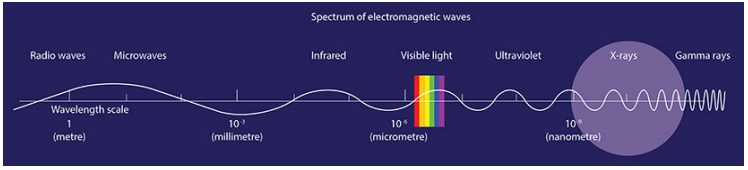
Research data: the case of synchrotrons in Metallurgy

Guillaume Geandier

Sciences ouvertes 2020 – 8 octobre 2020 – Nancy

Context

Synchrotrons offer a lot of possibilities using X-ray



All science fields can use synchrotron light to aquire data.
Experiment possiblities are large on the different sources.
`www.esrf.eu` – `www.spring8.or.jp/en/` – `www.aps.anl.gov/` – `www.synchrotron-soleil.fr`

For metallurgy, due the samples, we use high energy X-rays (80-120 keV) :

For IJL, hard X-rays are used since more than 20 years.
Most of the experiments are done to study in-situ behaviors :

- thermal treatment
- mechanical behavior
- thermo-mechanical behavior

Overview

Research data: the case of synchrotrons in Metallurgy

Science using synchrotrons

Synchrotron experiments
- Metallurgycal studies : in-situ High energy diffraction

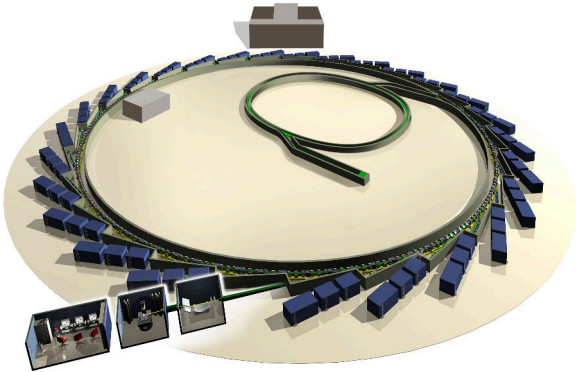
Data Management
- synchrotron sources level
- Laboratory/team level

Conclusions

Acknowledgments

Synchrotrons

lightsouces.org



Schematic of Diamond Light Source, showing the components that make up the synchrotron.

→ more than 50 light sources worldwide (synchrotron, XFEL)

Energy : 1meV to 750 keV —- beam size : 50nm – cm

Synchrotrons

How to get beamtime ?

Public access

- write a proposal (2 pages):
  Including state of the art, experiment description and expected results.
- contact beamline scientists.
- submit proposal in time (March or September).
- proposal evaluation (April / October).
- results of proposition (June / December).
- Perform the experiments : several days 24h/24.
  2 to 6 persons
- Analyze data : days / months / years ...
- Write articles.
- redo ?

→ almost free of charge for 3 persons.
→ need publications to redo ...
→ Data stored on some synchrotron sources.

Experiment schedule : 1 year

Industrial access

- contact beamline scientists.
- contact Business Office.
- Paid ±4000 € per shifts (8h of beamtime).
- Perform the experiments : several days 24h/24 or paid people to do it.
- Analyze data : days / months / years ...
- redo ?

→ need money to redo ...
→ Data not stored on synchrotrons.

Experiment schedule : 1 month

Experiments on synchrotrons

Example of ESRF

ESRF - Grenoble

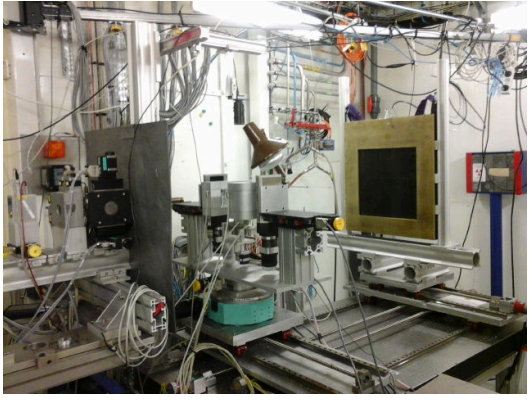
(Credit: P.Ginter/ESRF)

