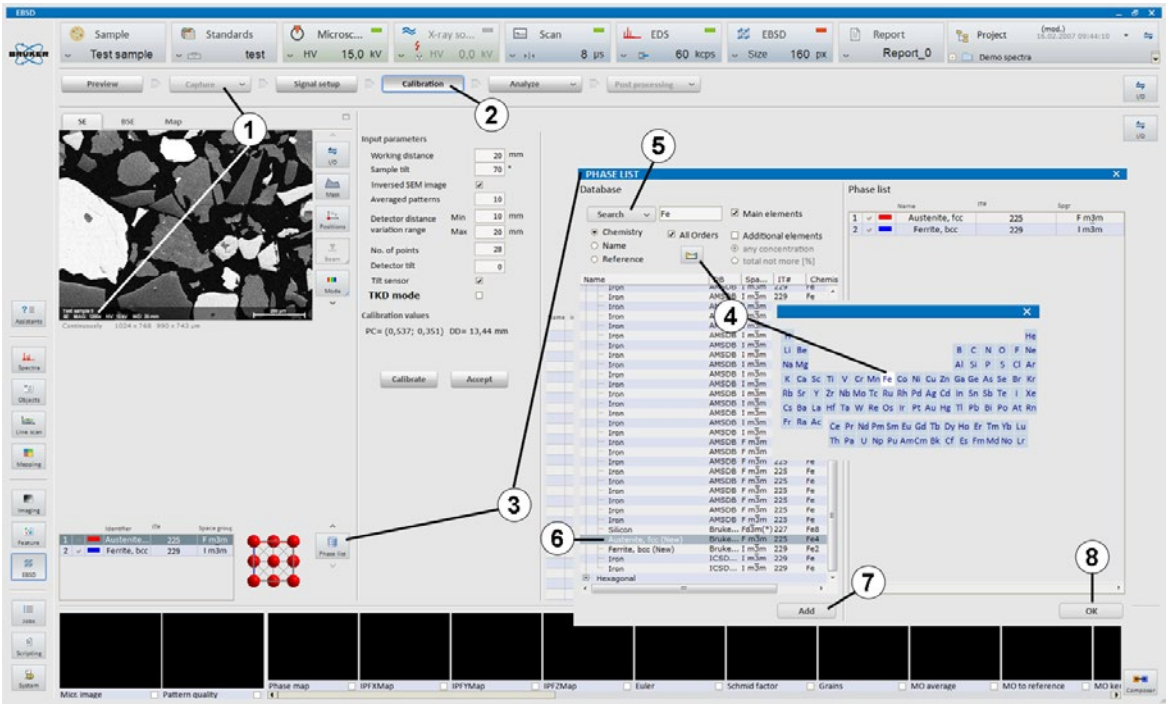


Fig. 5.3-1 Pattern center calibration – Part 1

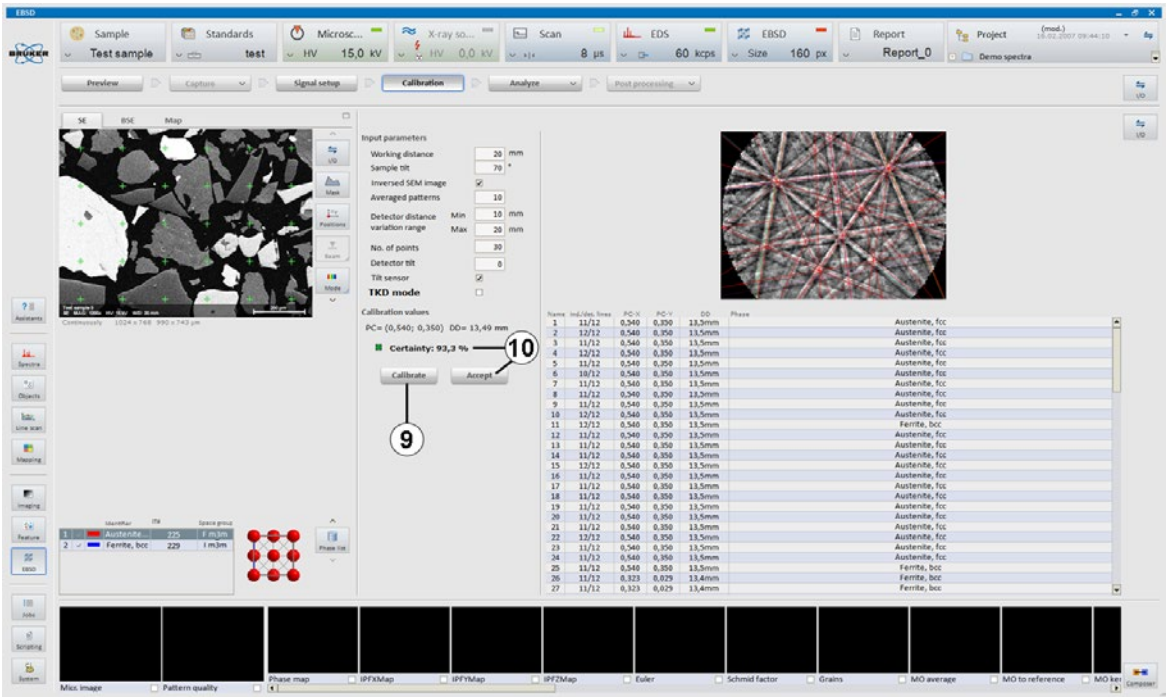


Fig. 5.3-2 Pattern center calibration – Part 2

5.4 Crystallographic Phase Editor

This section describes how to create a new phase file.

Step	Example/hints
1 Click on the  icon to open the **PHASE EDITOR** dialog.	
2 Click on the  icon and select **New** in the drop down menu.	*All shown parameters can be edited now.*
3 Click on the space group button  to access the **SPACE GROUP SETTING** dialog containing all space groups sorted by crystal symmetry.	*This button shows the last used space group and it will change as soon as a new space group is selected from the list. The dialog closes automatically after selecting the space group type.*
4 Insert the **Lattice parameters**.	*The software automatically fills in values based on the crystal symmetry, e.g. all angles to 90° for a cubic or tetragonal phase.*
5 Click on the  tab to open the atom positions interface.	
6 Click on the Ion column to modify the current atom type.	*A periodic table opens to choose a new element. Choose the atom or the given ions options depending on what is required.*
7 Insert the atom positions for the new atom type in the related columns.	*Once all atoms positions are inserted, the Wyckoff positions will be automatically added by the software. If only one atom type is used, the site occupation factor (SOF) is automatically set to 1.*
8 If another atom type or position has to be inserted, click on the  button.	*An additional atom position line will be added automatically using the values in the line above. Modify the atom type as described in step 6.*
9 Modify the position values for the added type of atom as described in steps 6 and 7.	
10 If the newly added atom uses the same positions as the already existing atom(s), change the SOF value according to the stoichiometry so that the sum of all SOF values for the same position equals 1.	*For example, in a stainless steel containing 10 % Ni, 18 % Cr, and the balance Fe the SOF values should be 0.10 for Ni, 0.18 for Cr, and 0.72 for Fe.*
11 Edit/modify the phase name as **Identifier** and the **Chem. Formula**.	*More details on editing the atom positions table can be found in section 4.7.3 of the QUANTAX EBSD User Manual.*
12 Click on the  icon again and choose **Save** to open the **SAVE TO DATABASE** dialog.	

13 Select an existing user database or type in a name to create a new one. The newly created phase will be added to the selected user database.

Once added to a user database a new phase will immediately become available during advanced phase ID or phase search, i.e. there is no need to restart the software.

