EASI-STRESS

EUROPEAN ACTIVITY FOR STANDARDISATION OF INDUSTRIAL RESIDUAL STRESS CHARACTERISATION

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Deliverable Report:

D3.4 Ontologies and Complex Workflows

EASI-STRESS

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Authorship	Written by	Sandra Cabeza
	Contributors	Caroline Boudou David Canelo Yubero Ennio Capria Mohamed Fares Slim Hanna Leemreize Juan Manuel Martinez Marko Marton Arnold Paecklar Thilo Pirling Kousika Rajendran Simon Robbe Matthew Roy Peter Staron
	Reviewed by	Nikolaj Zangenberg
	Approved	

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List of Figures

List of Tables

List of Abbreviations

AE	Acoustic emission
BC	Boundary conditions
CAD	Computer Aided Design
CFD	Computational fluid dynamics
CHADA	Characterization Data
CSC	Conical slit cell
DIC	Digital image correlation
EMMC	European Materials Modelling Coucil
EMMO	European Materials Modelling Ontology
FDM	Finite Difference Method
FEM	Finite Elements Method
FVM	Finite Volume Method
FWHM	Full width half maximum
GV	Gauge volume
IGV	Insrumental gauge volume
ISM	Inherent strain method
MODA	Materials Modelling Data
NGV	Nominal gauge volume
SGV	Sampled gauge volume
LRI	Large-scale research infrastructure
NQL	Neutron Quality Label
RS	Residual stress/es
VSM	Volume Shrinkage Method

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Table of Contents

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 953219.

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Executive summary

The formulation of transversal ontologies between diffraction-based residual stress characterization is proposed including neutron, synchrotron and laboratory X-ray methods.

Complex workflows from idea or conception of a measurement to exploitation of results are rationalized for all participating facilities in EASISTRESS project, identifying the interfaces and gaps to address for a fluent exchange and collaboration.

This document also enhances the homogenization of definitions towards common procedures and protocols in WP3, common RS software development addressed in WP4, nurturing the set of metadata descriptors, and ultimately promoting an easier exploitation for industrial simulation activities in WP5.

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1. Introduction

Residual stress determination through measurement of elastic lattice strains using X-ray or neutron radiation, both at laboratory (X-ray) and at Large-scale Research Infrastructures (LRIs synchrotron and neutron sources) have been used for around three decades [1-5] and standards for some of these techniques are already available [6-9]. Despite previous round-robin tests to demonstrate the feasibility and precission of the method as well as the resulting guidelines and standards, the knowledge of these techniques at LRIs is not yet extended nor consolidated within the industry. Additionally, there are currently no general stress measurement guidelines for synchrotron X-ray, let alone a harmonised guideline which encompasses the different techniques. The project EASI-STRESS aims to address some of these gaps through its work packages (WPs): industrial confidence in the methods is enhanced by validation and benchmarking of neutron, synchrotron X-ray, and lab-based techniques with predictive numerical model using relevant reference samples in WP2; residual stress determination using different methods at the LRIs are harmonised in terms of measurement protocols (by WP3) and data analysis algorithms and software (by WP4). Hence, a setup of industrial service functions for residual stress is initiated through a series of round-robin measurements of industrial cases in WP5 whereas WP6 aims a technical specification for synchrotron X-ray to bring the method closer to a standardized techniques.

Looking at the European landscape, the European Materials Modelling Council (EMMC) join together modellers, materials data scientists, software providers, translators and engineering designers in Europe. The EMMC considers the integration of materials modelling and digitalisation to be critical for a more agile and sustainable product development. The EMMC Roadmap from November 2020 highlights that industrial R&D is driven by a need of fast adaption to market and optimising processes considering also the environment, so disruptive processes and introduction of novel materials comes at a very high risk for them, hence the materials modelling approach is crucial. Also, there is a recommended action in line with increasing the understanding of complementary roles from different stakeholders (academics, software providers, industry) and raise the awareness of free open source software, both of which are contained within the EASI-STRESS objectives. The European Materials Modelling Ontology (EMMO) is the result of a multidisciplinary effort within the EMMC, aimed at the development of a standard representational ontology framework based on current materials modelling and characterization knowledge and developed from the very bottom level (physical events). Notably, the Materials Modelling Data (MODA) is a standardized documentation for simulations proposed by the European Modelling Council summarized in the CWA 17284 “Materials modelling – terminology, classification and metadata” [12]. In particular, there are on-going efforts to integrate these new approaches in the domains of mechanical testing and in crystallography. An example for spectroscopy characterization in industry is addressed by Charisma project[1].

This document aims towards the same direction of those actions applied to multiple characterization approaches for residual stress characterization.

In the first part of the present deliverable D3.4 on *ontologies and complex workflows*, we aim to document the effort in harmonising RS definitions at LRIs for different methods (synchrotron X-ray and neutron diffraction) aiming to form the basis for the development of a common software for residual stress determination and a standardisation of data output formats in WP4. Therefore, general descriptors for residual stress determination using neutron and synchrotron radiation are described, as well as their related instrumental and software specifications. The information has been gathered and

[1] CHARISMA project EU Horizon Europe, grant ID: 952921 (https://cordis.europa.eu/project/id/952921)

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discussed with the concerned EASI-STRESS partners for each diffraction method. The report describes the harmonised ontologies at LRIs and X-ray labs. This report is to be used also as a guidance for the work of WP4, which is the development of the common software for residual stress determination at LRIs and, to some extent, at X-ray labs.

In a second part of this report, complex workflows at LRIs are detailed taking as guideline the reported CHADA approach in the previous Deliverable 4.1.

2. Ontologies for General Definitions at LRIs

2.1 Ontology: definition of the relationships between the concepts of a domain or area of knowledge.
2.2 LRI: Large-scale Research Infrastructure including synchrotron and neutron radiation facilities.

2.2.1 Access:

2.2.1.1 Collaboration: non-confidential project involving LRIs as partner or led by those. Access open all year.

Academic: internships, master and PhD thesises, postdoc.

Internal: in-kind contribution from partners for a common development at LRIs

EU funded: European commission funded projects such as in Horizon calls (Sine2020, Calipso+, Brightness2, etc).

National/ International funded: government dedicated funding for access or collaborative research or instrumentation such as sweedish Vinnova's LRIs call Industrial utilization of neutron and synchrotron light-based technologies in large-scale research infrastructure; ESA General Support Technology Programme (GSTP); round robind tests, etc.

2.1.1.2 Feasibility test or easy access: all year, fast track access, not charged.

2.2.1.3 Proposal (non-confidential): usually 2 calls per year, subjected to external peer-review evaluation, competition based on scientific excellence. If granted beam time this usually takes place the following semester.

2.2.1.4 Proprietary (confidential): commercial access all year, fast track.

2.2.2 Method:

2.2.2.1 Source of radiation:

2.2.2.1.a) X-ray: Soft (often used in the laboratory) or hard (often produced at synchrotron facilities) X-rays. White or monochromatic beam can both be produced and used.

2.2.2.1.b) Neutron: reactor or spallation source

2.2.2.2 Technique:

2.2.2.2.a) Angle-dispersive diffraction: Uses a monochromatic beam (constant wavelength/energy). The diffraction pattern is collected by scanning the scattering angle or by intercepting a specific portion of the totality of the Debye-Scherrer ring using a two-dimensional detector.

2.2.2.2.b) Energy-dispersive diffraction: Uses a white beam covering a broad energy spectrum (variable wavelength/energy). The diffraction pattern is collected at a fixed scattering angle using an energy-resolving detector.

2.2.2.2.c) Time-of-Flight diffraction: uses a pulsed or chopped beam and detects the different times of neutron arrival on the detector, that is, having different wavelengths for a fixed angle.

2.2.3 Standard:

2.2.2.3.a) Guideline: recommendations, standard operating procedures (SOPs) and best practices information to users when specific standards do not apply.

2.2.2.3.b) ISO: International Organization for Standardization. Nongovernmental organization that comprises standards bodies from more than 160 countries.

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Comprises international standards (IS), technical reports (TR), technical specifications (TS), technology trends assessment (TTA), international workshop agreements (IWA), etc.

2.2.2.3.c) **NQL®:** Neutron Quality Label. Trademark No. 018531682 from 09.12.2021. Internal certification process achieved between neutron strain scanners at ILL, ISIS, FRMII and NECSA under Brightness2 project grant 823867.