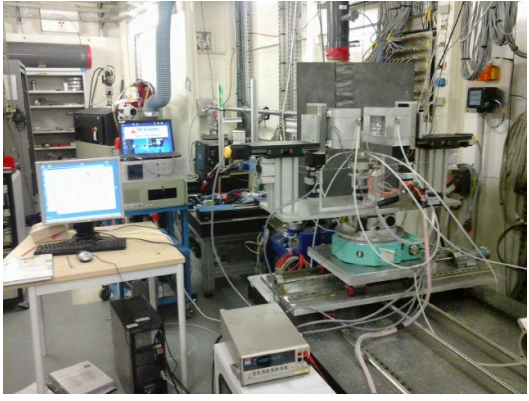
on top of the beamlines

Experiments on synchrotrons

Example of ESRF - ID15

inside experimental hutch

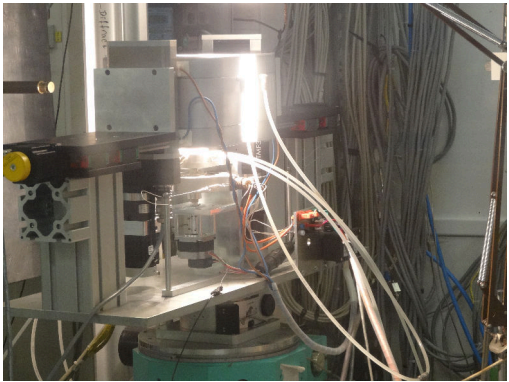




Experiments on synchrotrons

Example of ESRF - ID15

Furnace in action. . .



control room

Several computers, screens and a huge amount of information to manage . . .

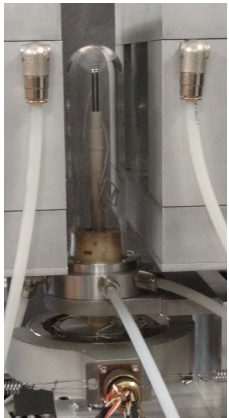
Users need to mange the samples, sample environment, some parts of the beamline (beam, detectors control) during several days 24h/24.
Experiments time : 5 min to days . . .

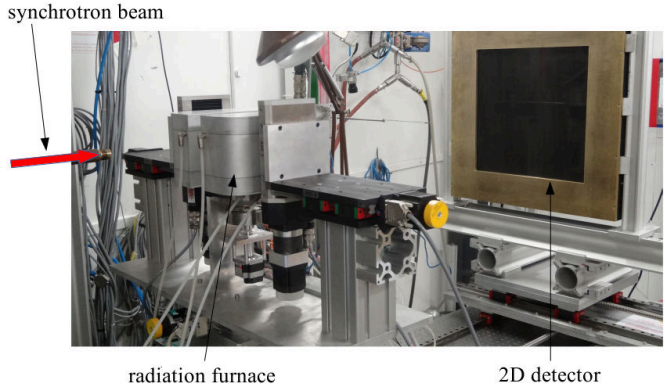
Experiments on synchrotrons

at ESRF-ID15 : high energy diffraction

- Radiation furnace
- Welded thermocouple
- Argon atmosphere
- Sample rotation
- ID15B (ESRF)

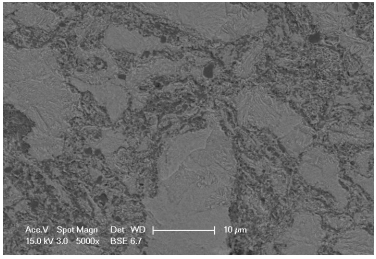
- High energy beam (87 keV)
- Transmission geometry
- 2D detector
- Acquisition rate : 10 frames / s
- Beam size : 400 x 400 μm^2





Experiments on synchrotrons

at ESRF-ID15 : raw data

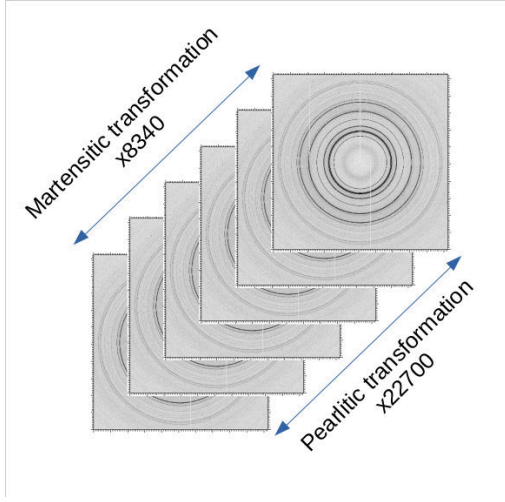


Development of automatic procedures in python langage

- large data set
- up to three phases to analyse

One data set :