14 Save all changes.

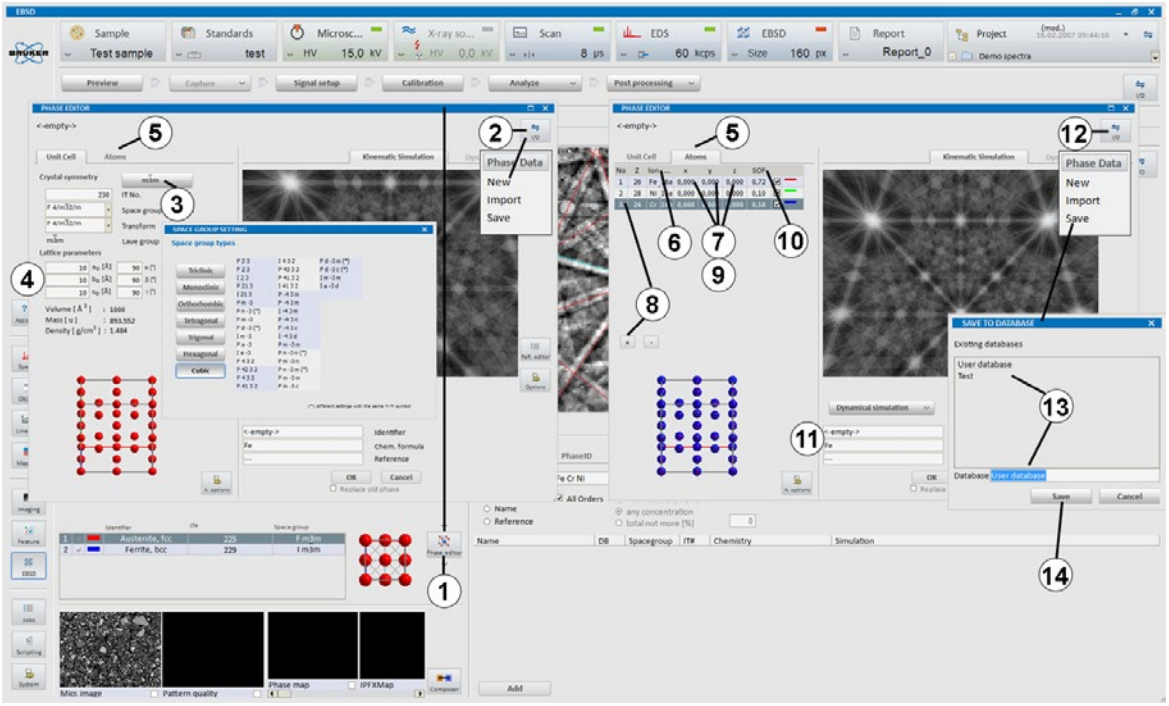


Fig. 5.4-1 Crystallographic phase editor

5.5 Automatic Data Acquisition

This section explains the steps to be taken before launching an automatic data acquisition.

	Step	Example/hints
1	Click on the Analyze button to open the analysis parameters menu.	
2	Go to the **Quantification** sub-menu and check the **EDS spectra acquisition** to acquire simultaneously EBSPs and EDS spectra.	*This step is optional.*
3	If necessary, the total acquisition time can be drastically shortened by using the slider in the **Pixel size** sub-menu.	*Please be aware of the fact that by using the raster feature the step size or pixel size will increase according to the raster size.*
4	Go to the **After measurement** submenu and select the options required for the current measurement.	*These actions are performed automatically. Check the corresponding boxes to activate each feature. For example, check the Retract detector and Switch off camera boxes for these actions to be taken automatically at the end of the measurement.*
5	**Retract detector**	
6	**Switch off camera**	
7	**Beam off**	
8	**Automatically save data**	*When checking **Automatically save data** a dialog opens where the file name and the location/folder can be entered.*
9	**With patterns**	*Patterns can also be added to the file as well as EDS spectra if they were acquired during the measurement by checking the corresponding boxes.*
10	**With spectra**	