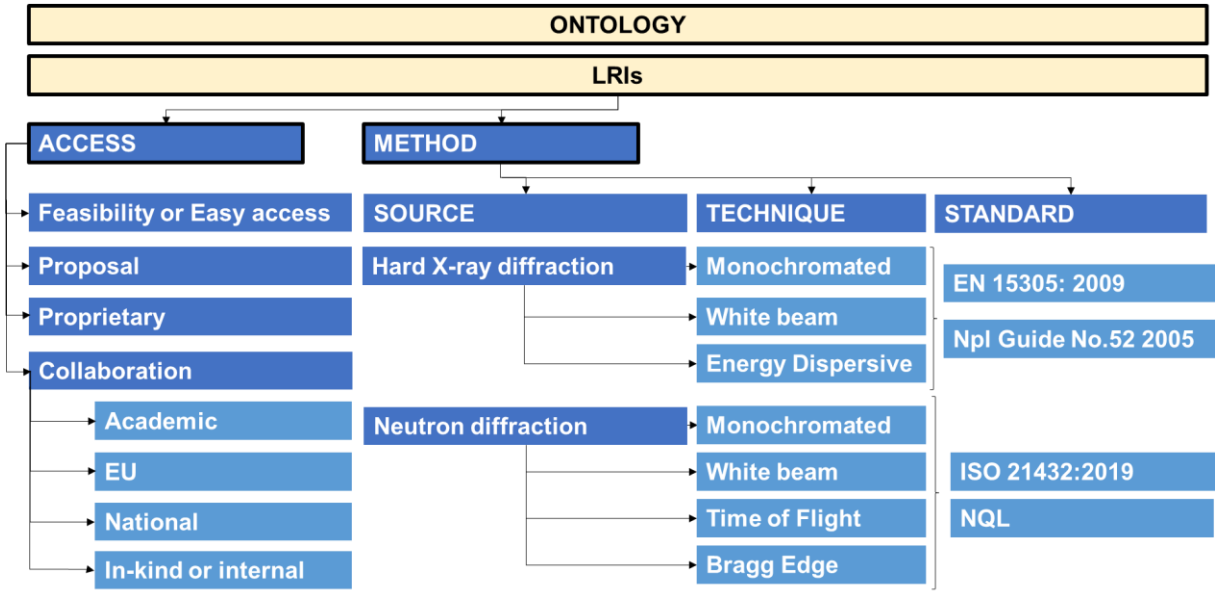

Figure 1. Ontologies and LRIs: access and method branches.

2.2.4 **Experiment:** measurement designed to prove/investigate an hypothesis.

2.2.3.1 **Beam time:** days or shifts allocated to perform an experiment at LRIs.

2.2.3.2 **Beam line:** instrument where an experiment is performed at LRIs.

2.2.3.3 **Benchmarks:** quantitative values used against a measurement to compare it.

2.2.3.4 **Remote access:** ability for an authorised person to acces an LRI network to control a particular computer to program and perform an experiment or data processing without physical presence.

2.2.3.5 **Sample:** particular material selected to prove an hypothesis in an experiment.

2.2.3.6 **Support labotratories:** facilities at LRIs for sample preparation and/or complementary or necessary characterization related with the beam time.

2.2.5 **Data Processing:**

2.2.4.1 **Raw data:** signal acquired at the detector and saved at the instrument together with part of the metadata (instrumental).

2.2.4.2 **Data reduction:** conversion of detector signal to angle/energy by integration and peak fit.

2.2.4.3 **Data analysis:** interpretation of the peak fit and shifts, that is strain-stress analysis considering the unstrained reference d_0 (microstructural dependence) and other contributions (externally applied temperature, load, etc). Could also extend to interpretation of further properties such as FWHM and intensity evolution, failure analysis, etc.

2.2.4.4 **Meta data:** group of data necessary to interpretate the set-up and conditions of the experiment related to the acquisition of the raw data in order to ensure reproducibility.

2.2.6 **Report:** presentation of results and interpretation.

2.2.7 **Data exploitation:** publication of results (peer reviewed article, master or PhD thesis, conference, etc) or internal implementation into industrial FEM, design and processes.

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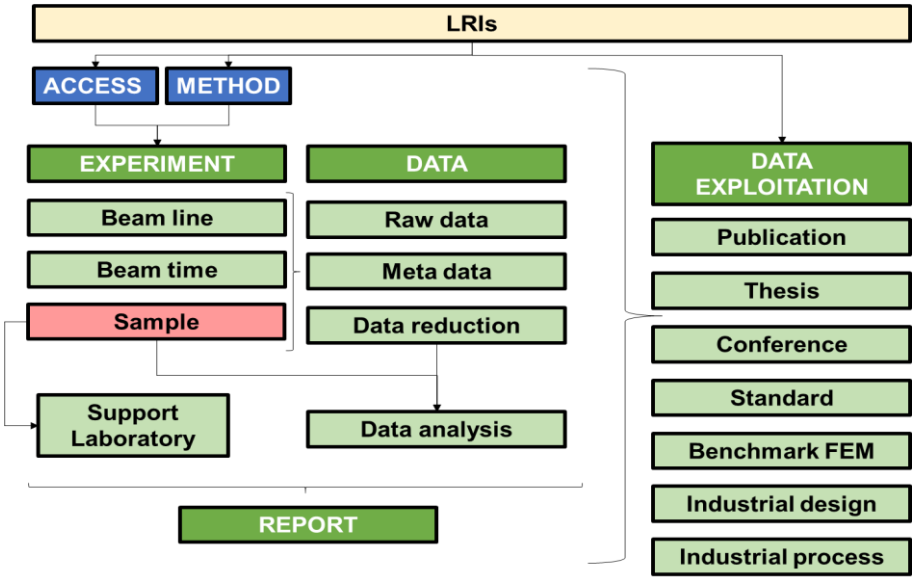

Figure 2. Ontologies and LRIs: experiment and data branches.

3. Ontologies for diffraction characterization and instrumentation

3.1 Instrument set-up:

3.1.1 Alignment: adjustment of the sample position and orientation and also all the components of the instrument such that measurements can be performed precisely at the desired location in the specimen and the desired strain direction.

3.1.1. 1 Beam alignment: intensity scan procedure to determine the position of the gauge volume in the system of the instrument to set the reference point using a special calibration sample (i.e. thin foil).

3.1.1.2 Entry scan, surface scan or wall scan: intensity scan procedure to determine the position of a specimen surface or interface with respect to the reference point.

3.1.2 Beam:

Energy (eV): kinetic energy of the photon/neutron beam defined by its mass and speed.

Wavelength (λ): relationship between mass and speed of a particle (neutron or photon) through De Broglie equation.

Energy or Wavelenght calibration: powder reference measurement to determine the precise value of the beam energy or wavelength and its error.

3.1.2.1 Incident beam: beam illuminating the sample

3.1.2.2 Diffracted beam: beam emanating from the sample due to interaction between the incident beam and the sample.

3.1.2.3 Scattering Vector (Q): difference between scattered and incident wavevector. In elastic scattering it bisects incident and diffracted beam.

3.1.2.4 Beam-defining optics: arrangement of devices used to define the properties of a beam such as wavelength and intensity distributions, divergence, and shape.

The beam width is characterized by its FWHM and typically defined by:

3.1.2.4.a) Soller Collimator: device which narrows a beam of particles or waves with parallel absorbing foils. Beam size in one direction is then defined considering FWHM width of a peak-profile at half the peak height above background.

3.1.2.4.b) Radial Collimator: device which narrows a beam of particles or waves with radially arranged absorbing foils, collimating tube with absorbing or reflecting walls.

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Beam size in one direction is then defined considering FWHM width of a peak-profile at half the peak height above background.

3.1.2.4.c) Planar Slit: Beam size definition in one direction considering a straight, narrow opening or apertureaperture of plates.

3.1.2.4.d) Curved or Conical Slit: Beam size definition in one direction considering a curved or conical, narrow opening or aperture of surfaces.

3.1.2.1.d) Neutron chopper: neutron absorbing rotating disk with a given opening where there is no absorber. It defines either the time-width of the neutron beam at the starting position or the difference between the smallest and largest wavelength in the beam.

3.1.2.5 Primary optics: component/s defining the wavelength and the shape of the incident beam shape (usually 2 dimensions of the later gauge volume).

3.1.2.6 Secondary optics: component/s selecting or filtering the diffracted beam (usually 1 dimension) from the sample towards the detector.

3.1.2.7 Gauge volume: 3D volume defined by the intersection of primary and secondary beam. Volume from which information of the sample is obtained.

3.1.2.7.a) Instrumental gauge volume (IGV): (measured) volume of space defined by the actual beam paths through the defining apertures, taking into account the beam divergence and the beam intensity profile. The IGV dimensions can also be defined in terms of the FWHM of the beam intensity profile.

3.1.2.7.b) Nominal gauge volume (NGV): (theoretical) volume of space that is occupied by the intersection of parallel beams, which are transmitted through the defining apertures (e.g. slits, collimators) for both the incident and diffracted beams.

3.2.2.7.c) Sample gauge volume (SGV): IGV immersed within the sample. For bulk measurments IGV and SGV are identical.

3.1.2.8 Reference Point or center: centroid of the instrumental gauge volume.

3.1.2.9 Beam path:

3.1.2.9.a) Neutron absorption: neutron capture by an atomic nucleus in the matter.

