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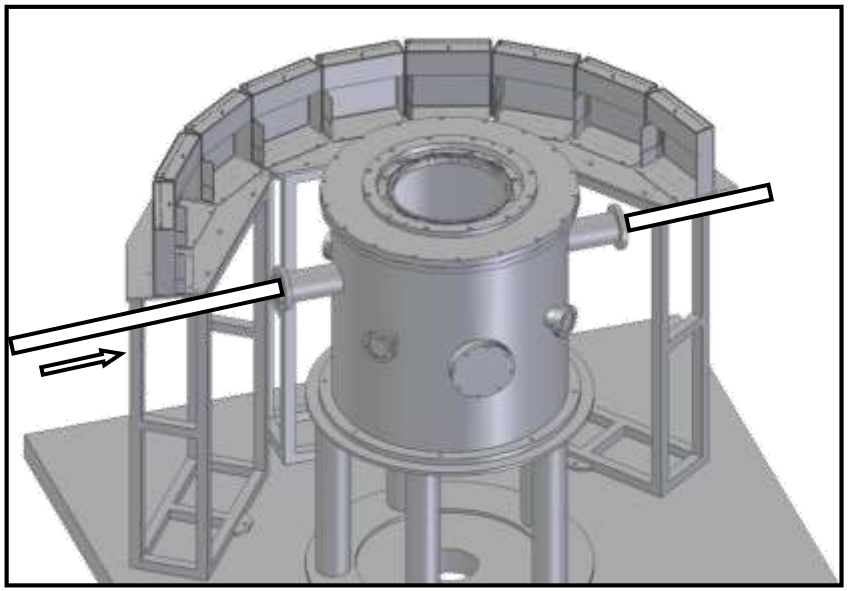
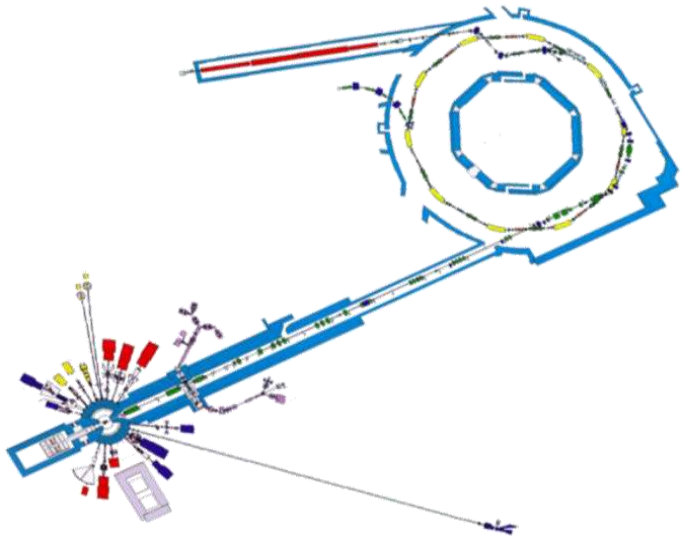
Managing data as part of research infrastructure

Antonella Scherillo

ISIS facility, STFC, UK





Outline

- Who am I?
- Where do I work?
- Access and data management at ISIS – STFC
- Example of data collection, treatment and results

About me….

- Since 2010 I am the INES instrument scientist
- I support users during they experiment and data treatment
- I develop and mantain the instrument
- My main research interest is material science, in particular archaeometry

About INES@ISIS....

- **INES is a powder diffractometer built and managed within the collaboration between CNR (IT) – STFC (UK), operating at the ISIS spallation source, UK**

- **INES became fully operational in 2007, since then it is open to proposal from international community**

- **Your proposals are welcome and funds are available, depending of your nationality. UK users are funded!**