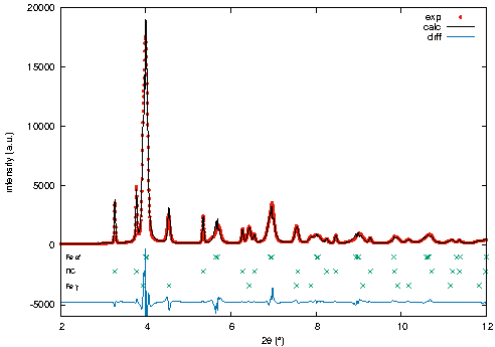
- up to 30000 2D diffraction frames
- 150-300 GB of raw data



Experiments on synchrotrons

at ESRF-ID15 : intermediate data

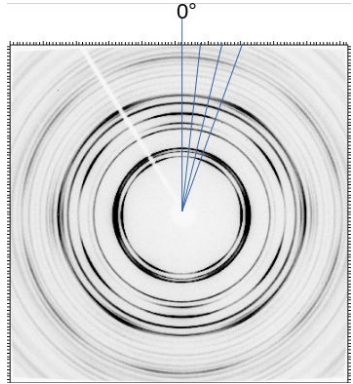
First step : Rietveld analysis
full image integration.



Microstructural parameters for each phase all along the thermal cycle.

- phase fraction
- cell parameters
- FWHM

Second step : strain/stress analysis
image divided in 180 to 360 sectors.

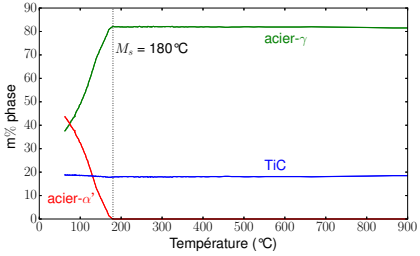


- peak positions for each phases
- up to 10.000.000 peaks per phase.

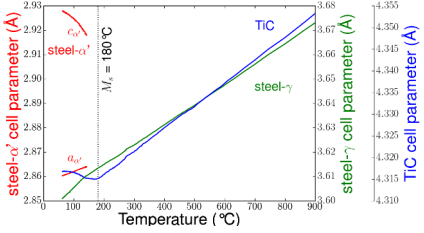
Experiments on synchrotrons

at ESRF-ID15 : Results – microstructural analysis

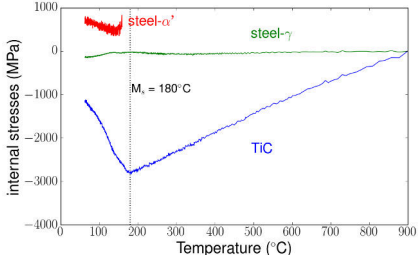
Phase fraction



Cell parameters



internal stresses



Geandier et al. Materials (2018)

www.mdpi.com/1996-1944/11/8/1415

Data Management

Synchrotrons point of view

Old model :

- data stored for 3 months.
- users need to save their data at laboratory and at their own will (raw, reduced, ...).

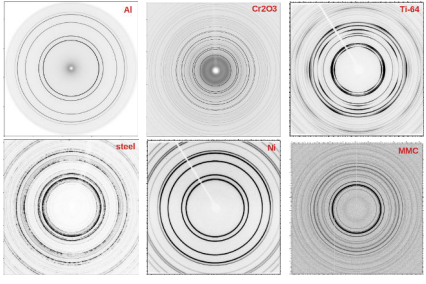
New model :

- data stored at synchrotron source (up to 10 years).
- metadata generated by beamline and users.
- doi associated to experiment:
  article related to data-set must include the doi.
- limited time embargo (3-5 years).
- public access after embargo.

→ only for raw data

More details at :
`www.esrf.eu/datapolicy`

`www.desy.de/data_privacy_policy`



Data Management

Synchrotrons sources point of view

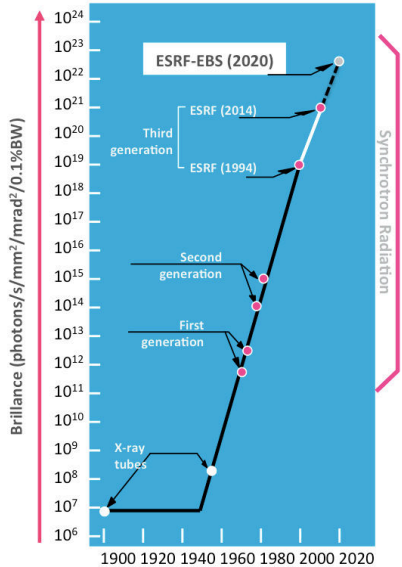
New IV^{rth} generation sources : EBS at ESRF
`www.esrf.eu`

Start of the EBS on 22th August 2020.
20 months closure for the upgrade.