3.1.2.9.b) X-ray absorption: photon transfer of energy to an electron in the matter (photoelectric effect).

3.1.2.9.c) Extinction: decreasing of the intensity along the beam path in the sample by scattering .

3.1.2.9.d) Filter: material device used to filter/absorb undesired waveleegth/energy.

3.1.2.9.e) Path-length: total length of trajectory of the beam inside the sample material.

3.1.2.9.f) Time-of-flight: time needed for the neutron to arrive from the pulse of the pulsed source or from the firs chopper to the detector.

3.1.2.9.g) Flight path: the total path in neutron TOF measurement from the source of the pulsed source or the first chopper till the detector.

3.1.3 Detector: combination of hardware and software tools for the effective quantification of photon/neutron events.

3.1.3.a) Proportional detector: type of gaseous ionization detector used to count particles of ionizing radiation. It is able to measure the energy of the incident radiation. It is widely used to discriminate between radiation types.

3.1.3.b) Scintillator: the material of the detector surface is excited to luminescence by the absorbed photons or particles.These are subsequently converted to voltage pulses. It can measure the position in one or two-dimensions.

3.1.3.c) Position sensitive detector (PSD): gas-filled detector with a long conducting wire to which a high tension voltage is applied at both ends. By measuring the rate

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at which the pulse arrives at both ends of the wire, it is possible to determine at which position on the wire the pulse originated.

3.1.3.d) Area detector: defined by its array and the pixel size. The whole or a large portion of the diffraction rings can be measured simultaneously.

3.1.3.1 Detector Calibration: powder reference measurement to determine sample-detector distance (synchrotron diffraction with a monochromatic beam), the 2θ angle (synchrotron diffraction with a white beam) of each pixel / channel of the PSD and the relative efficiencies of the pixels / channels.

3.1.3.2 Position (2θ): for PSD area detectors the positioning around sample's bragg peak selected for measurement.

3.1.3.3 Distance (D): distance from the reference point to the detector.

3.1.3.4 Resolution: angular or channel width/ time/ energy.

3.1.3.5 Time-of-flight: time needed by a neutron of a given speed to cover the distance from a defined starting point to the detector.

3.1.4 Sample stage:

3.1.4.1 XYZ table: stage design which allows the sample movement in 3 orthogonal directions. Could also be reduced to 2 orthogonal movement in XZ or XY.

3.1.4.2 Hexapod: parallel kinematic stage design which allows the sample movement in 6 degrees of freedom including 3 Cartesian position parameters (x, y, z) and 3 Eulerian angles (intrinsic rotation or commonly known as ω, χ, ϕ), enhancing complex motion profiles. Well suited for highly accurate positioning and heavy samples (more than 500 kg). Limited workspace.

3.1.4.3 Robotic Arm: serial kinematics 6-axis arm allowing 6 degrees of freedom for sample movement including 3 Cartesian position parameters (x, y, z) and 3 Eulerian angles (intrinsic rotation or commonly known as ω, χ, ϕ), enhancing automatized sample exchange and complex motion profiles, Large workspace, medium positioning accuracy, light and medium sample weight (typically up to 30 kg).

3.1.4.4 Eulerian Cradle: mechanical device on which the sample is mounted for angular motion to select different χ angles, usually between 0-90° for samples up to 30kg.

3.1.4.5. Goniometer: mechanical device on which the sample is mounted for angular motion about its center axis to select a different angle, usually ψ or ϕ, with 360° range.

3.1.4.6 Rotation stage: mechanical device on which the sample is mounted for angular motion about its center axis to select a different angle (χ, ψ or ϕ) with 360° range.

3.1.4.7 Positioning angles:

χ (chi): Angle of rotation in the plane normal to that containing omega and 2θ about the axis of the incident beam.

ω (omega): Angular rotation about a reference point -the angular motion of the goniometer of the diffraction instrument in the scattering plane.

ϕ (phi): Angle between a fixed direction in the plane of the sample and the projection in that plane of the normal of the diffracting plane.

ψ (psi): Angle between the normal of the sample and the normal of the diffracting plane (bisecting the incident and diffracted beams).

3.1.5 Sample environment: External condition applied to the sample or component under investivation (in-situ, operando):

3.1.5.a) Cryostat: apparatus for cooling and maintaining a sample at a very low temperature.

3.1.5.b) Furnace: device used to provide sample heating

3.1.5.c) Load rig: apparatus to deform the sample

3.1.5.d) User supplied: in-situ instrumentation or processing equipment (i.e. DIC, AE, laser-based printers, etc)

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3.1.6 Sample holder: an extra device which fixes the sample or component in the desired position within the sample stage and/or environment to assure its correct position during the measurement.

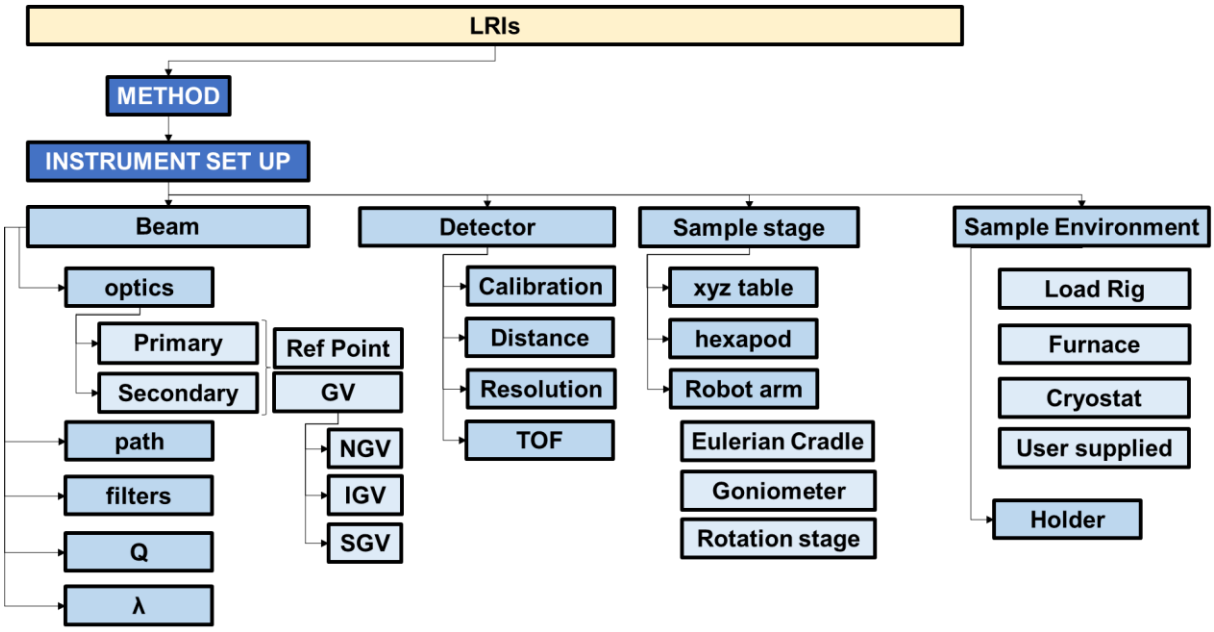

Figure 3. Ontologies for diffraction characterization: instrument set-up branches.

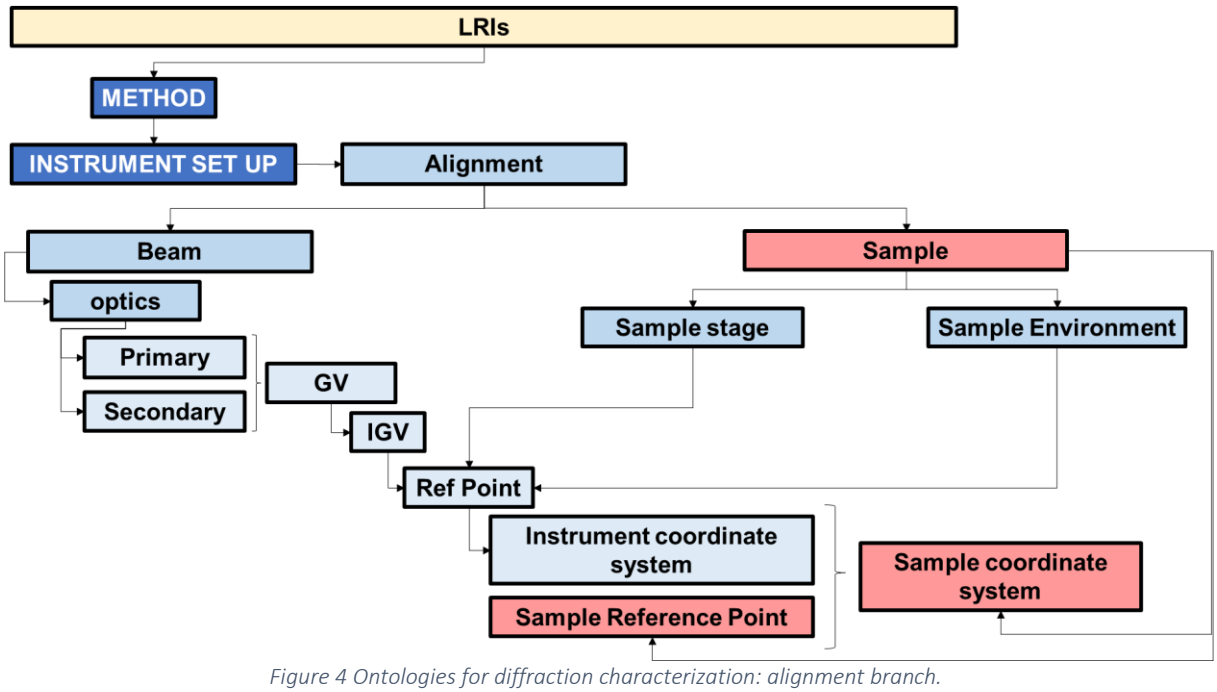

Figure 4 Ontologies for diffraction characterization: alignment branch.