RAL aerial view

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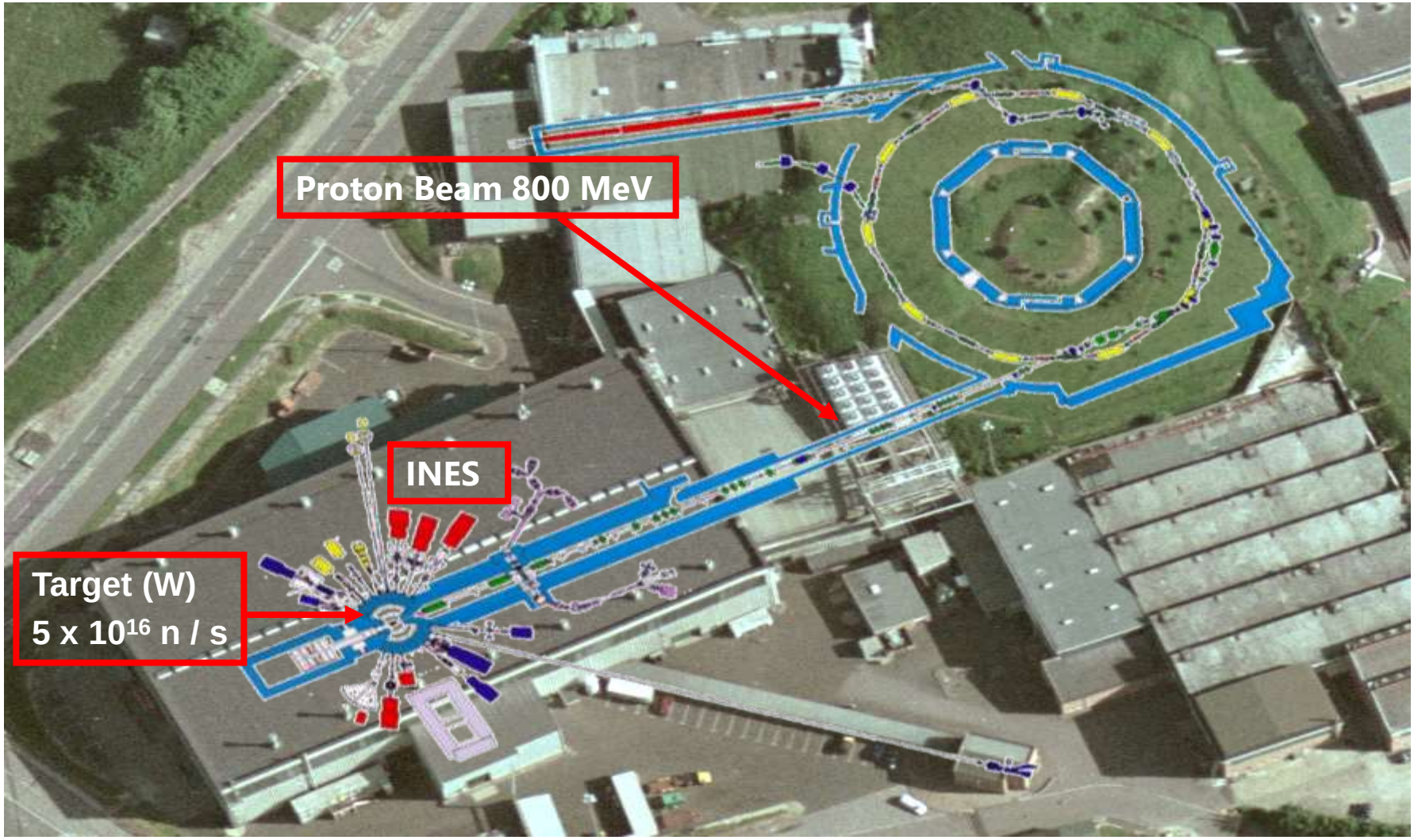
The ISIS Spallation Neutron Source -TS1



Neutron for Archaeometry

- All crystalline material – metal, pigments, rock, ceramics – can be analysed by neutron diffraction. Archaeological object in most cases can be considered randomly oriented polycrystalline material (powders)

- Neutrons are non-destructive and can penetrate deep into the artefact to reveal micro-structure, phase composition or provide 3D images

- Whole artefacts can be placed in the neutron beam and analysed at room conditions, without sample preparation

ToF -ND for Archaeometry

- Determine the wt% of crystal phases present in the sample
- Binary alloys composition (elements wt%)
- NRCA, PGAA etc...

Composition

- Texture (preferred cristallites orientation)
- Cristallite size
- Residual stress

Working techniques

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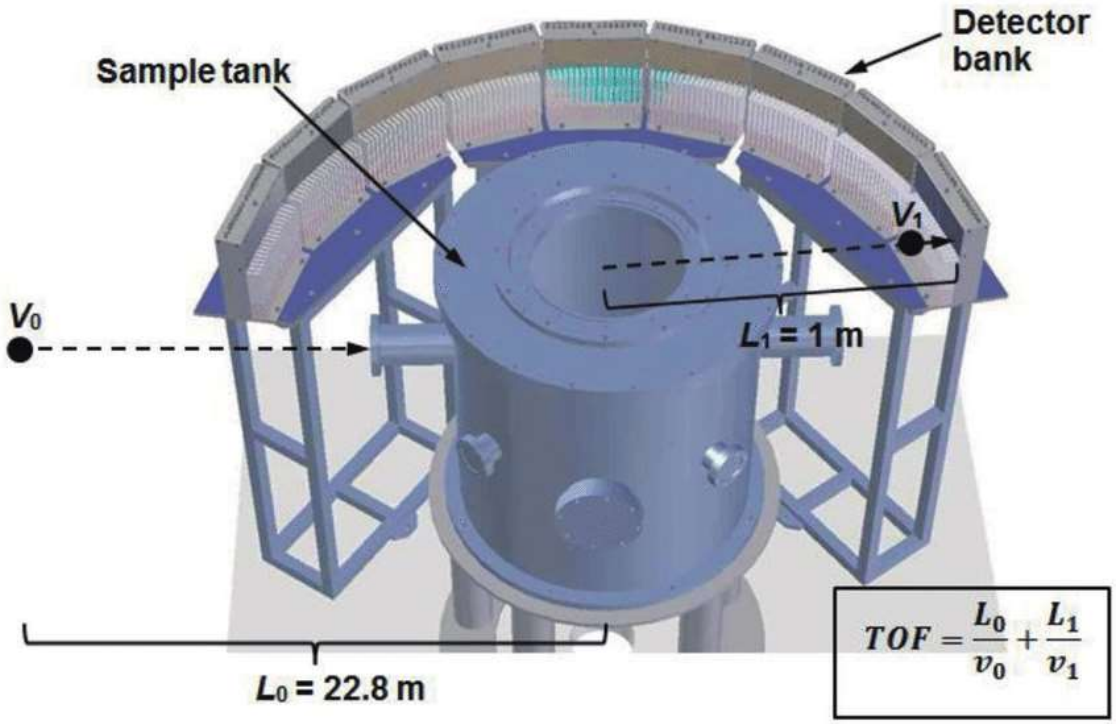