- increase of beam brillance
- increase of coherence.
- increase of flux by factors 10 to 100.
- New types of experiments : narrow beam, small objects ...
- New science ...

Plans on the way at SOLEIL, DESY (almost all recent sources) to go to IV^{rth} synchrotron sources.

`www.esrf.eu/about/synchrotron-science/synchrotron-light`



Data Management

Synchrotrons sources / Metallurgy point of view

IV^{rth} generation sources for Metallurgy

Ex-situ :

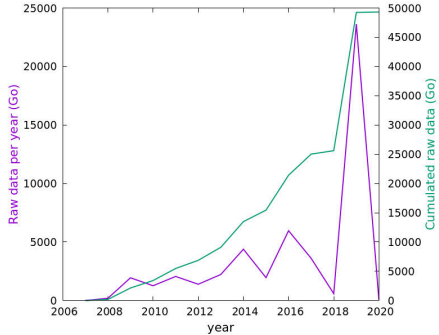
- experiment will be done quicker → more experiments with the same amount of time.
- better discrimination (spatial, angular, ...) → more data.
- high dynamic for data (signal to noise ratio) → bigger data format.

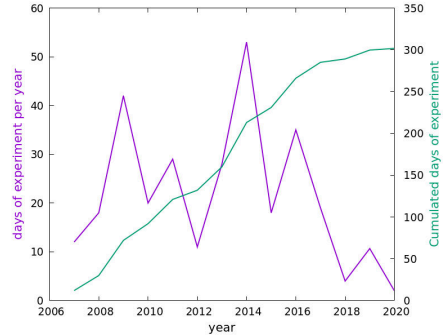
In-situ / in-operando :

- experiments will be done quicker ?
  → for Metallurgy not really relevant.
- higher temporal discrimination → more data.
- better spacial discrimination → more data.
- combination of spacial and temporal discrimination → more data.
- high dynamic for data → bigger data format.

Data Management

IJL-SI2M point of view



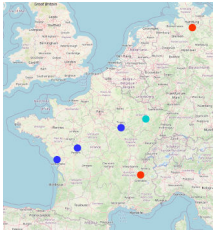


- Large data-set on different materials : Fe, Ti, Al, MMC, ...
- Large data-set on configurations : sources, beamlines, detectors, ...
- Old data are still used : comparison with more recent experiments, machine learning / deep learning studies

Data Management

multi-Users point of view

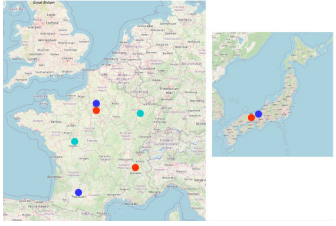
Project Oxydation
raw data : 3 To



Collaboration:

- Institut Jean Lamour (Nancy)
- UTT (Troyes)
- Institut PPrime (Poitiers)
- LaSie (La Rochelle)

Project ANR HighS_Ti
raw data : 8 To



Collaboration:

- Institut Jean Lamour (Nancy)
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- CEMES (Toulouse)
- LSPM (Villetaneuse)
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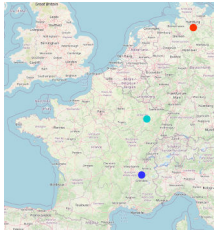
Project thèse I. Benrabad (SIMAP, Grenoble)
raw data : 16 To



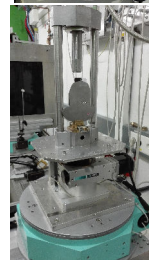
Collaboration:

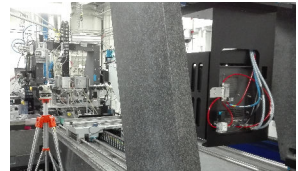
- Institut Jean Lamour (Nancy)
- SIMAP (Grenoble)

Conclusions : Open data / Science for Metallurgy

Synchrotrons case

- new IV generation sources / III generation sources
  → new experiments to imagine ...
  → faster experiments.
  → more data ...
  → new models for data management → open data in several years.
  → metadata ?
- lot of raw data
  → several Terabytes for each experiment.
  → difficulties to store data at laboratory scale (transfert, space, secure storage, ...)
- lot of intermediate data
  → need spaces to share data between teams.
  → at national and international level.
- metadata for synchrotron data ?
  → synchrotron sources level
  → laboratory / team level
  → collaboration level





Acknowledgments

Metallurgy with synchrotrons

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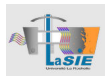

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