

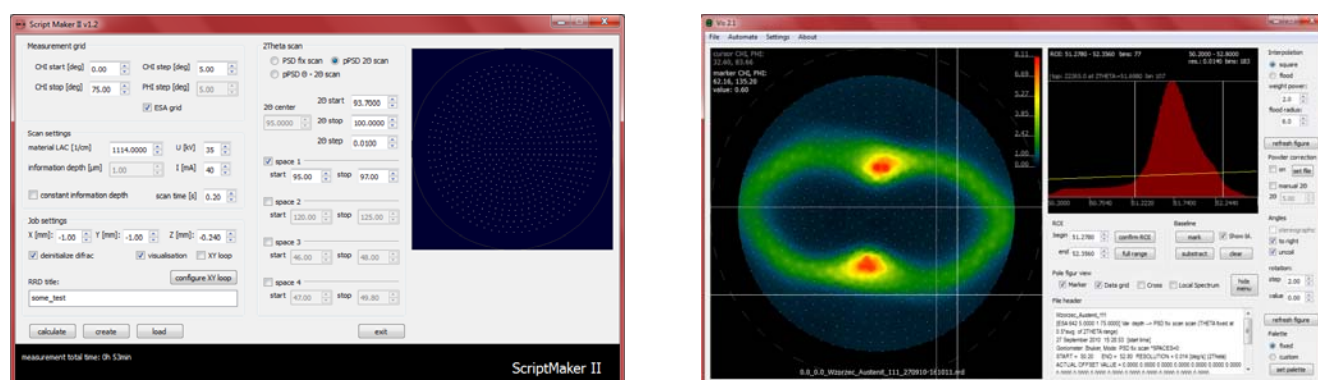


## Custom Measurement Software (CMS)

### General description

Custom Measurement Software (CMS) **Script Maker**- and **Vis**- programs (Fig. 1) have been developed at the Institute of Metallurgy and Materials Science of the Polish Academy of Sciences in Kraków (Poland). The CMS package is dedicated for *Bruker D8 Discover* diffractometer controlled with Windows XP/Windows 7 based computer, and in each aspect of the software-hardware communication is entirely based on the *Bruker User Manuals*;

- Diffrac Plus Basic, Part 11, Release 2005
- Diffrac Plus Scripting Language, Release 2000



**Figure 1.** The main screens of the CMS package consists the Script Maker (left) and Vis (right) programs

Software solutions utilized by the CMS are delivered and documented as a part of the Bruker's system, thus shouldn't interfere with its guarantee terms. Moreover, the CSM is partially run under a guidance of the standard *XRD Commander* controller to ensure the high level of technical and content-related security. Each of the programs' commands transmitting to the diffractometer processor is evaluated beforehand by Bruker's software modules supplied with the original system to check their syntactic conformity and to ensure the particular actions are in the range of the hardware limits. If any action initialized by the CMS, for some reason, is considered as impossible or forbidden (unsafe), the activated CMS's program will most likely stop before triggering of any hardware brakes.