3.2 Measurement:

3.2.1 Attenuation: reduction of the beam intensity.

3.2.2 Background: intensity considered not belonging to the sample's diffraction signal.

3.2.3 Continuous radiation : continuous X-ray or neutron spectrum that contains every wavelength (interval of real numbers) between the wavelength on which the spectrum starts and the wavelength on which the spectrum ends.

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3.2.4 Pulsed radiation: X-ray or neutron spectrum that takes only distinct values, with gaps between one value and the next between the wavelength on which the spectrum starts and the wavelength on which the spectrum ends.

3.2.5 Acquisition modes: X-ray or neutron detection and saving modes

3.2.5.a) Time: count events for a given time.

3.2.5.b) Monitor: count for a given number of events. Acquisition time is automatically adapted. i.e. neutron monitor counter in incident beam: allows precise intensity normalization, number of detector events: assures equal statistics in detected peak.

3.2.5.c) Continuous: event mode: a detector event is stored with a coordinate and time stamp. Time binning and reconstruction of detector image is done during data reduction. Well suitable for in-situ studies.

3.2.5.d) Stroboscopic: the sample is exposed to a reversible process (e.g. temperataure, pressure, etc) and data are acquired synchronously. Data acquired under equal conditions can be binned together to improve the signal to noise ratio.

3.2.6 Diffraction: scattering arising from coherent interference phenomena

3.2.6.1 Bragg's law:

Bragg edge: sharp change in the neutron intensity as a function of the wavelength or monochromator take-off angle corresponding to the condition $\lambda = 2d_{hkl}$, where hkl indicates an (hkl) diffracting lattice plane of the sample under investigation

Bragg angle or Bragg peak or Diffraction peak: intensity distribution of a neutron or X-ray beam diffracted by a specific (hkl) lattice plane. While the equavency of the three terms is not the same in different types of literature, it is commonly assumed to be similar within the strain-stress user community.

3.2.6.2 Characteristic lines: Lines of the X-ray emission spectrum, coming from electron transitions within an atom. Selected lines from laboratory X-ray sources are used for investigations.

3.2.6.3 Characteristic radiation: radiation arising from the electronic transition in an exited atom. Exitation refers to removal of an electron from an inner shell.

3.2.6.4 Debye-Scherer cone:

Debye-Scherer ring: concentric diffraction ring produced by Bragg reflection which are obtained when polycrystalline samples are illuminated with a X-ray or neutron beam.

Debye-Scherer arc: section of a Debye-Scherrer ring recorded in an area detector

3.2.6.5 Diffraction pattern or Diffractogram: intensity distribution of photons/neutrons diffracted from a crystalline material over the available wavelength, time-of-flight and/or diffraction angle ranges.

3.2.6.6 Orientation Distribution Function (ODF): quantitative description of the crystallographic texture.

3.2.6.7 Intensity: it is generally taken to be synonymous with "peak area" since it represents the sum of all the diffracted photons/neutrons that have been detected regardless of the peak shape.

3.2.6.8 Pattern: Intensity within a unit wavelength / energy range as a function of wavelength / energy. Gives information on the structure of the crystal of different crystallographic planes or the identity of a crystalline material causing the diffraction.

3.2.6.9 Incoherent scattering: material scattering in an uncorrelated way thus giving rise to a strong background signal and not contributing to the Bragg peaks or only some with low amplitude.

3.2.6.10 Spectrum: pattern from coherent scattering.

3.2.7 Measurement direction or component: direction parallel to the direction of the scattering vector and therefore specific strain component under examination.

3.2.8 Measurement approach or strategy:

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3.2.8.1 Equilibrium conditions: sample at room temperature (RT) and atmospheric pressure (P_{atm}) and without any other external condition applied.

Layer removal: (destructive) variation of residual stress determined as a function of depth by successive material removal by electro polishing and subsequent diffraction measurement.

Line scan: (non destructive) line formed by the points measured in the sample by diffraction.

Mapping: (non destructive) 2D or 3D region in the sample anaylzed by diffraction.

Sin²ψ: (non destructive) method based on the diffraction measurement at several ψ sample projections. Can be used to evaluate stress differences between principal stresses at ψ = 0° and ψ = 90° directions as well as the presence of shear stresses without the need for precise d_0 determination.

Step size: linear or angular variation of the sample positioning.

Depth profiling: (non destructive) Uses the information collected in a reflection $\sin^2\psi$ measurement in energy dispersive mode. Since each peak is at a different energy, it delivers information from a different depth.

3.2.8.2 In-situ: sample subjected to an external condition such as temperature, load, magnetic fields, etc (see also section 3.1.5).

3.2.8.3 Operando: sample subjected to external conditions identical or representative to the requirements during in-life service.

3.2.8.4 Stroboscopic: technique which involves the division of the physical phenomemon into discrete time segments. Photons/neutrons collected during each segment are stored separately and added to that collected during the same segment of subsequent cycles.

3.2.8.5 Phase measurement:

Single peak: one hkl measurement (single phase) to extrapolate to residual stress analysis.

Multi peak: multiple hkl peak positions averaged to calculate residual stress from the same or from multiple phases.

3.2.8.6 Uncertainty: non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurement, based on the information used.

3.3 Data processing

3.3.1 Data reduction: using the raw data, collected on the instrument, for the calculation of the angle-dependent intensity distribution. This is done for each data acquisition from a sample including additional information such set-upand calibration files. This also considers the sorting of output data it in a convenient shape for strain/stress analysis.

3.3.1.1 Binning or integration: data that fall in a given interval are replaced by one representative value, i.e. their sum, mean… according to Deby-Scherer cone.

3.3.1.1.a) Azimuthal integration: from an angular range of the Debye-Scherer ring or arc.

3.3.1.1.b) Spatial binning: from various measured points within the sample volume.

3.3.1.1.c) Time binning: from various diffraction events at the same sample location.

3.3.1.2 Peak: Bragg angle or Bragg peak

3.3.1.3 Peak fit:

3.3.1.3.a) Full pattern analysis: determination of the crystallographic parameters and/or strain from a measured (multi-peak) diffraction pattern of a polycrystalline sample.

Rietveld refinement: diffraction pattern refinement method that uses the total integrated intensities of the separate groups of overlapping peaks in the least-squares refinement of structures. Requires initial

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input of the approximative crystal structure such as the space group, atomic positions, site occupancies, and lattice parameters.

Le Bail refinement: diffraction pattern refinement method where the intensities of the individual peaks are no refined but instead set to an initial arbitrary value.

Pawley refinement: diffraction pattern refinement method that is based on Rietveld refinement but in this case every reflection is assumed to have a peak position, a peak width determined by the resolution function parameters and a peak intensity. In contrast, the Rietveld method calculates the intensity of the peaks from the structure factures, which are themselves calculated from the parameters of the model structure.

3.3.1.3.b) single peak analysis: statistical procedure to determine the characteristics of a peak and the background from the measured diffraction data.

3.3.1.3.c) Peak Profile or peak shape: intensity distribution (typically in arbitrary units) of colletected photons/neutrons. It is usually described by individual or convolued probability density functions as Gaussian, Lorentz, or Voigt distributions.

3.3.1.3.d) Peak Function: analytical expression to describe the shape of the Bragg peak

Gaussian: probability density function of the normal distribution.

Lorentzian: distribution function in the Cauchy distribution.

Pseudo-Voigt: approximation for the Voigt function, which is a convolution of Gaussian and Lorentzian functions. In this case it allows the refinement of a mixing parameter determining the fraction of Lorentzian and Gaussian components.

3.3.1.3.e) Full width at half maximum (FWHM): width of the Bragg peak at half the peak height above the background.

3.3.1.3.f) Peak height: maximum number of counts of the Bragg peak above the background.

