Scientific computing in x-ray microscopy

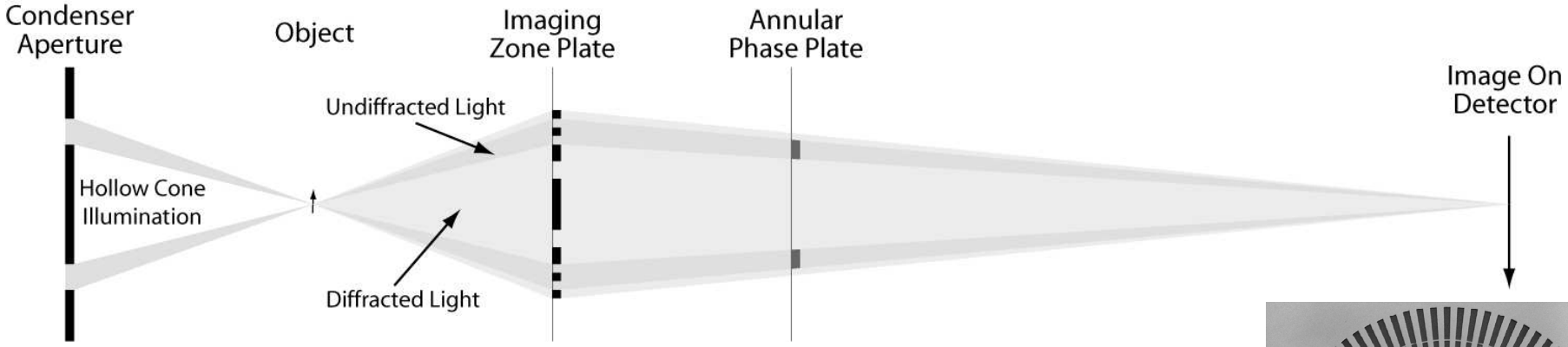
F. Meirer[1], Y. Liu[2], J.C. Andrews[2], A. Mehta[2], P. Pianetta[2]

[1] MiNALab, CMM-irst, Fondazione Bruno Kessler, Via Sommarive 18, 38123 Povo, Trento, Italy

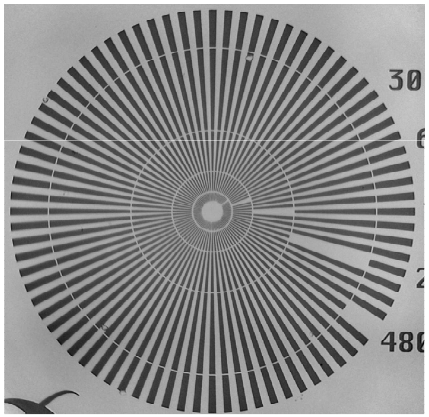
[2] Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

Full field X-ray transmission microscopy

Schematic diagram of the Zernike phase contrast X-ray microscope



- Full field X-ray transmission microscopy:
  - -) typical FOV: 15x15 or 30x30 microns^2
  - -) typical image size: 1024x1024pixels, 12bit grayscale
  - -) typical exposure times: 0.25 – 1 second
  - -) typical file size: 2 Mb (including metadata)
  - -) total writing speed (including overheads for motor movements): ~0.85 seconds per file for 0.25 sec exposure time