- Large sample holder tank (1 m^3)
- 144 ^{3}He diffraction detectors
- 9 banks
- d-spacing: 0.4-12.0 Å
- High resolution: 0.10% backscattering
- Beam size: 30x30mm
- Jaws to shape the beam: min 2x2mm
- Laser pointer to align the sample
- Neutron Radiography apparatus to align and scan through the sample
- X-Y precision positioning table
- NRCA - YAP detector

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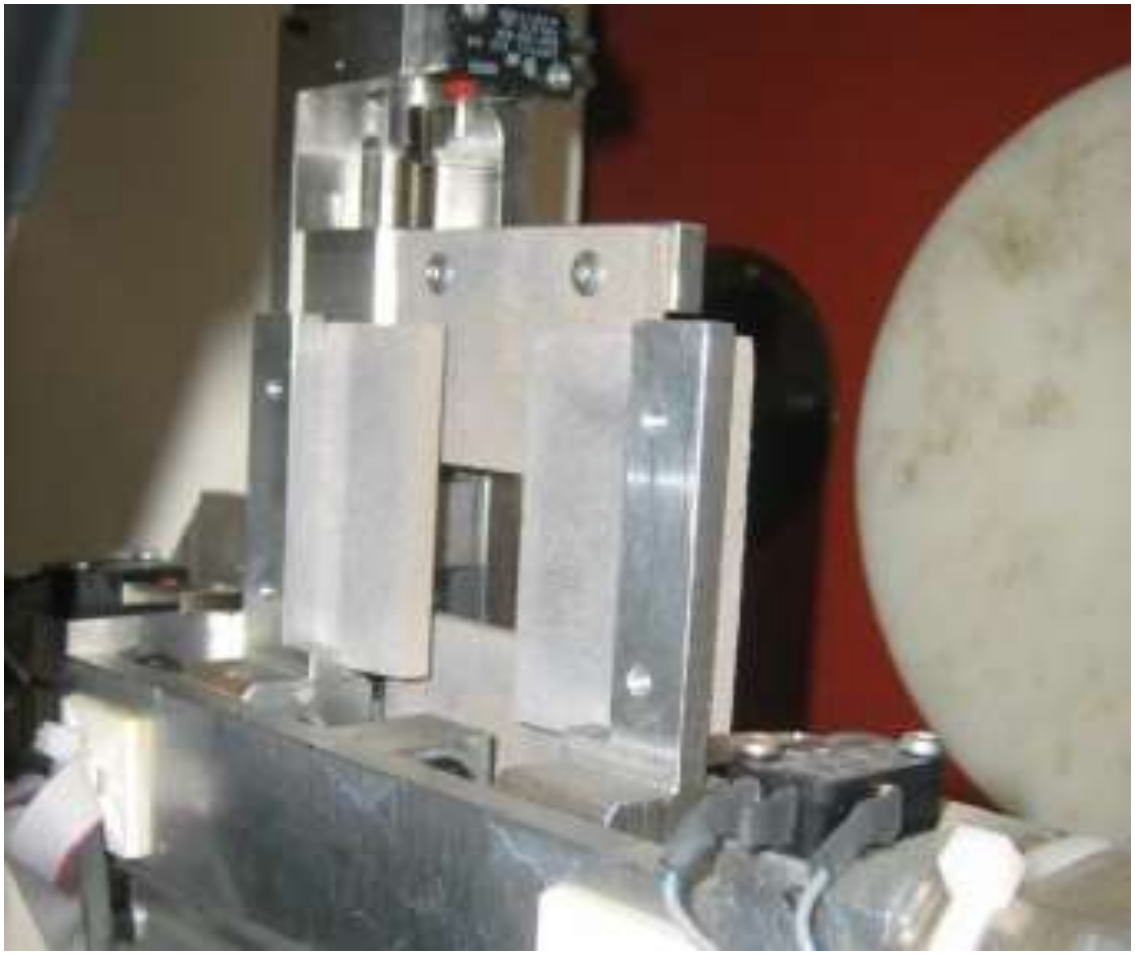