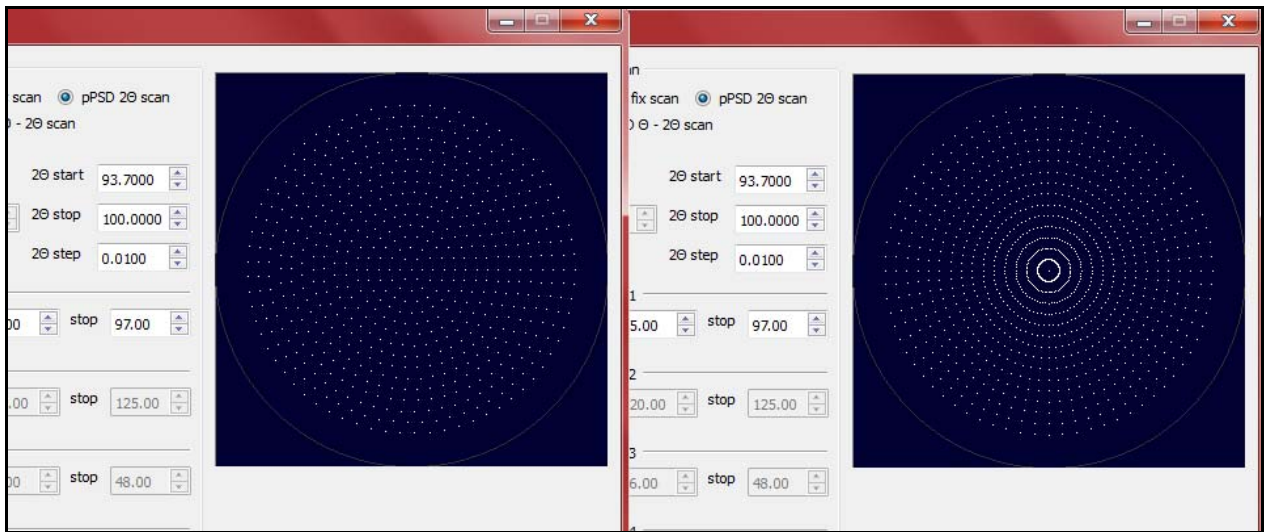
The Custom Measurement Software operates with both the point- and linear (LynxEye) detector mounted in the Bruker's diffractometer system. Anatomy of the CMS tries to overcome limitations of original Bruker's software and it is often impossible to generate a proper \*.raw file on-line. Instead of this, CMS provides procedures of exporting the obtained data to the \*.epf format file, accepted by the *LaboTex* package(LaboTex, 2010).

### Main advantages

Among a few advantages of the CMS package compared to the Bruker's standard measurement software, the following ones are the most essential:

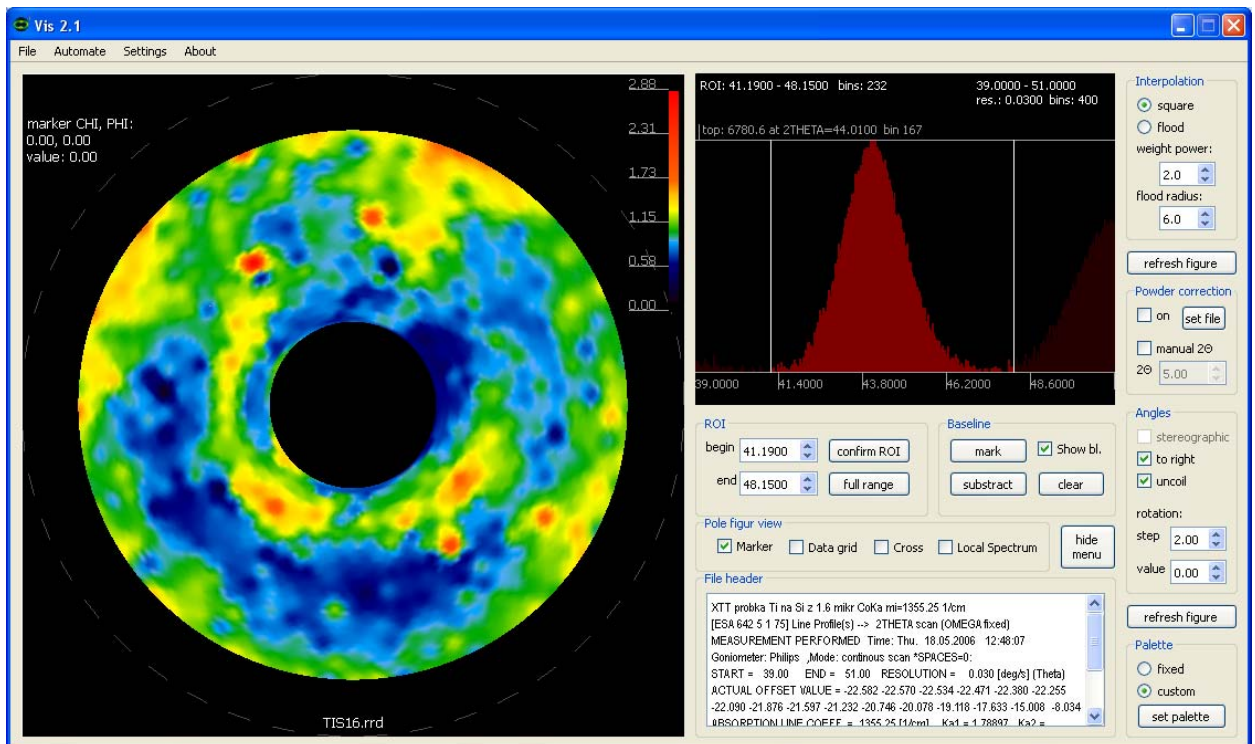
- Equal Solid Angle (ESA) measurement grid (Tarkowski, 2002) of the back-reflection pole figures (Schulz, 1949), implemented for any type of measurement, resulting in significant (above 40%) time- and electrical power saving by eliminating the resolution inconsistency across a various  $\chi$ -angles during measurement. For example, the standard (traditional) grid with a constant  $\chi/\phi$  angle step produces 1152 points for gathering data set ( $\chi$  from 0 to 75°, assuming  $\delta\chi = \delta\phi = 5^\circ$ ), but the ESA-grid consists of 642 points only, giving the results with the same