3.3.1.3.g) Peak Intensity or integrated intensity: area under the diffraction peak above the background, normally calculated from the associated fitted parameters of a selected peak function and a background function.

3.3.2.3.h) Peak position: (2θ) single value describing the position of a Bragg peak in the direction of the measurement (i.e. component) in angle, energy or time condition.

3.4 Reproducibility: closeness of agreement between indicators or measured quantity values obtained under conditions of measurement, out of a set of conditions that includes different locations, operators, measuring systems, and replicate measurements on the same or similar objects.

3.5 Data format:

NeXus: data format for experimental science that is commonly used in the neutron, x-ray, and muon scientific communities [13]

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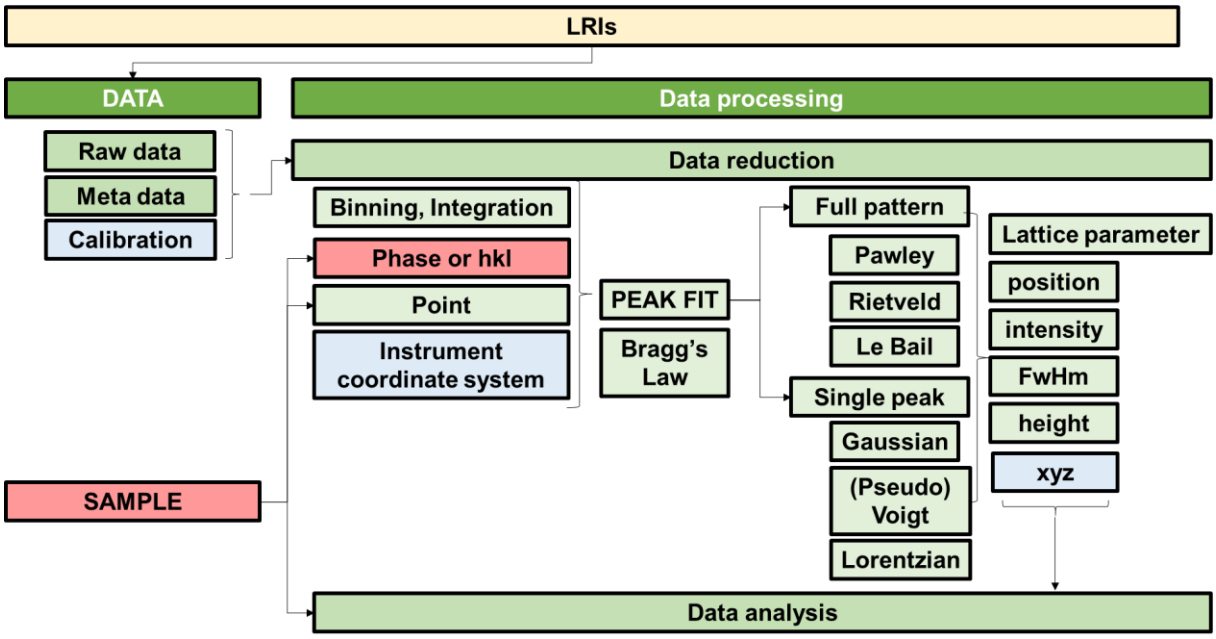

Figure 5 Ontologies for diffraction characterization :data processing and data reduction branches.

4. Ontologies for residual or internal strain/stress determination

4.1 Sample microstructure: grain size, phases and crystallographic information.

4.1.a Polycristalline sample: material comprised of many small crystallites with different crystal orientations that are separated by grain boundaries

4.1.b Single crystal sample : material comprised of one crystallite

4.1.1 Anisotropy: dependence of material properties on the direction with respect to the sample orientation.

ARX: anisotropy factor - a measure of the elastic anisotropy of a material considering for example texture effects such as in directional materials processing (e.g. welding, rolling, casting, additive manufacturing, etc).

Texture: crystallographic texture, or other microstructural features, referred to as morphological texture, within a sample.

4.1.2 Homogeneity: Information about any spatial variation in the composition, microstructure or phase distribution that is germane, affecting the confidence in the measurements obtained at a particular location in a sample dictating its validity to be representative of the sample as a whole. Inhomogeneities in the microstructure and composition can lead to variations in the stress-free lattice spacing with position in the specimen or component, necessitating specific approaches and inherent uncertainties.

4.1.3 Interplanar spacing, lattice spacing or d-spacing: (d): perpendicular distance between adjacent parallel crystallographic planes

d_0: strain-free interplanar spacing

4.1.4 Lattice parameters: linear and angular dimensions of the crystallographic unit cell

a, b, c: lattice parameters

α, β, γ: lattice angles

a_0, b_0, c_0: strain free lattice parameters used as reference for strain calculations

4.1.5 Miller indices or Miller-Bravais notation (hkl): Indices of a crystallographic lattice plane

hkl: set of equivalent crystallographic planes

hkil: alternative index notations of a crystallographic lattice plane for hexagonal structures.

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4.1.6 μ (m): Linear absorption coefficient.

4.1.7 Processing history: thermomechanical routes used to shape, form or join the sample, including deformation and heat processes, modifiying the underlying microstructure and/or residual stes state.

4.1.8 Operando history: concerns previous operating conditions for samples that have been removed from service use and may have alter the underlying microstructure and/or residual stes state.

4.2 Internal strain/ stress

4.2.a Strain:

Principal strain directions: maximum/minimum axial deformations, no shear deformation. Denoted by e_1, e_2 and e_3.

Plane strain: condition where e_3=0.

Intergranular strain: developed due to a) variation in elastic properties of single crystals with direction and b) crystals deform on specific crystal planes in specific directions.

4.2.b Stress:

Principal stress directions: maximum axial forces, no shear forces: S_1, S_2 and S_3.

Plane stress: condition where S_3=0.

Type I: stress that self-equilibrates over a length scale comparable to the dimensions of the sample, thereby spanning multiple grains and/or phases.

Type II: stress that self-equilibrates over a length scale comparable to the grain size.

Type III: stress that self-equilibrates over a length scale smaller than the grain size.

4.2.1 Component

A/R: Axial/**R**adial component in cylindrical geometries.

L/T/N: Longitudinal / **T**ransverse / **N**ormal components in prism geometries.

1, 2, 3 Invariant principal directions and magnitudes of strain/stress

x, y, z Directions defining a right-handed Cartesian co-ordinate axis

Normal: component oriented perpendicular to the surface of the sample denoted by**S.**

Shear: component oriented within the surface of the sample denoted by **T.**

Compressive strain/stress: negative strain/stress values.

Tensile strain/stress: positive strain/stress values.

4.2.2 Elastic regime: linear relationship between force and deformation

Elastic constants: macroscopic relationship in the linear regime between force and displacement defined by modulus (E) and Poisson's ratio (ν)

Diffraction elastic constants: elastic constants associated with diffraction from individual (hkl) lattice planes for a crystalline material

Diffraction Elastic modulus: E_{hkl},

Diffraction Poisson's ratio: ν_{hkl}

Hooke's law: tensorial equation describing the linear dependence of stress and strain through the elastic constants

Compliance Tensor: C tensor qualtity as a function of E_{hkl} and ν_{hkl} and applied to the stress tensor as e=C:S.

Lamé constants: Functions of elastic constants for simplifying inverted compliance tensor needed to calculate stresses from strain.

Load partition: measure of the participation of each phase materials in carrying internal or external loads, a function of properties and phase fraction/orientation.

4.2.3 Plastic regime:

Elastic limit, or Yield stress (YS): Greater than the stage 1 yield stress and less than or equal to 0.2% proof stress.

Strain to failure: elongation capability of the sample at the breaking point.

Ultimate Tensile Strenght (UTS): maximum load bearing capacity of the sample before necking and/or breaking.

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Striction or Necking: effect of cross section reduction in the sample subjected to externally applied tensile load.

Failure Criteria: structural condition to assess the capability of a structure to operate under safe conditions.

Von Mises equivalent stress limit: maximum elastic distortional energy criterion that combines the three principal stresses into a scalar value. A ductile material starts to yield at a location when the von Mises stress becomes equal to the stress limit.

4.2.4 Data correction: When performing layer removal for X-ray residual stress depth profiling it is important to consider any redistribution or relaxation in the residual stress in the exposed surface, particularly if the component is relatively thin. Solutions are available to correct the stress values obtained considering flat samples and/or hollow cylinders.