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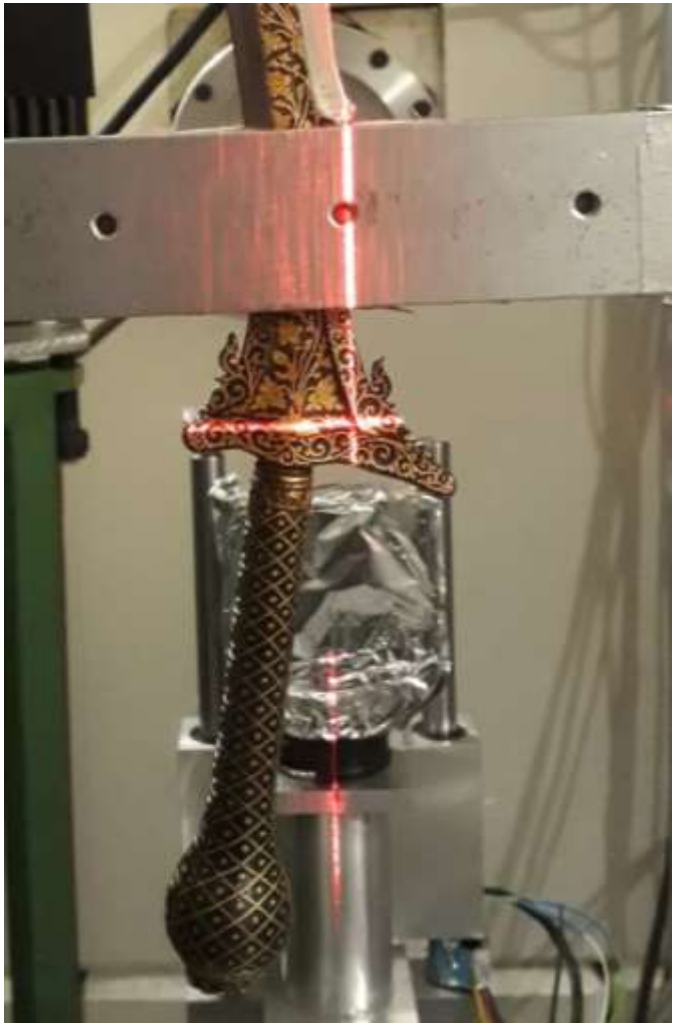

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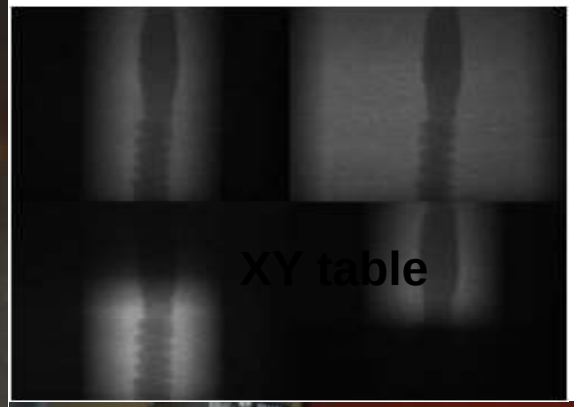