quality (Fig. 2). Experimental data based on the ESA-grid can be easily converted to the standard grid with any arbitrary (like  $5^\circ \times 5^\circ$ )  $\chi$  and  $\varphi$  steps, and, of course, the software enables to perform also the standard measurement by the constant-step grid.



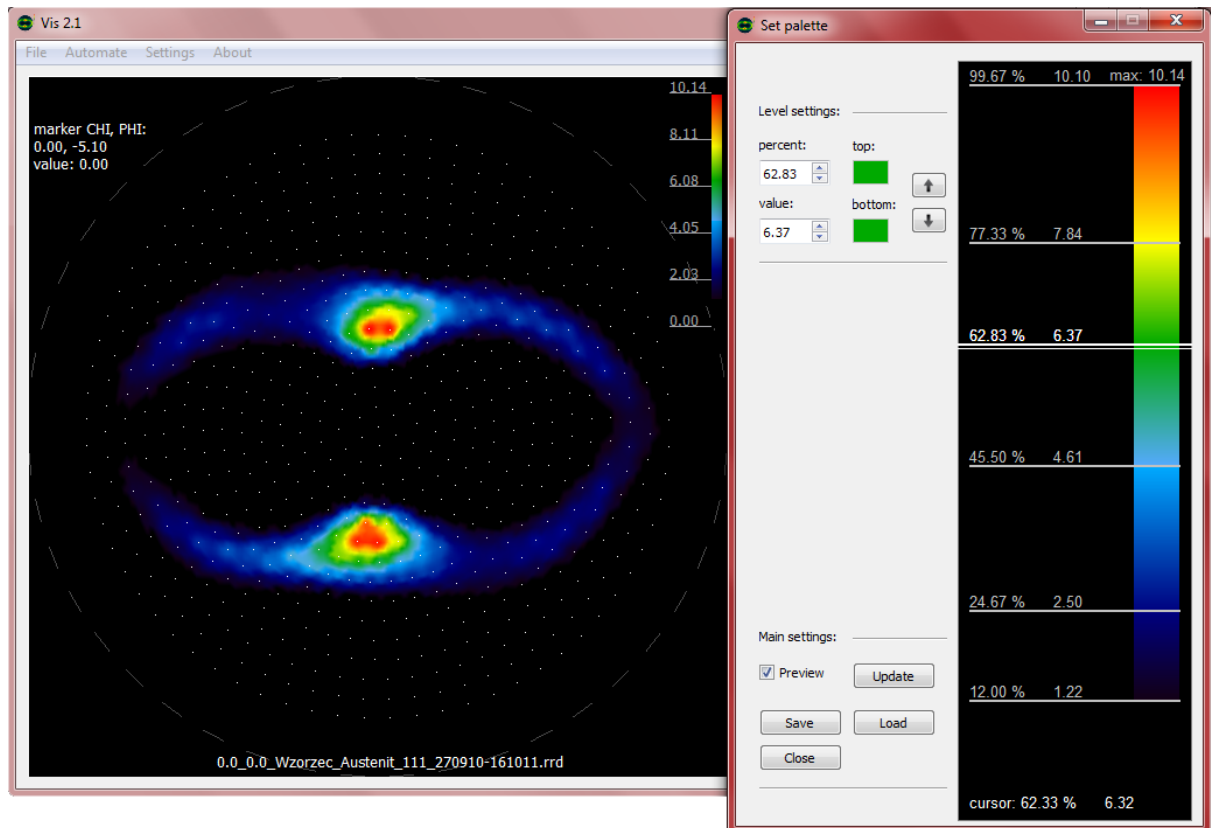
**Figure 2.** The ESA- (left) and its counterpart ( $5^\circ \times 5^\circ$ ) standard (right) measurement grid available in the Script Maker program