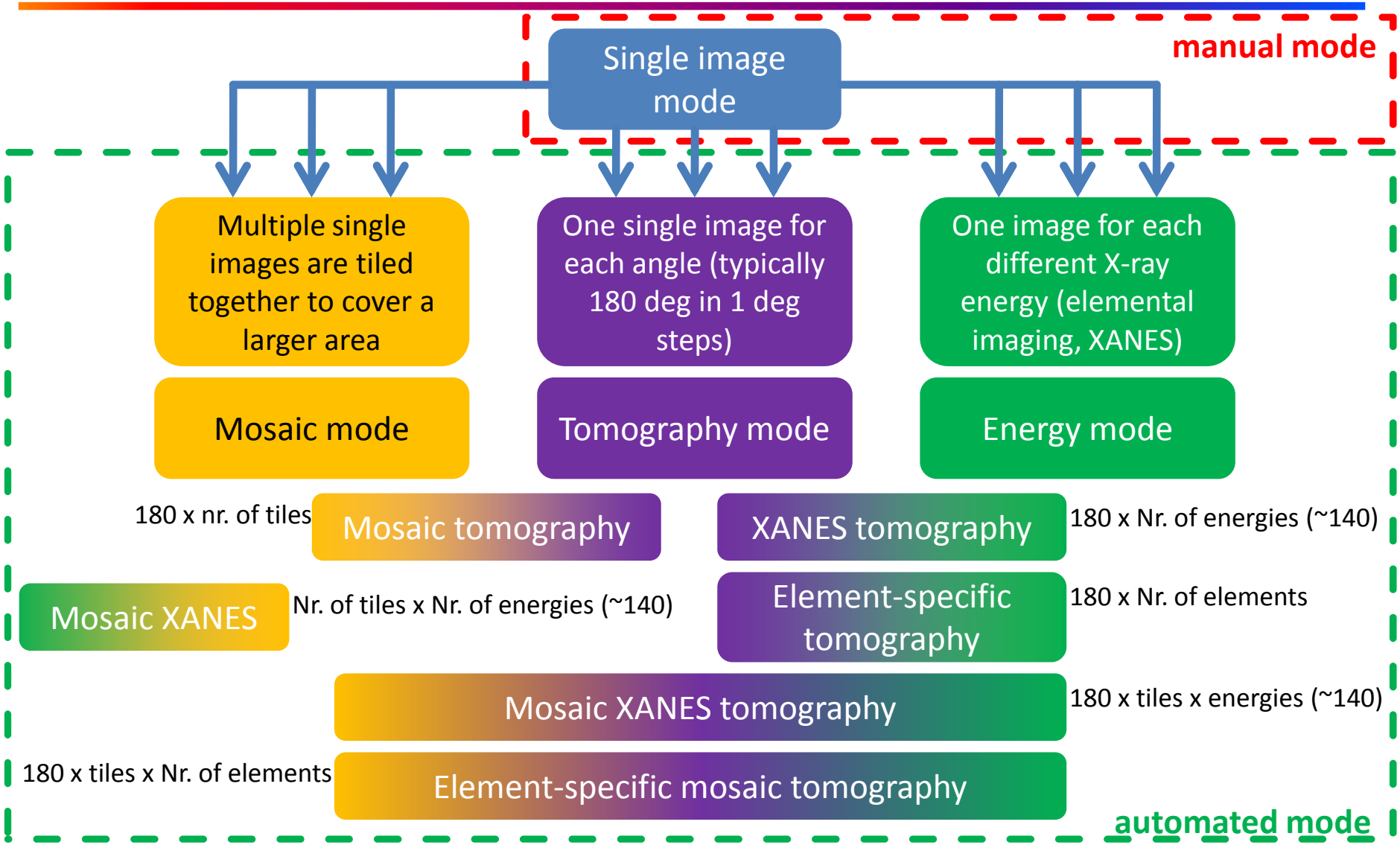


X-ray transmission image of the Siemens calibration standard with 30 nm minimum features. FOV: 30x30 microns^2

How many files are needed per experiment?