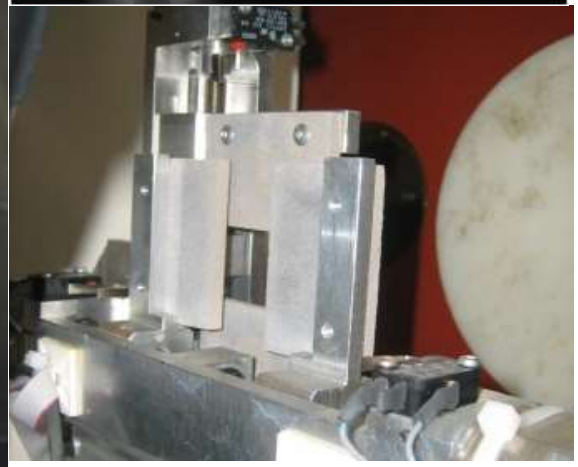

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XY table

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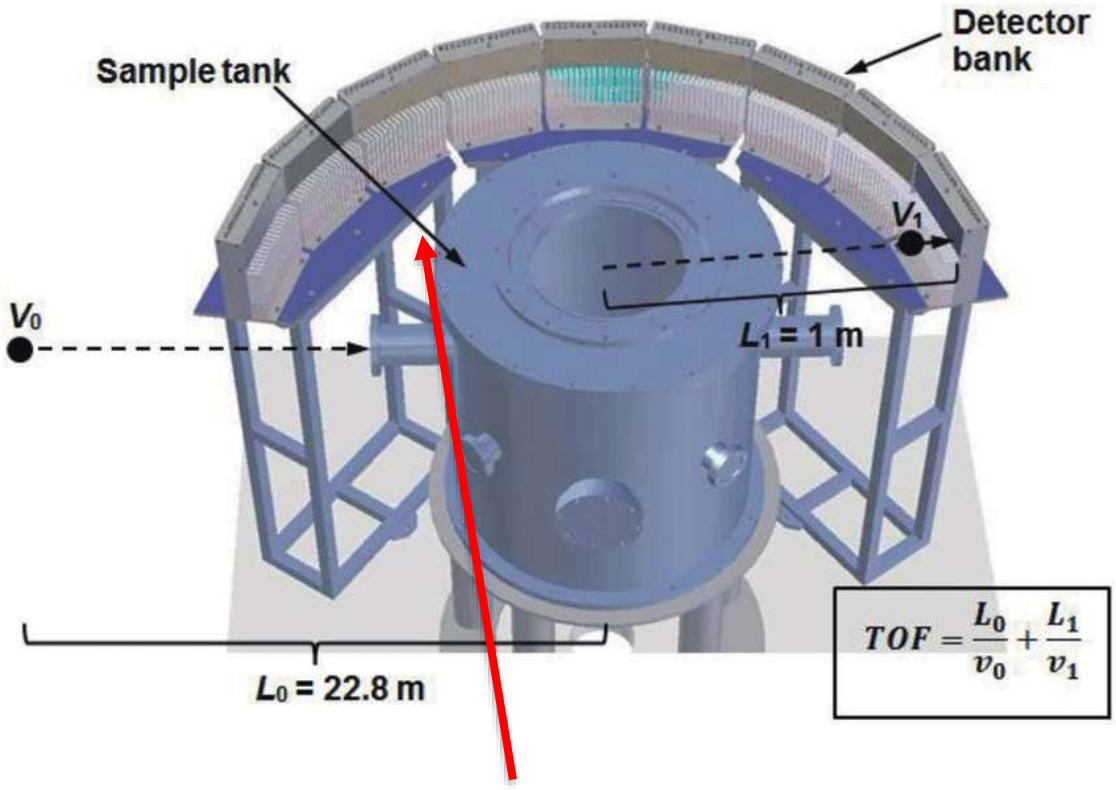

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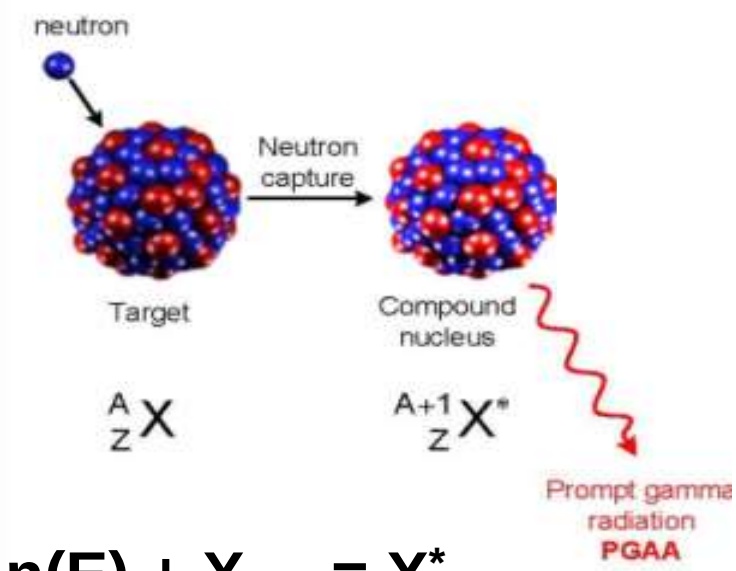
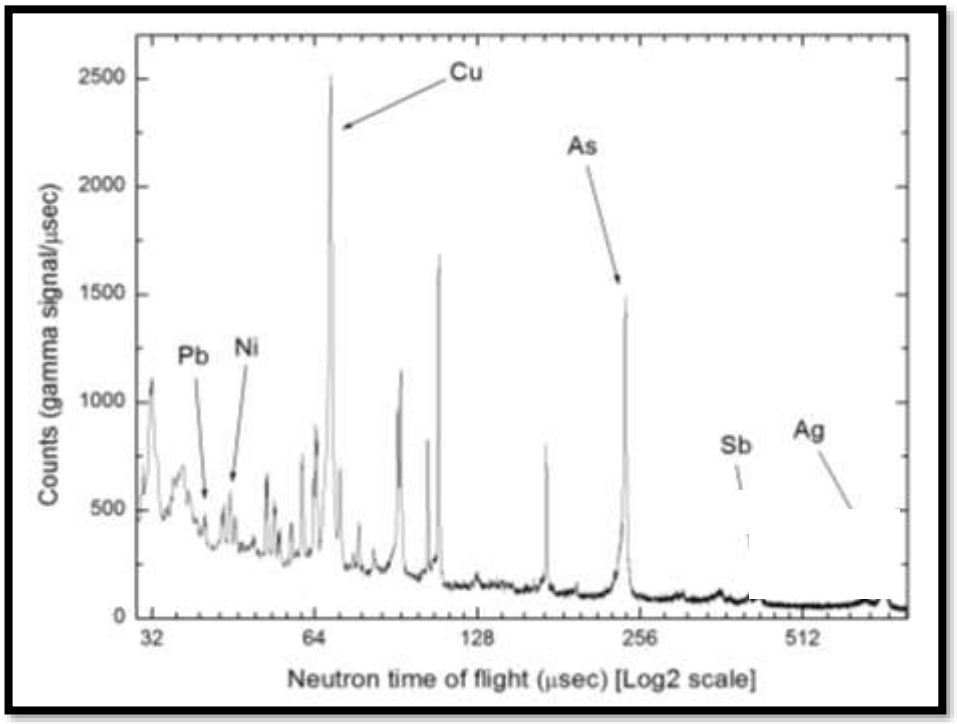
Neutron Resonance Capture Analysis