- Ability to registration of diffraction reflections at a specified information depth (Bonarski, 2006), regarding the examined material by introducing an additional degree of freedom (angular rotation) during the measurement procedure.
- The CMS package extends the *Bruker D8 Discover* to a tomographic XRD-system only with a new control paradigm for the existing equipment. Tomographic pole figures geometry is translated by software to the standard grids (constant  $\chi/\varphi$  step) with a modified initial  $\chi$ -angle range, making this new type of measurement as universal as standard one (Fig. 3).



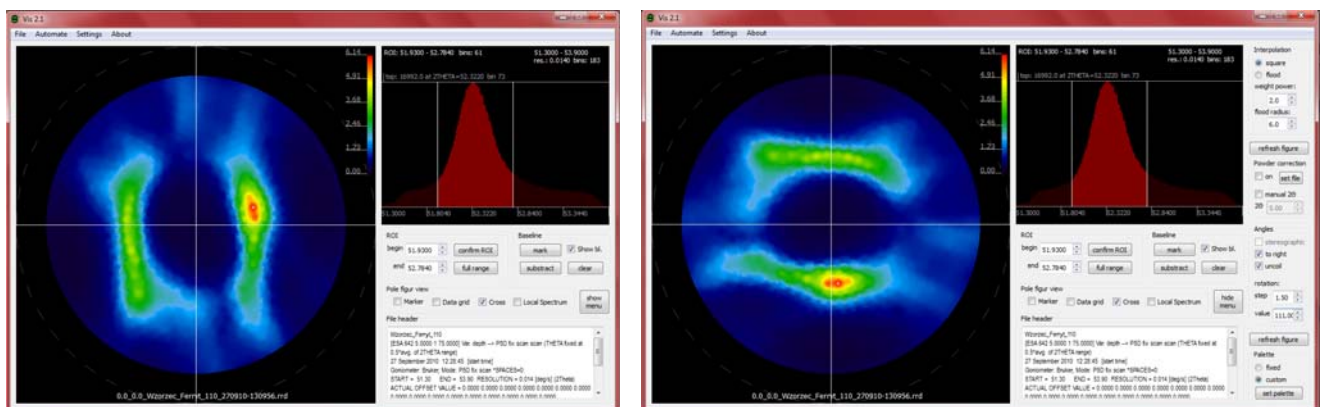
**Figure 3.** X-ray Texture Tomography: (10 -11)-pole figure of Ti (with constant information-depth = 1.6  $\mu\text{m}$ ) deposited on Si-crystal substrate obtained in measurement controlled (and monitored) by the CMS package

- On-line visualization of registering pole figures with possible definition of the spectral range of the interest for imaging, baseline subtraction, real-time color scale modifications and view of the measured spectrum for each grid point or the pole figure value at any  $(\chi, \phi)$ -coordinates (Fig. 4).