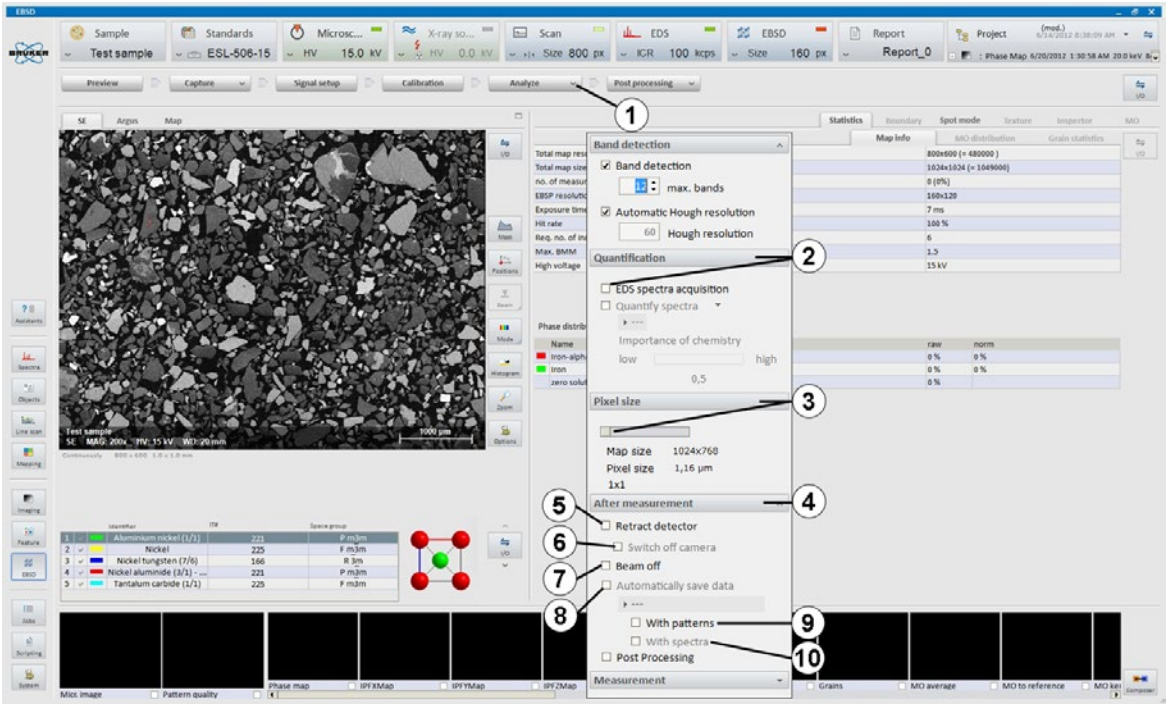


Fig. 5.5-1 Automatic data acquisition options

5.6 Spot Mode Analysis

The Spot mode is mainly used for phase identification analysis but can also be used for acquiring high quality patterns and/or spectra for publication purposes. This section briefly describes the main options available in spot mode. For a detailed description of all features and capabilities please consult the QUANTAX EBSD User Manual (section 4.6).

	Step	Example/hints
1	Select the Spot mode tab to access the corresponding Spot mode workspace.	
2	Select a particle/grain in the EM image that produces good quality patterns.	*A small red cross hair on the EM image defines the selected spot.*
3	Go to the Spectrum tab situated below the Spot mode tab to access the corresponding Spectrum workspace.	
4	Acquire a spectrum.	
5	Use the Elements icon and the **Auto-ID** or **Finder** function to identify the major element(s) present in that selected spot.	
6	Write the found elements in the box next to the **Search** button.	*Use space as a separator between the elements.*
7	Select the Pattern tab (next to the Spectrum tab) to access the EBSP workspace.	
8	Search for candidate phases through the available phase databases.	*Use the major elements found in the EDS spectrum (steps 3 - 5). If the major elements are known, they can be manually inserted without the need to use the* **Spectrum** *workspace.*
9	Go to the PhaseID tab.	*The* ***Phase ID*** *tab is situated next to the* ***Database*** *tab (right above the* ***Search*** *button.*
10	Press the PhaseID button.	*The software will automatically test all the phase candidates against the current EBSP and sort the solutions based on the quality of fit. For more details on the phase identification procedure please refer to section 4.6 in the QUANTAX EBSD User Manual).*
11	Click on one of the phases appearing in the list to check the quality of fit to the experimental pattern visually.	*The list contains all candidate phases sorted based on the fit quality. Due to duplicate phases present in the crystallographic databases or to the presence of very similar phases there could occur many phase candidates with the same good fit. In this case the user will have to use other details related to the sample to decide which phase will later be used for mapping.*

12 Drag & drop the newly identified phase to the phase list below the EM image.

The phase ID procedure can be used "online" at the SEM as well as "offline" on already acquired EBSD/EDS data. When working offline it is recommended to use files containg the EBSPs to allow the manual band re-detection which is critical for accurate phase identification.