$$n(E) + X_{A,Z} = X^{*}_{A+1,Z}$$



- **We can have detailed semi-quantitative information on the composition of our sample**
- **It is isotopic selective**

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Access to ISIS

- **ISIS instruments are free at the point of access for academic and industry researchers, provided the results from experiments are published in the public domain. Fully confidential fast-tracked use of the instruments is also available for industrial and commercial customers.**

- **Proposals should have a Principal Investigator (PI), an experimental team able to conduct the experiment, with the support of the local contact, and to analyse the data. Proposals should clearly state the relevance and impact of the proposed experiment.**

- **ISIS operates nine Facility Access Panels (FAPs) to peer review all beamtime proposals. Panels meet twice a year, in June and December. Proposals are ranked on a scale from 10 (world class) to 1(unsatisfactory). Beamtime is awarded to the highest scoring proposals, subject to instrument availability.**

- **New users are always welcome at ISIS Neutron and Muon Source and we are constantly encouraging new areas of research that can flourish.**

Access to ISIS data

- **All data produced at ISIS is catalogued into ICAT – the ISIS data catalogue. You can log in to ICAT using your account.**
  The PI and the experimental team will have an ISIS account when the register to the proposal system to submit their proposal.

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Data set, especially for imaging or position sensitive detectors can be very large!!!

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Access to other large scale facilities (beamtime and data)

- Similar policies are in place in several large scale facilities like ILL (high-flux neutron source in France).
- The raw data and metadata are managed by the facility, and made available firstly to the experimental team, and then – possibly- open access.

Is our data management ideal?

- At present, in most of the cases the raw data and metadata are stored by the facility in a “safe” repository, and made available firstly to the experimental team, and then –possibly- open access.
- Should the community be able to reuse the data after the publication process? If yes, how?
- Science funders, publishers and governmental agencies are beginning to require data management for data generated in publicly funded experiments with the goal that they should be re-used for downstream investigations, either alone, or in combination with newly generated data.
- What constitutes ‘good data management’ is, however, largely undefined, and is generally left as a decision for the data or repository owner….

FAIR data management concept

- **FAIR**—Findable, Accessible, Interoperable, Reusable

Courtesy of “The FAIR Guiding Principles for scientific data management and stewardship.”, Published online 2016 Mar 15. doi: 10.1038/sdata.2016.18

How can we make data FAIR?

- **FAIR**—**Findable**, Accessible, Interoperable, Reusable

The FAIR Guiding Principles

To be Findable:

F1. (meta)data are assigned a globally unique and persistent identifier

F2. data are described with rich metadata (defined by R1 below)

F3. metadata clearly and explicitly include the identifier of the data it describes

F4. (meta)data are registered or indexed in a searchable resource

How can we make data FAIR?

- **FAIR**—Findable, **Accessible**, Interoperable, Reusable

The FAIR Guiding Principles

To be Accessible:

A1. (meta)data are retrievable by their identifier using a standardized communications protocol

A1.1 the protocol is open, free, and universally implementable

A1.2 the protocol allows for an authentication and authorization procedure, where necessary

A2. metadata are accessible, even when the data are no longer available

How can we make data FAIR?

- **FAIR**—Findable, Accessible, **Interoperable**, Reusable

The FAIR Guiding Principles

To be Interoperable:

I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.

I2. (meta)data use vocabularies that follow FAIR principles

I3. (meta)data include qualified references to other (meta)data

How can we make data FAIR?

- **FAIR**—Findable, Accessible, Interoperable, **Reusable**

The FAIR Guiding Principles

To be Reusable:

R1. meta(data) are richly described with a plurality of accurate and relevant attributes

R1.1. (meta)data are released with a clear and accessible data usage license

R1.2. (meta)data are associated with detailed provenance

R1.3. (meta)data meet domain-relevant community standards

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Are ISIS data FAIR?