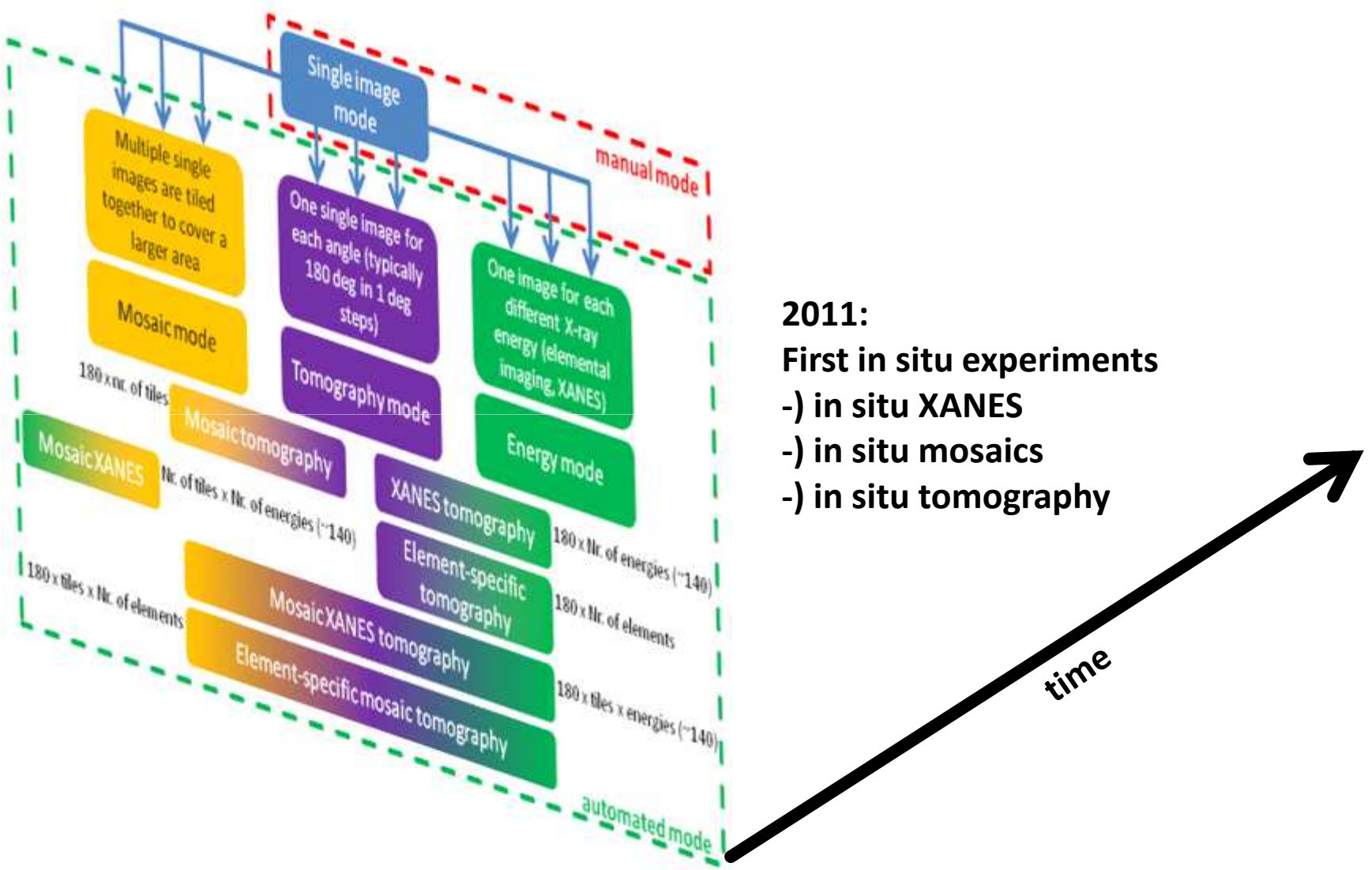
The instrument was upgraded with the capability to execute scripts
-> sophisticated experiments involving complex motor movements are now possible
-> the number of files per experiment increased drastically (from <100 to several 10000) during the last year and depends on the measurement mode used

X-ray microscopy – measurement modes



MATLAB software packages for data collection and evaluation have been developed for all measurement modes

X-ray microscopy – measurement modes



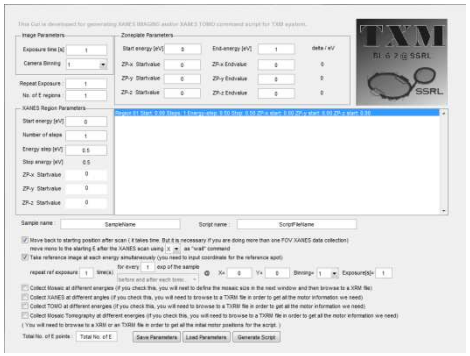
2011:
First in situ experiments
-) in situ XANES
-) in situ mosaics
-) in situ tomography

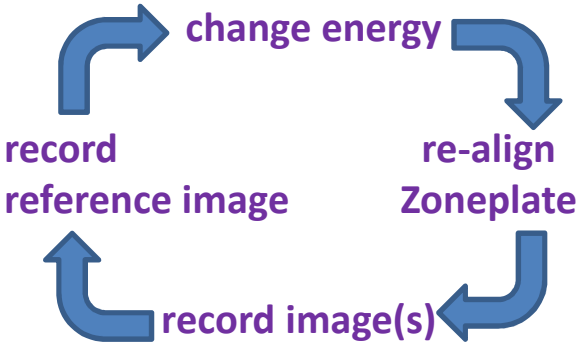
MATLAB software packages for data collection and evaluation have been developed for all measurement modes

Example: XANES tomography

XANES tomography

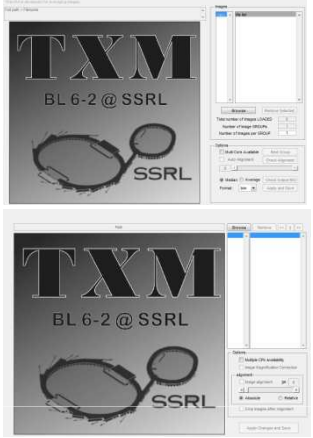
measurement





Code & GUI generate script for automated measurement
Several 1000 commands (motor movements) are necessary

data pre-processing



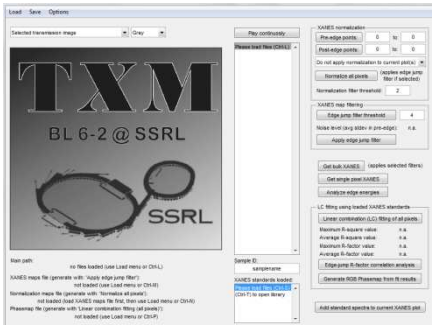
Code & GUI for:
- reference correction
- averaging
- image alignment (PhCo, SIFT)
- cropping
- filtering