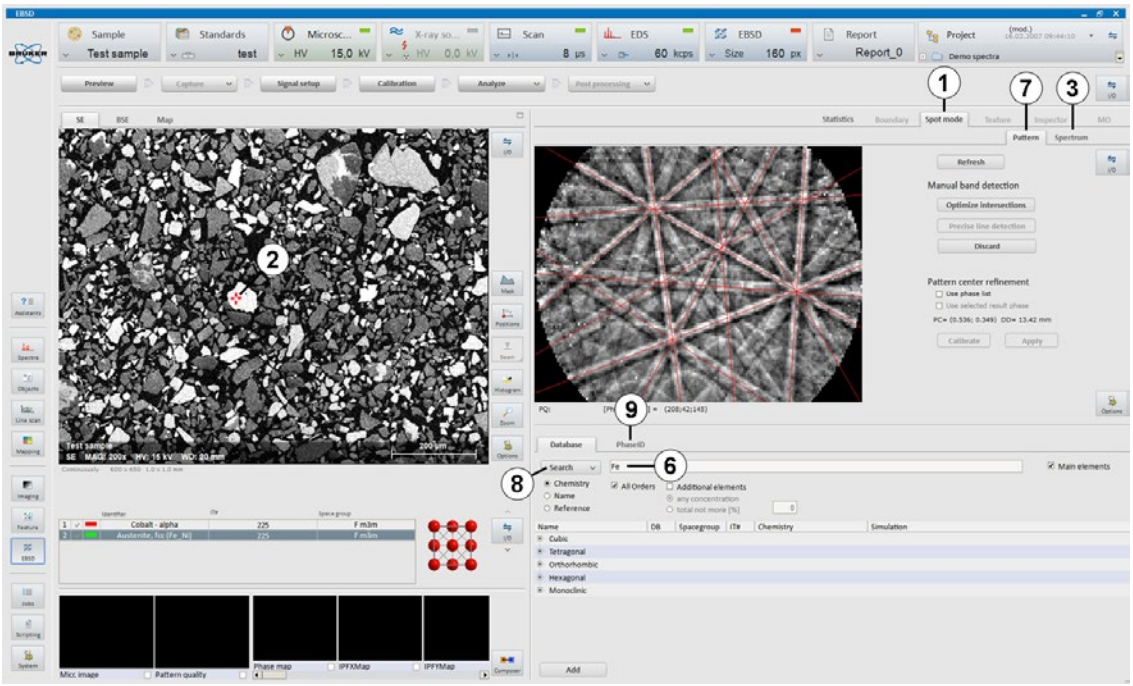


Fig. 5.6-1 Spot mode analysis – Part 1

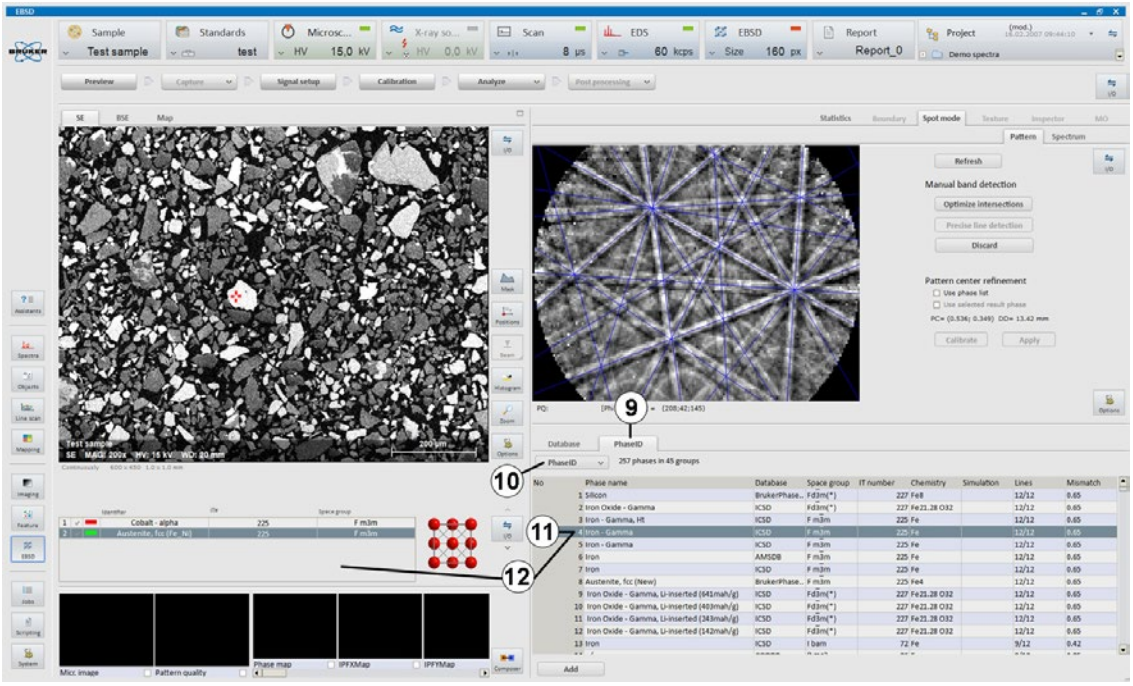


Fig. 5.6-2 Spot mode analysis – Part 2

5.7 Data Analysis and Post-Processing

This section describes the data analysis and post-processing options available during and/or after the measurement.

	Step	Example/hints
1	Load an EBSD map using the workspace I/O button	
2	Use the Options icon in the **Map** window to open the corresponding menu.	
3	Go to the **Shown solutions** sub-menu.	
4	Remove misindexed points by controlling the minimum number of bands to fit the simulation and the maximum band mismatch.	*Try with 5 bands and a band mismatch of 1.8°. Refer to section 4.9.6 in the QUANTAX EBSD User Manual for more details on this topic. This data filtering works during the measurement as well as on loaded maps.*
5	The following options are available for visualizing and/or interpreting EBSD data during the measurement as well as on loaded data:	
	Tab **Statistics/** Tab **Map Info**	*Displays a multitude of measurement parameters as well as the phases fraction in the scanned area.*
	Tab **Statistics/** Tab **MO distribution**	*Displays the misorientation angle distribution histogram.*
	Tab **Statistics/** Tab **Grain statistics**	*Only available after running the postprocessing step (see step 5) and displays grain size, shape and main axis inclination angle statistics and histograms.*
	Tab **Texture**	*Texture analysis workspace with multiple capabilities, e.g. pole figures, inverse pole figures, ODF.*
	Tab **Inspector**	*Allows to check the quality of band detection, indexing, comparing the real EBSP with a simulation, check the EDS spectrum if available, etc.*
	Tab **MO**	*Displays the misorientation profile along a line which can be calculated in relation to the first or to the previous point along the line.*
	Tab **Boundary**.	*The grain boundary analysis workspace becomes available only after running the postprocessing step.*
6	Click on the Post processing button to open the corresponding menu.	
7	Go to the **Grain detection** sub-menu.	
8	Define the **Max. misorientation angle** and the **Min. grain size**.	*To be used for grain detection.*

9 Select the **Kernel size** in the **Misorientation kernel** sub-menu to be used for calculating the Kernel Average Misorientation (KAM) map.

10 Go to the **Grain boundaries** sub-menu.

11 Check the **Remove 60°<111> twins** option to disregard this special type of boundaries during the grain detection process.