H2020 project PaNOSC officially started to contribute making FAIR data a reality 17 Dec 2018

- Large-scale research infrastructures produce a huge amount of scientific data on a daily basis.
- For storage and future use, data need to be managed according to the FAIR principles.
- The adaptation and development of both policies and technologies are key to making FAIR data a reality.
- The project, which will run until December 2022, is coordinated by the ESRF (European Synchrotron Light Source, Grenoble, France). Other member are ILL (neutron source, Grenoble, France) and ESS (European spallation source, Lund, Sweden, operational from around 2025)
- The project will work closely with the national photon and neutron sources in Europe in order to develop common policies, strategies, and solutions in the area of FAIR data policy, data management and data services.

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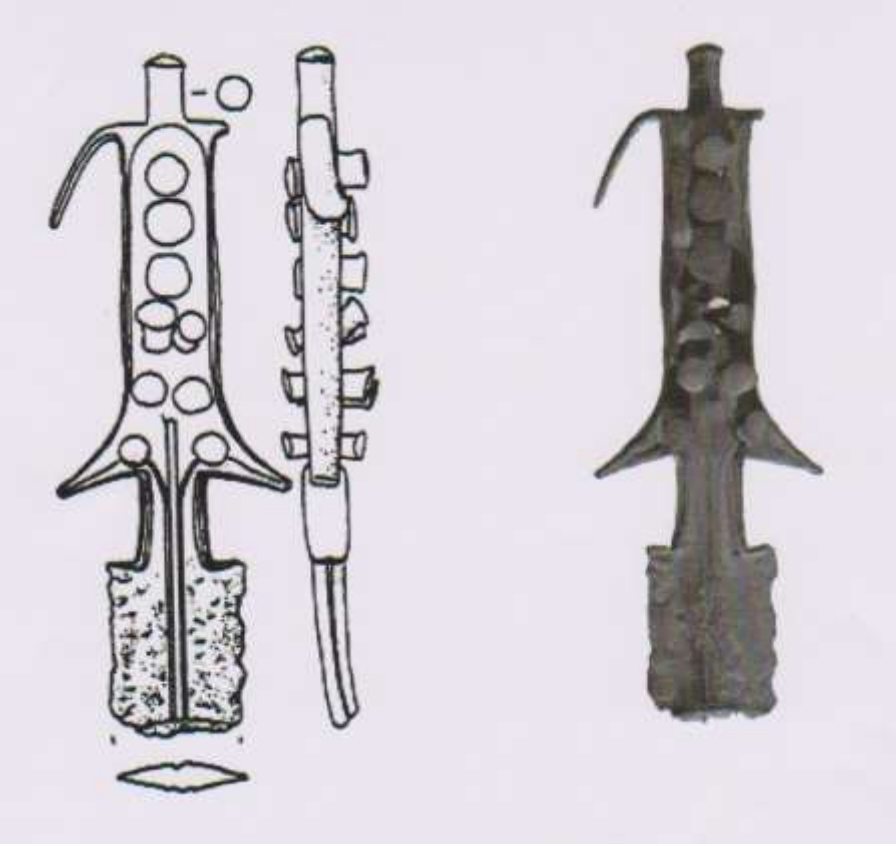
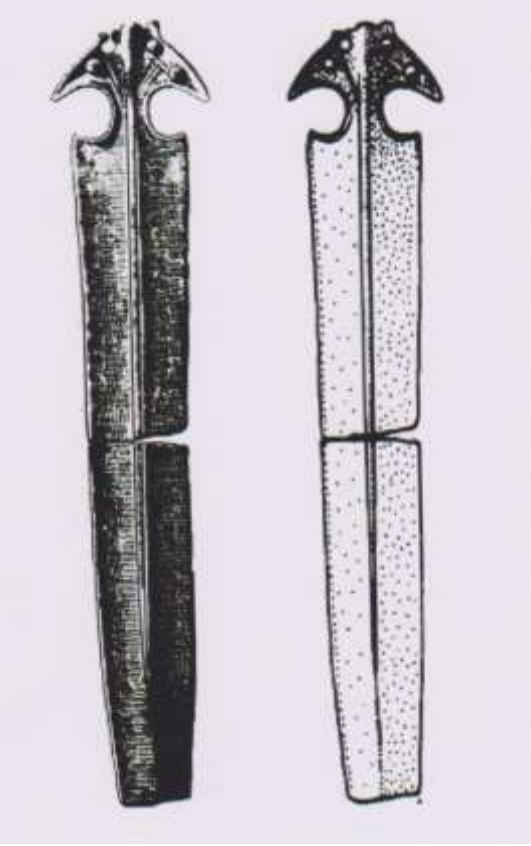
Characterization of Sardinian bronze age swords of *Monte Sa Idda* type



Riveted Sa Idda sword (type A)



Ringed Sa Idda sword (type B)

Antonella Scherillo

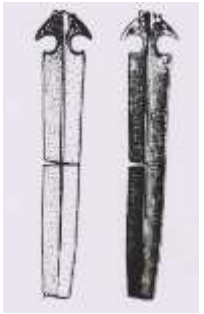
Francesco Grazzi

Università degli Studi di Sassari

Antonio Brunetti, Anna Depalmas

Ministero
dei beni e delle
attività culturali
e del turismo

Marco E. Minoja, Gianfranca Salis, Sergio Orru'