**Figure 4.** User-defined palettes can emphasis characteristic elements of pole figures

- Pole figures registered in one type of measurement-grid can be easily transformed to the other grids with different  $(\chi, \phi)$ -parameters. Visual results of the transformation are available immediately.
- Arbitrary software rotation of the registering (or earlier registered) pole figure and its extraction for export and further analysis related to a chosen, valuable part of the obtained diffraction spectrum, as well as by the *LaboTex*-package (Fig. 5).

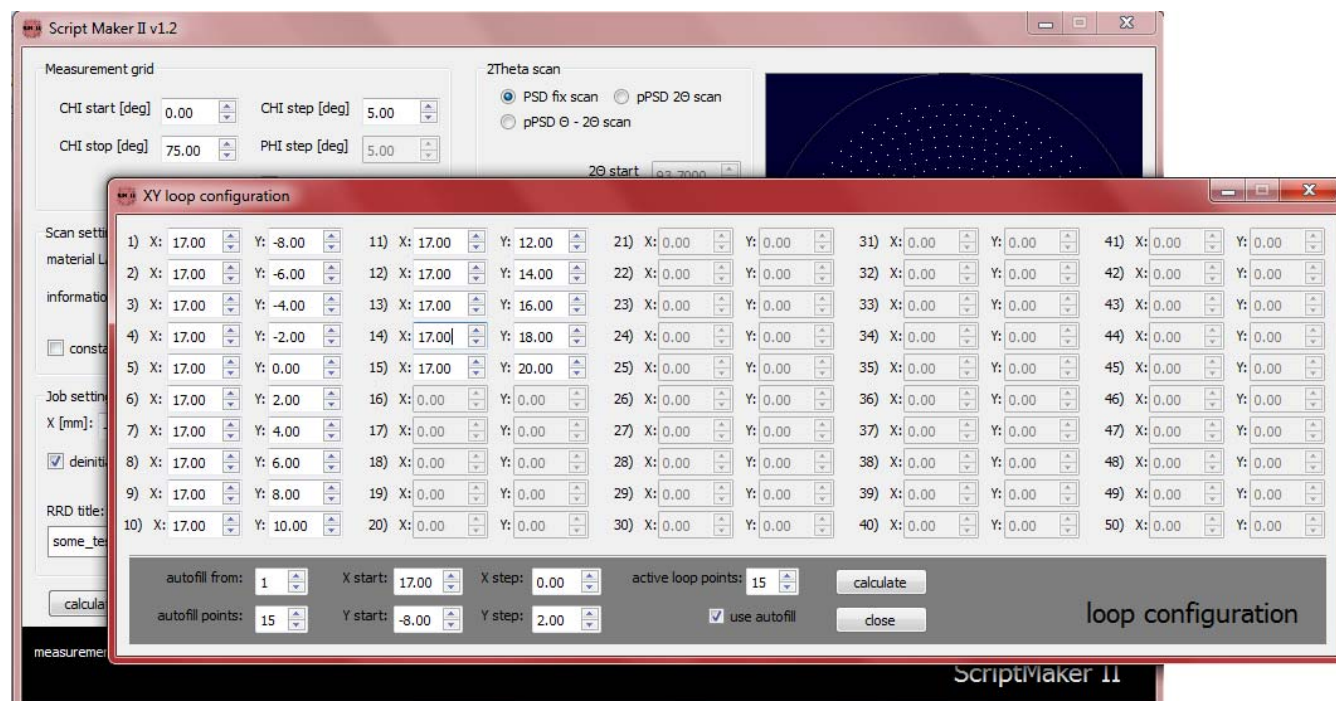


**Figure 5.** Export results only from interesting parts of spectrum and in most convenient orientation

- Ability to defining a big variety of results or procedure correction in function of  $\chi$ -,  $\phi$ -,  $\theta$ - and  $2\theta$  angles. For example, the CMS can correct the intensities in each

of the measurement ( $\chi, \phi$ )-point as a function of  $\chi$ - and  $2\theta$  value to utilize the calibration curves based on a suitable powdered sample, previously registered.