12 Check the **Sub-grain boundary** option.

13 Select the minimum misorientation angle criterion for the detection of sub-grain boundaries.

14 Click OK to start all calculations.

*The Kernel and the Grain Average Misorientation maps will not be calculated if the **Remove 60°<111> twins** option is activated.*

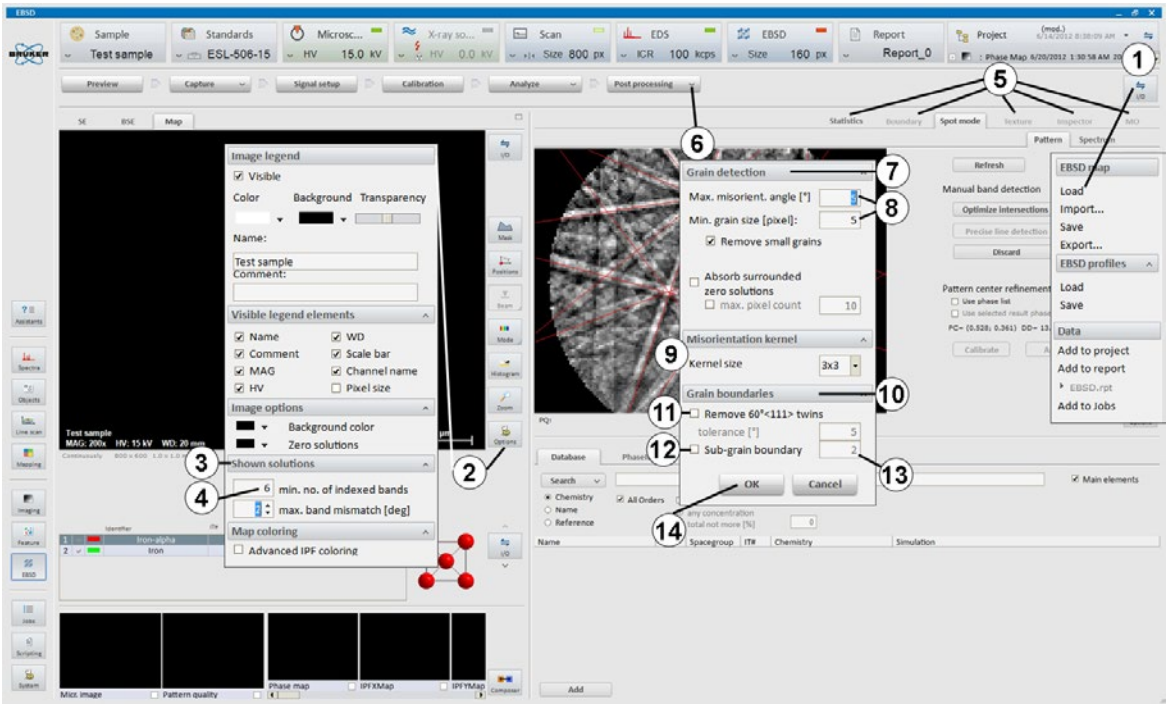
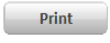


Fig. 5.7-1 Post-processing options

5.8 Creating a Report

This section describes how to create a report based on the data obtained or processed by QUANTAX ESPRIT.

Step	Example/hints
1 Select a workspace and perform an analysis or process data.	
Add data to report:	
2a Use the workspace  icon and select **Add to report**	*All results contained in the workspace will be added to the report.*
2b Use the chart  icon and select **Add to report**	*Alternatively, right click into the chart and use the local menu.*
2c Use the thumbnail bar  icon and select **Add to report**	*Available in the **Mapping** or **Line scan** workspace. Alternatively, a right mouse click into the thumbnail bar opens the corresponding local menu.*
2d Use the right mouse click and select **Add to report**.	
3 Use the  icon at the bottom left corner of the report configurator to open the **Report**.	*The **Report preview/Report** is either docked to the right side of the screen or to the configurator bar. The display can be changed using the icon in the **Project** tool.*
4 Edit/ review the report	
a) Use **Zoom** to set display	
b) Use **Properties** to set object layer order	*Objects are displayed as layers. Uncheck **Fixed** when moving an object. Check **Pass on** to show object on every page.*
c) Use **Objects** to add text	
d) Use **Tools** for drawing	*Draw **Point, Arrow, Line, Rectangle, Circle/Ellipse**. Set fill/color/size options for selected element.*
e) Use the  icon in the **Report** editor to import data.	*Open image, spectrum or text.*
5 Rearrange order of items.	*Drag objects (maps, images, spectra…) and move them to the desired position.*
6 Use the **Report**  icon to **Save as** report.	*Alternatively, use the **Report Preview**  icon. The report is saved as .rpt.*
7 Use the **Report**  icon to **Export to WORD**.	*If Microsoft Word© is available*
8 Click the  button to print the report.	*Check page **Setup** before printing. Use printer or generate a .pdf file.*