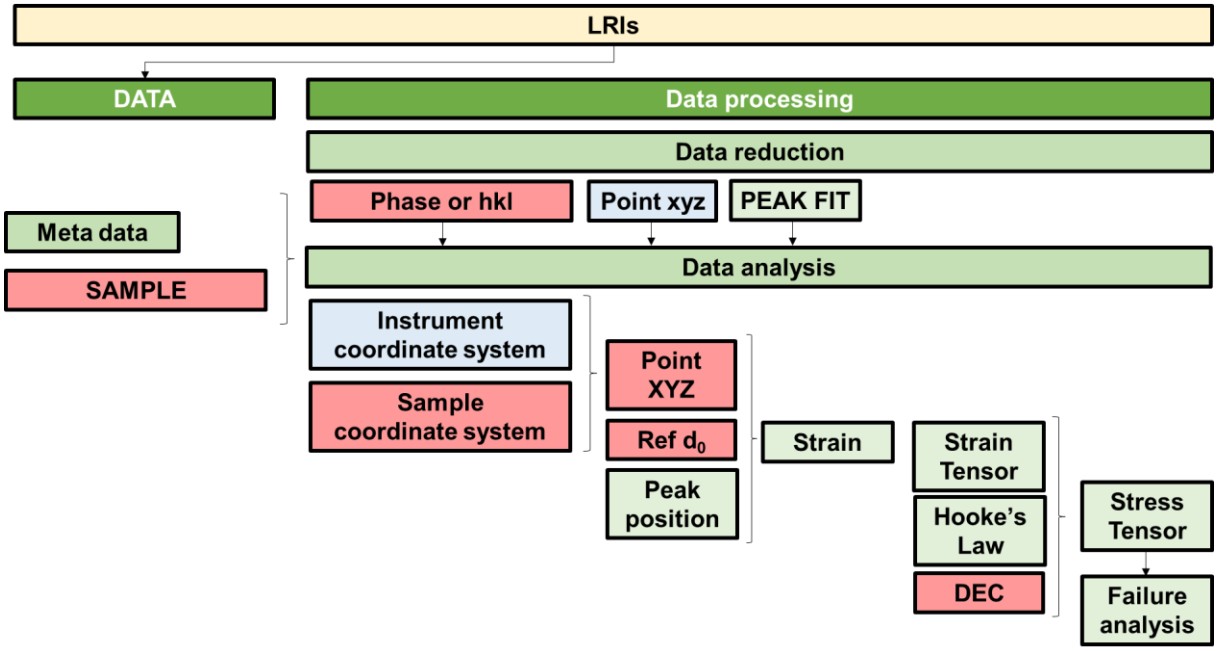

Figure 6 Ontologies for residual or internal strain/stress determination: data analysis branch.

4.3 Report and Data Exploitation

4.3.1 Report: summary of background and RS measurement results.

4.3.1.1 Background and/or Scope: motivation and aim for the measurement in the context of the sample and its applications.

4.3.1.2 Error: Difference between stresses captured (measured) and those predicted (model) or measured by other methods (deep hole drilling, contour method, etc).

4.3.1.3 Precision: Minimum distance between distinguishable stress predictions, e.g. length of domain decomposition. For measurement, the details of orientation and positioning of gauge volumes such that they do not intersect, and deconvolution methodologies for those that do. Strain resolution.

4.3.1.4 Results: peak position (2θ), FWHM and intensity values related to one or multiple locations in the sample. If d0 and DEC are provided the results may extend to strain and stress values. Trend analysis may also be debated in terms of microstructure and/or external conditions applied such as load and/or temperature.

4.3.1.5 Reproducibility: Datum/location features of components and orientation of geometry relative to model. Number of strain components/orientations measured and any assumptions made. Material conditions such as baseline composition, processing history including temper as measured. Measurement conditions for departures from ambient conditions. Details of stress-free reference.

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4.3.1.6 Uncertainty: Range of values of stress which modelling assumptions can provide, range of values of stresses measured. Positional tolerances of measurement points and location.

4.3.2 Data Exploitation: impact and use of a measurements such as input for FEM or publication (peer reviewed article, thesis, conference, etc)

5. Ontologies for RS software and stress simulation

5.1 European Materials Modelling Ontology **(EMMO):** bottom-up ontology framework based on current materials modelling and characterization knowledge.

5.2 Materials Modelling Data (MODA): standardized documentation for simulations proposed by the European Modelling Council.

5.3 Input: conditions necessary to be detailed in order to run a simulation for stress analysis.

5.3.1 Boundary conditions (BC): constraints and external inputs which can evolve to affect the mechanical state of the component, which along with initial conditions and methodology dictate the system of partial differential equations to be solved. Boundary conditions could just used to prevent rigid body motion. For example pre-load and gravity loads. The most important BCs during fabrication are:

- Contact between the material and the cruzible or buildplate (Conduction)
- The heat extraction (Convection)
- The heat emitted to the ambient (Radiation)

Complementary BCs are:

- Clamping
- Anyother heat source involved in the process

5.3.2 Geometry: domain (outer periphery of component), and domain decomposition (e.g. mesh arrangement and type).

CAD: Computer Aided Design which file format is used to describe 3D objects.

Element type: recognised based on their shapes and grouped as 1D element, 2D element, and 3D element.

Geometry Cleanup: Making model FE ready by removing non-critical features from CAD model.

Mesh: splits the domain into a discrete number of elements for which the solution can be calculated.

Mesh convergence: number of elements required in a model to ensure that the results of an analysis are not affected by changing the size of the mesh.

Mesh resolution: size of the sampled volume or element

Element Type: Hexa, Quad, simple, double, etc.

Node or Connections: Joint creation or contact creation. The interaction between adjacent mechanical components to build mechanism/sub-system.

5.3.3 Initial conditions: starting point of component conditions, e.g. stationary, ambient temperature.

5.3.4 Material Properties: thermomechanical properties of the materials.

Mechanical Properties: Young's Modulus, stress - strain curves, S-N curves

Physical Properties: solidus & liquidus temperatures, density, melting point, solid state transformations, precipitation Mechanics, absorptivity / emissivity.

Thermal Properties: Conductivity, specific heat, expansion coefficient.

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5.3.5 Simulation method or Solver: resolution of differential equations in engineering components and structures concerning the equilibrium of forces (including the scale: micro-, meso-, macroscale). They are usually based on:

Finite Element Method (FEM): numerical method that provides a contimuous solution with values stored at the element nodes.

Finite Difference Method (FDM): numerical method that provides a discrete solution.

Finite Volume Method (FVM): numerical method that provides a discrete solution with values stored at the center of the finite volume.

5.3.6 Simulation Type or Code:

5.3.6.a) Mechanical:

Inherent strain method (ISM): consists in simulating the thermal stress build up at component scale by using a residual plastic strain (inherent strain) tensor which is activated in the individual hatching regions of a macro-scale mechanical model in a layer-by-layer fashion.

Fatigue Analysis model: relates damage accumulation to the number of load cycles while taking into account the loading conditions (load ratio, energy release rate, and mode mixity).

Static Structural model: describes the static structure of the system being modeled, which is considered less likely to change than the functions of the system

Volume Shrinkage Method (VSM): linear elastic finite-element modelling that assumes that the linear thermal contraction of a nominal shrinkage volume is the main driving force for distortion; the model solution times are reduced significantly.

5.3.6.b) Thermomechanical:

Thermal elastic-plastic model: temperature history is employed as a thermal load in the mechanical elastic–plastic calculation of the residual stress field. Phase volume fractions and the lattice change due to phase transformation is considered through modifying the thermal expansion coefficient over the temperature range of interest. Note that variation of yield strength goes together with phase variation in the modelling.

Layer by Layer approach: regarding additive manufacturing processes, this is a simplified model where instead of activating the real path of the laser, a macrolayer is activated with an activation energy equivalent to its volume. It is then allowed to cool, simulating the cooling that the recoater would expect, and it continues. This method is very widespread for thermomechanical simulation in LPBF given the computational efficiency, on the contrary, it is a method that requires calibration since it is a rather crude simplification of the real physics of the process.

Segment by segment approach: in comparison with previous point in this model instead of activating the real path of the laser it activates sub-segmentations within a layer, that is, there will be N time steps (defined by the user) that will correspond to the activations of mesh segments within each layer. This allows capturing macrotrends in thermal gradients, although not all the information related to the manufacturing strategy. The computational cost is an exponential function of N time steps.

High fidelity approach: thermomechanical simulation activating exactly the path traveled by the laser during manufacturing, it is the most accurate way to have a detailed thermal history at the layer level as well as the thermal gradients within each layer. Its computational cost is enormous and in industrial cases it is considered incomprehensible.

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5.3.6.c) Computational fluid dynamics (CFD): produces quantitative predictions of fluid-flow phenomena based on the conservation laws (conservation of mass, momentum, and energy) governing fluid motion.

5.4 Output: Stresses and strains over the entire or subset of a domain at specific points, averaged at mesh junction points (nodes) which is a feature common to all simulation methods.

5.4.1 Centre: location of the stress value (in sample xyz) defined by the centre of the mesh volume.

5.4.2 Distortion: shrinkage or expansion of the sample, deviation form the planned geometry.

Angular distortion (deflection): angle formed between the original CAD file or geometry and the resulting displaced/deformed geometry.