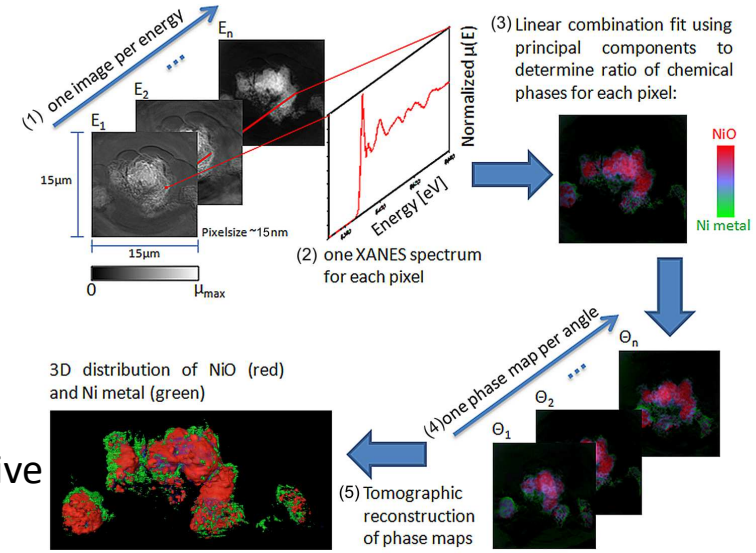
...

data analysis

Code & GUI for XANES analysis: (up to 10^6 spectra have to be processed for each single FOV)
- filtering & XANES normalization
- edge energy clustering
- least squares LC fitting
- PCA & target transformation

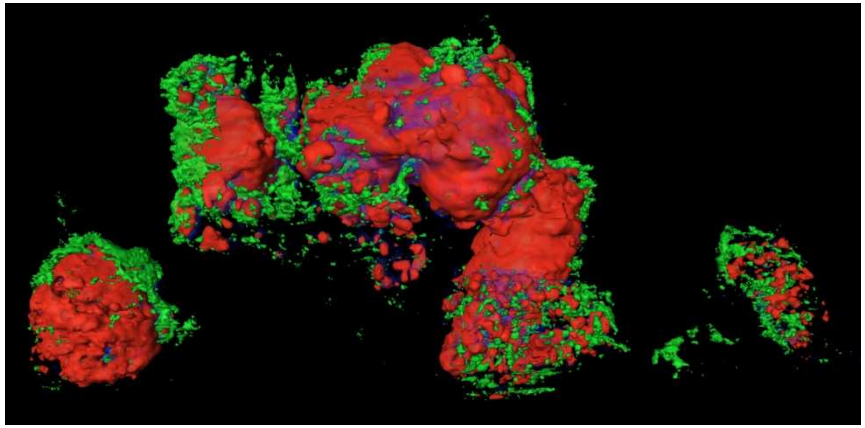
...





Code & GUI for tomographic reconstruction using Filtered Backprojection (FBP) or Iterative Algebraic Reconstruction Technique (i-ART)

X-ray microscopy at BL6-2 – state of the art



Nanostructure & phase imaging of battery electrodes:
XANES tomography of NiO/Ni metal particles
3D resolution: ~60nm
Total measurement time: ~18h
Data processing time:
~5 days (old system, single CPU)
20x faster with new system
Visualization: Avizo Fire

- 16 different user groups at 6-2 Jan-June 2011
- 100% of experiments use automated measurement mode
- developed software package is freeware and used by 15 groups and beamline scientists at 4 synchrotrons (SSRL, APS, BSRF, NSLS-2 and NSRL)
- only 2 dedicated workstations for data evaluation at BL 6-2: 12Gb Ram, 8 CPUs
  32Gb Ram, 24 CPUs
- average amount of data collected per week:
  ~1Tb (x2 after processing)
  >150.000 files
- 24h non-stop data collection: ~250Gb

Next steps:
- improved data management
- improved automation of data pre-processing (pre-processing during collection)
- use of GPUs for parallel processing?

To be improved:

Hardware needs
a) Data is transferred (also for backup) via network or external drives
b) Software is not optimized for read/write operations and disk space usage
c) User often don't have access to necessary hardware

Software needs
d) Users still need help with data evaluation -> improve software documentation
e) Need for human interaction during data pre-processing and evaluation