- X/Y loops in control scripts with automatically- or manually defined coordinates of measurement areas on the sample surface (Fig. 6).



**Figure 5.** Tilting angle time correction for measurements would be part of the Script Maker program, similar to a loop configuration

- Implementing the correction of measurement time as a function of the  $\chi$ - or  $\omega$ -tilting angle adapted to parameters of the Buyer's experimental set up.
- Providing an open and easy to read collected data format (in ASCII text file) for the experimentally registered pole figures with a possibility to export to the \*.epf format accepted by the *LaboTex*-package.
- The Buyer of the CMS package can also benefit from future variant of the ESA-grid developed especially to incorporate a procedure of stress measurement simultaneously with registration of related pole figure(s) in one experimental session without increasing time, including a tomographic texture- and stress measurements.

## References

- Bonarski J.-T.: (2006), *X-ray texture tomography of near-surface areas*, Progress in Materials Science, **51**, 61–149
- Schulz LG.: (1949), *A direct method of determining preferred orientation of a flat reflection sample using a Geiger counter X-ray spectrometer*. J Apply Phys. **20**, 1030–3.
- Tarkowski L., Lankosz L., Bonarski J.: (2004), *Optimisation of X-Ray Pole Figure Measurement*, Eighth European Powder Diffraction Conference, Uppsala, Sweden: Materials Science Forum, **443-444**, 137-140.
- LaboTex. (2008). *The Texture Analysis Software*. by LaboSoft s.c.

### **Remarks on installation procedure**

The Custom Measurement Software needs to be installed and tuned to particular diffractometer and computer system by representatives of the Author's team from the Institute of Metallurgy and Materials Science of the Polish Academy of Sciences in Kraków (Poland). The installation process involves evaluation of the present *Bruker* software, controlling computer OpenGL compatibility for CMS, testing of the system's visual basic scripts interpretation consistency, calculation and setting proper measurement time estimation for CMS procedures, realization of a full-scale testing measurement and a potential real-time trouble shooting of encountered compatibility issues.

The CMS installation requires administration privileges on diffractometer's controlling computer for registering the *dll*'s in the operation system and effective potential problems solving. Each part of the CMS package can be adjusted to needs of particular user's laboratory during the installation process.

After installation procedure the CMS software is strictly related to Buyer's equipment and software configuration. Any changes in the diffractometer's controlling computer hardware and some changes in its original Bruker's software can lead to incorrect functioning or disabling the Custom Measurement Software. In the case of the above mentioned modifications, contact with CMS Authors is needed to ensure further operation of the software.

## Price and sale terms / conditions

Item No.	Description	Quantity	Price (Euro €)
1	SCRIPT- MAKER programme	1	2 500,- €
2	VIS programme	1	2 000,- €
<b>Total price *</b>			<b>4 500,- €</b>

\* The price not includes costs related to installation of the CMS package at the Laboratory indicated by the Buyer.

### Shipment/Installation:

Four (4) weeks after acceptance of purchase order.

Shipment/Installation Seller's research group, Kraków, Poland, with IMMS PAS chosen carrier.

Customer pays for the shipping/Installation, insurance, taxes and duties under prepaid and billed arrangements.

### Installation & Warranty:

Installation by the representatives of Seller's research group. A standard installation process at the Buyer's laboratory needs 2-days engagement of 2-persons of the Seller's research group and is not included in the price of the offered CMS package. The costs related to the installation process (travel, 2-days accommodation and travelling allowance for 2 specialists) are extra paid by the Buyer.

### Terms of Payment:

Payment in Euros

50 % of the purchase price shall be prepaid at ordering and the remaining 50 % due within 10 days on Delivery (installation).

### Other Terms and Conditions:

Institute of Metallurgy and Materials Science, Polish Academy of Sciences: Standard Terms and Conditions of Sale

Institute of Metallurgy and Materials Science, Polish Academy of Sciences may make changes to specifications and product descriptions at any time, without notice.