5.4.3 Mesh volume: size in cubic mm of the mesh element related to the location of a strain/stress value.

5.4.4 Strain/Stress:

Contact pressure: the ratio of the normal load to the true contact area

Displacement Plots: display the deformed model geometry either alone, with the undeformed edge, or overlaid on an outline of the undeformed geometry.

Principal Stress Plots: gives the maximum normal stress and its position acting inside each element.

Reaction forces and moments: are the resulting loads seen at the restraints of a model being analyzed.

Von Mises: failure condition when the shear strain energy per unit volume in the sample exceeds the shear strain energy per unit volume stored in the material in the one-dimensional loading test.

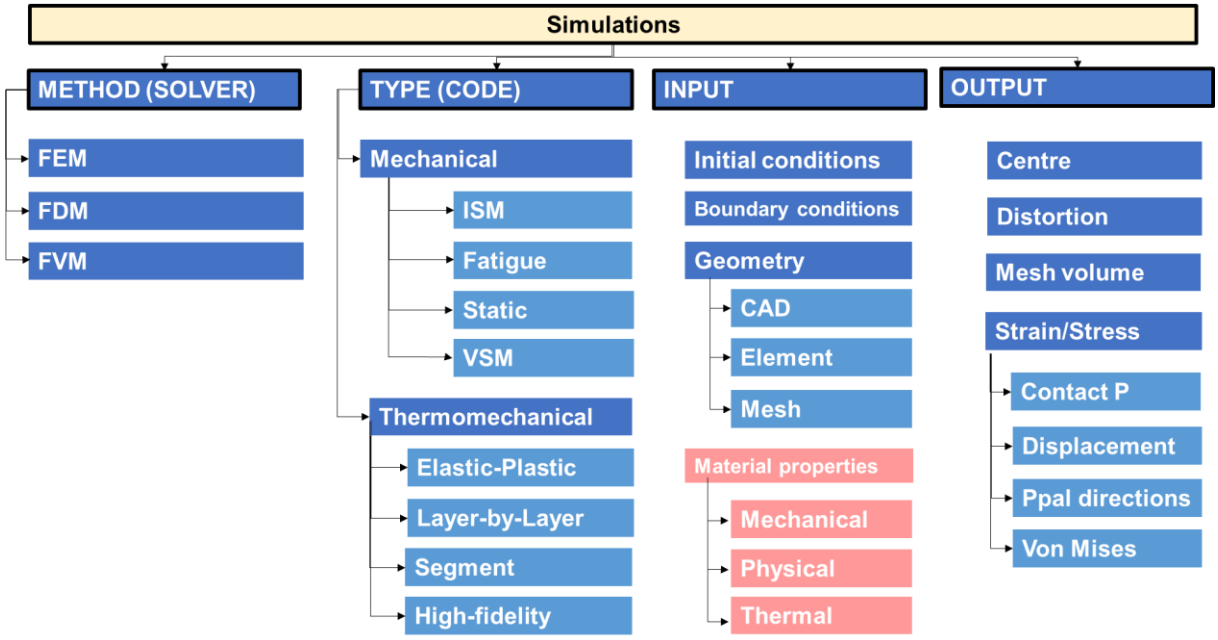

Figure 7. Ontologies for RS software and simulations

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6. Complex workflows at LRIs

This section describes the detailed workflow for characterization services at LSRIs with a selection of examples for neutron, synchrotron and X-ray instruments dedicated to residual stress measurement, which are involved in the EASI-STRESS project, namely ATHOS (neutron, EK, Budapest, HU), SALSA (neutron, ILL, Grenoble, FR), ID15A and ID31 (Synchrotron X-ray, ESRF, Grenoble, FR), P07 and P61A (Synchrotron X-ray, HEREON, Hamburg, DE) and X-Raybot/Set X (X-ray, CETIM, FR and DTI, DK). The description comprises the access to the facilities, steps before, during and after beam time, as well as reporting standards already in place as proposed before in CHADA format for D4.1 (based on ISO 21432:2019) and the NQL®. More comprehensive descriptions of the instruments are available in Deliverable 3.2 and theoretical equations and diagrams will be detailed in next Deliverable 4.2. Furthermore, the scope of LRIs is contextualized with laboratory x-ray method and industrial simulations to identify overlaps and gaps in RS characterization and analysis.

The process includes the CHADA classifications proposed in D4.1 (4 and **Error! Reference source not found.**, respectively), which is composed of 4 levels, to which we add 3 levels :

1. Access
2. Sample & measurement preparation,
3. Instrument calibration & alignment,
4. Sample & d_0-reference data acquisition,
5. Data reduction & post processing.
6. Reporting results
7. Exploitation of results

In the overall workflow in Figure 8 we include now level (0) for contact and access to the facilities and definition of the measurement or problem to solve. We include as well a level (6) for further exploitation of results – beyond the reporting measurements (level 5): comparison/ validation with FEM and/or publication (conference, scientific journal, thesis, etc).

Once the study case and measurements are identified, together with the corresponding confidentiality level, several access routes to large instruments can be proposed (see also Table 1 below):

- Collaboration access: under common project (academic or industrial), no confidentiality, beam time within 6 months and up to 3 years
- Proposal: peer-reviewed access with academy, no confidentiality, 2 calls a year, beam time within 6-12 months.
- Feasibility or Easy Access: For example, the Easy Access SYstem (EASY) grants beamtime to scientists from ILL member countries, who need a small amount of beamtime, to perform rapidly some measurements (not a full experiment). Access is open all year long, and it is not necessary to go through the ILL standard proposal round and consequent peer review system.
- Proprietary access: commercial access, under contract, confidentiality to be specified, paid access, usually within 3 months.

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Table 2. Access Routes to LRIs (adapted from an ILL original table)

	Selection of the request (peaceful end-use)	Cost	Delay to get measurements	Publication of results	Facilities involved in the project
Public Access (competitive, 2 calls/year)	Evaluation by a panel of experts, ranked according scientific relevance (rate of success ranging from 30% to 70% depending on the instrument and facility)	No costs in case the proposal is granted	Between 6 to 8 months	Results should be published in peer-reviewed scientific journals.	ILL ESRF HEREON BNC
Proprietary access	No selection	Depending on the facilty and instrument	As soon as possible (from 1 week, depending on the instrument and facility)	Confidentiality ensured Proprietary results	ILL ESRF HEREON BNC
Feasibility oe	Industrial R&D topics, few hours of measurements	Beam time and analysis not charged	When possible (from 2 weeks, depending on the instrument and facility)	No. Facilities are keen on making some of the tests visible for communication purposes.	ILL ESRF HEREON BNC
medium/long-term agreement	On an individual basis	On an individual basis (material, personnel, etc.)	On an individual basis	On an individual basis	ILL ESRF HEREON BNC

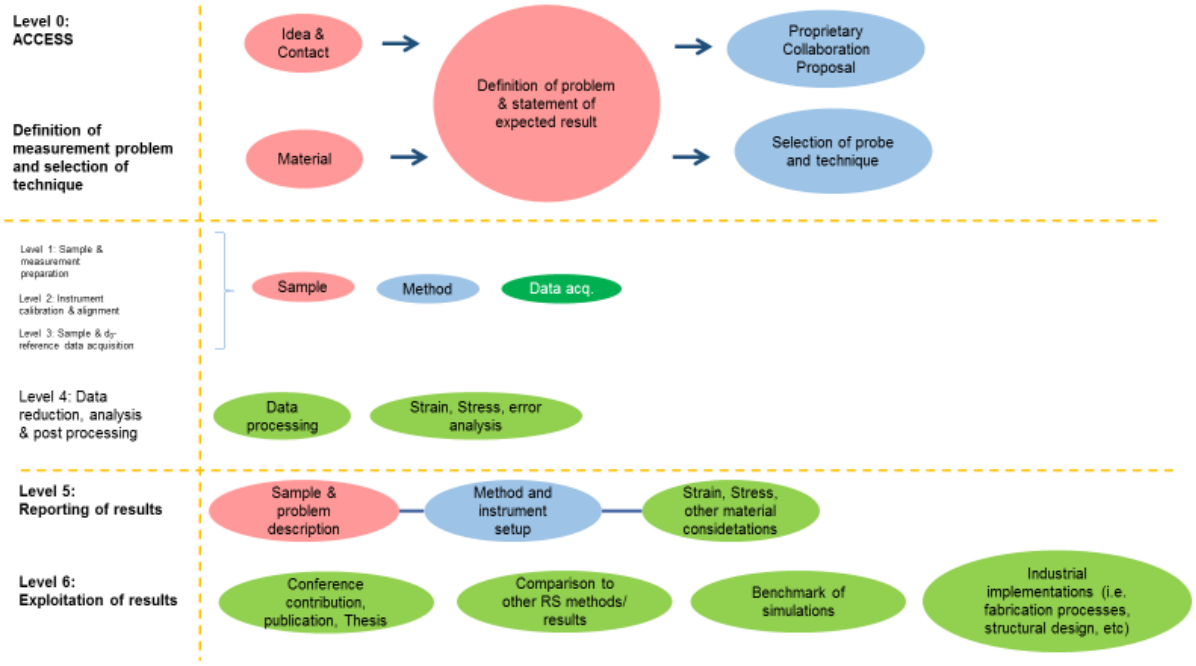

Figure 8 CHADA summary for access, measurement and data exploitation at LRIs.