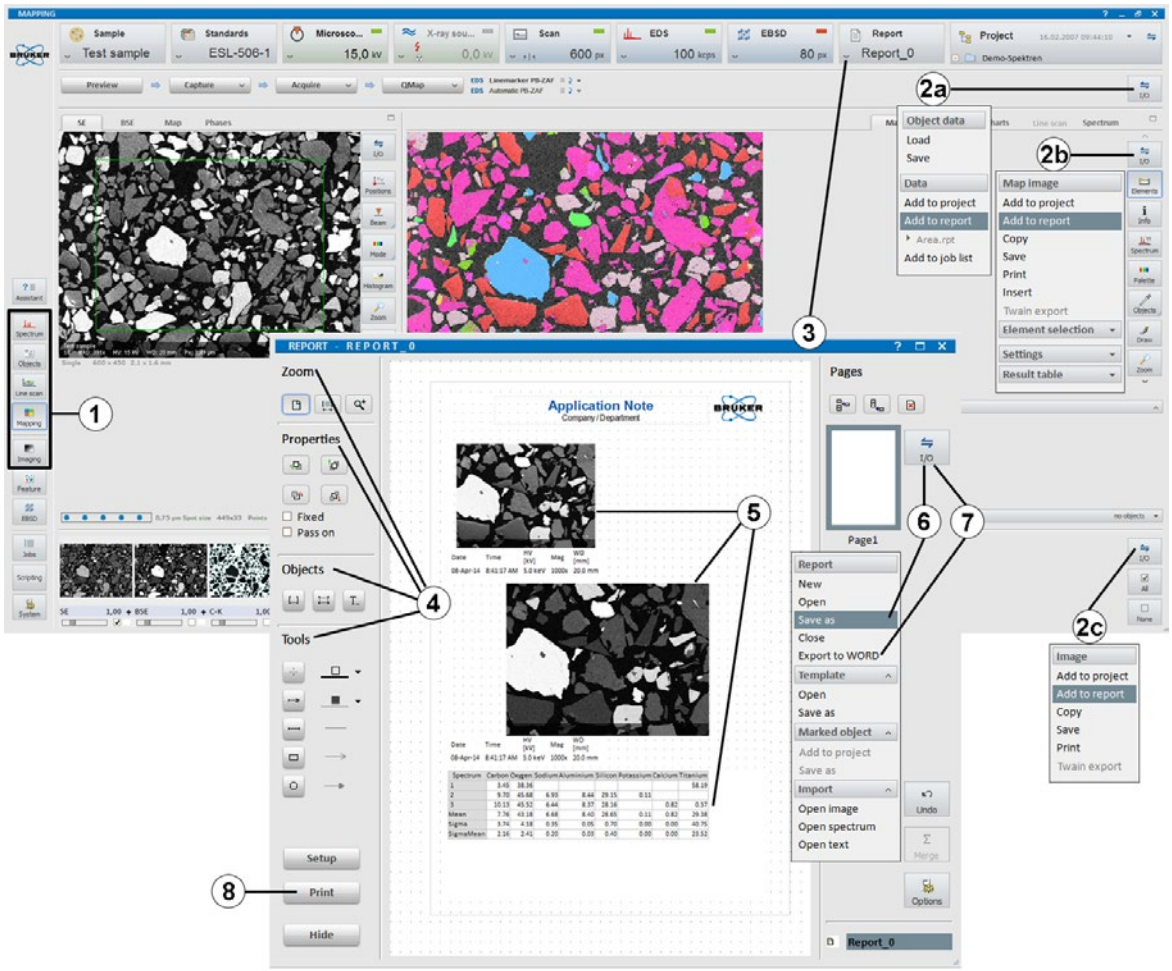


Fig. 5.8-1 Creating a report

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