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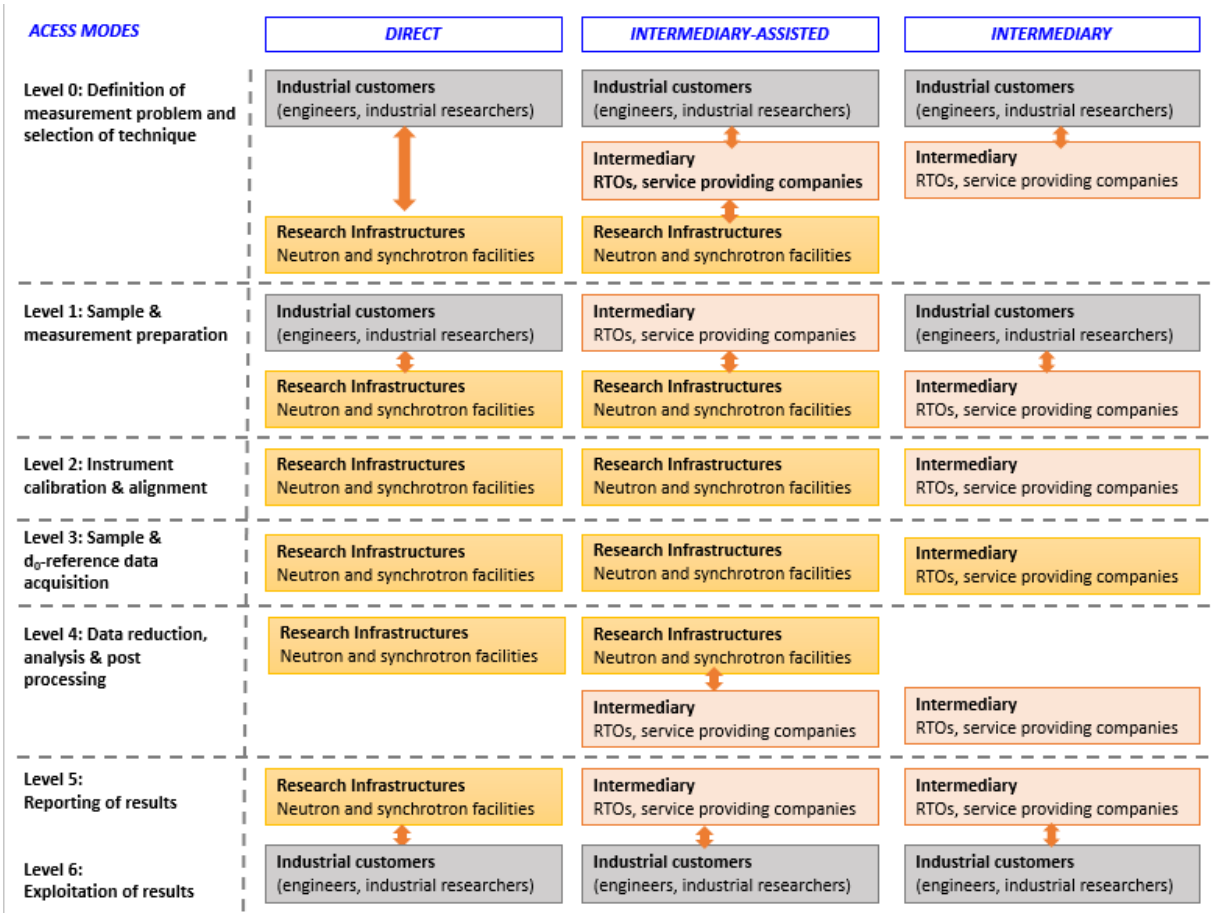

Figure 9. Complex workflow for the interactions and interfacing between the different levels in previous CHADA summary (Figure 8)

6.1 Scope, overlap and gap of RS characterization methods

For comparing the diffraction methods and simulation scopes Table 2 is presented. Furthermore, details of each participant RS characterization facility in EASI-STRESS and their instruments are detailed below.

a) BNC-ATHOS- neutrons

Beam line under development for RS analysis from a cold neutron three-axis spectrometer at the Budapest Neutron Centre (BNC) - part of the Energy Science Research Center (EK) in Budapest, Hungary. The instrument is used in a multi purpose regime, e.g. for high-resolution diffractometry, strain analysis, reflectometry, quasielastic and inelastic scattering as well. General access through proposal system at BNC is granted under review of an external panel of experts twice a year (70% of beam time). In-house beam time could reach up to 30% , shared with industry contracts representing 5 to 10% of that internal beam time.

b) ESRF – ID15- synchrotron

ID15A is an energy-dispersive diffraction (EDD) set-up at the ESRF which can be used for strain/stress mapping in the bulk of thick metallic components. Proposal access represents 70% of beam time whereas in-house development and collaborations take up to20 %. Industrial activity takes maximum 10%, depending on the demand.

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c) ESRF- ID31 - synchrotron

The high-energy beamline for buried interface structure and materials processing is dedicated for interface and materials processing studies using high energy x-rays. It offers a portfolio of hard X-ray characterisation techniques including reflectivity, wide and small angle diffraction (both in transmission and grazing incidence geometry), imaging methods, auxiliary techniques, coupled with a great versatility in choosing beam sizes, energy and energy-band. Proposal access and industrial/ in-house developments are equivalent to ID15.

d) Hereon – P07 High-Energy Materials Science Beamline (monochromatic) synchrotron

The High Energy Materials Science Beamline (HEMS) P07 at PETRA III satisfies high-energy X-ray diffraction (XRD) and imaging techniques. Measurements at P07 include both depth-resolved residual stress analysis, i.e. with conical slits, and fully transmission measurements. General user access through proposals is granted by a review panel twice a year (80%). 10% is for commissioning and 10% for in-house experiments. Industry access is between 5 and 10%.

e) Hereon- P61A White Beam Engineering Materials Science Beamline- synchrotron

The White Beam Engineering Materials Science (WINE) beam line P61A at Petra III is designed for the combination of energy dispersive X-ray diffraction (ED-XRD), angle dispersive X-ray diffraction (AD-XRD) and imaging techniques (radiography / absorption contrast). P61A is optimized for reasidual stress measurements within the bulk (transmission mode) and near the surface (reflection mode). Beamtime for users and industry follows the same rules as for P07.

f) ILL – SALSA - neutrons

SALSA – Strain Analyzer for Large Scale Applications is a monochromatic two-axes neutron diffractometer located at the Institut Laue-Langevin (ILL), Grenoble, France. Beam time distribution accounts for a dedicated industrial (proprietary access) of about 5% and collaboration (open) access up to 25% including internal time. General access through proposal system (70%) is granted under review of an external panel of experts twice a year.

g) CETIM – laboratory X-rays

Residual stress analyses by X-ray diffraction in laboratory are carried out with diffractometer as X-Raybot, Set-X or Bruker following the EN 15305 (2009) standard: Test methods for residual stress analyses by X-ray diffraction. The X-ray tube and filters will change in function of the characterised material and the analysis parameters will be adapted regarding the geometry of the analyzed area. CETIM's laboratory is available all the year to carry out some measurements, no particular process to follow, usually 20% time is dedicated to academic projects and 80% to industry.

h) DTI – laboratory X-rays

DTI operates a laboratory service function similar to CETIM with the X-Raybot also following the EN 15305 standard. The DTI measurement services is available to customers from both academia and companies. Most often, the academic users do not pay full fee if their usage leads to a case story that can be used by DTI to pomote the commercial service.

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Table 3. Characterization capabilities for residual stress anlaysis.

Method	Scope	Considerations
Neutron Diffraction	Complete stress tensor Non-destructive (NDT) Macro-stresses and micro-stress Bulk and near-surface: realistic sized parts and components In-situ and in-operando test conditions	Only elastic strain quantification; plastic strain only qualitatively Volume averaged stress values No microscopic stresses Access (>6 months) except feasibility or proprietary GV cubic geometry
Synchrotron Diffraction	NDT Macro- and micro-stress Bulk, surface & near-surface Ultra-fast acquisition In-situ and operando test conditions	Stress-tensor determination not always possible Only elastic strain quantification; plastic strain only qualitatively Small samples GV rhombohedral geometry (high lateral resolution) Access (>6 months) except feasibility and proprietary
X-Ray Diffraction	NDT (surface) or destructive (layer removal for bulk access) Surface Easily available Cheap	Only elastic strains Small samples Destructive bulk stress determination (layer removal max. 1-2mm) GV rhombohedral geometry (no lateral resolution) Restricted sample environment

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