Quantitative phase analysis + lattice parameter determination

⇩

Amount of Sn in the Cu-Sn alloy (bronze)

Conservation status of the swords (presence and amount of copper mineralization products)

Microstructural characteristics (texture, residual stress, grain size)

⇩

Manufacturing procedure and composition to compare with contemporary bronze artifacts produced in the other areas of the Mediterranean sea

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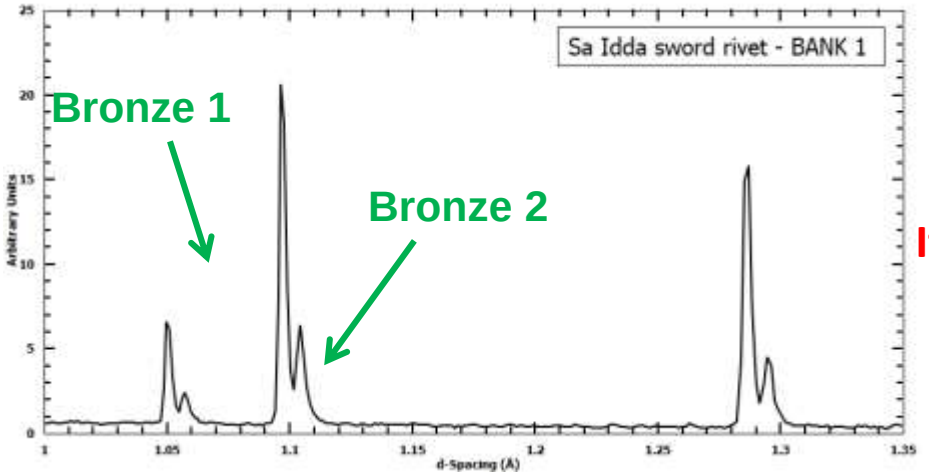
Riveted Sa Idda

Measuring point	Bronze dendritic #1	Bronze dendritic #2	Lead	Cuprite (Cu_2O)	Tenorite (CuO)	Nantokite (CuCl)
Edge right	33.1±0.2	66.5±0.2	0.3±0.1	0.1±0.1	--	--
Rivet	79.8±0.2	19.1±0.2	--	0.7±0.1	--	0.4±0.1

Dendritic segregation

⇩

the casting has been followed by a slow cooling, no annealing



Low amount of Cuprite

⇩

The sword was conserved in a low oxigen environment

It was possible to quantify Nantokite, even if it is located under other mineralization product since neutron penetrate deep into the artefact!!!

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Riveted Sa Idda

Measuring point	Lattice dendrite #1	Lattice dendrite #2	Tin weight concentration dendrite #1	Tin weight concentration dendrite #2	Tin average weight concentration
Edge right	3.63419(8)	3.6624(2)	3.3±0.1	8.1±0.2	6.5±0.3
Rivet	3.63576(2)	3.66036(6)	3.6±0.1	7.8±0.2	4.4±0.2

The rivets show a lower Sn content

⇩

more malleable bronze to be hammered

Measuring point	Texture index J	Strain level S400	Size parameter γ_2
Edge right	1.020(1)	6.2(2)	--
Rivet	1.011(1)	0.08(1)	--

Strain higher in the blade than in the rivet

⇩

The blade was cold worked to harden it, the rivet was shaped on the blade at high temperature

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Characterization of Sardinian bronze age swords of *Monte Sa Idda* type

Quantitative phase analysis + Microstructural parameter determination

⇩

Absence of lead and manufacturing technique are according with the information available on the *Monte Sa Idda* Iberian swords, possibly they were imported

Sword 2 and 3 should be conserved in a dry environment to avoid hydration of CuCl, detrimental for the sample integrity

Sword 3 was votive not a weapon as 1 and 2

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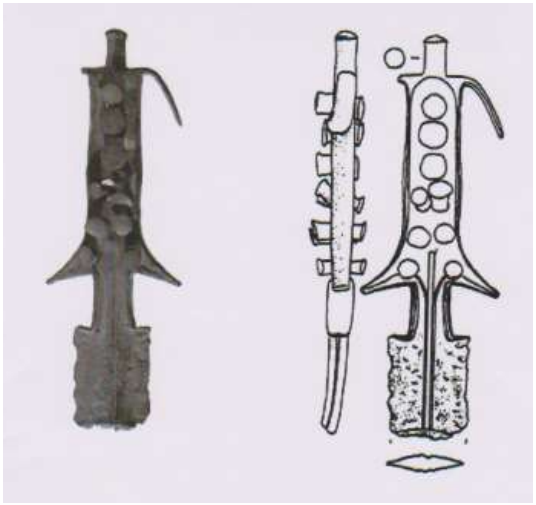
Characterization of Sardinian bronze age swords of *Monte Sa Idda* type – data management

- **The data collected in the several runs performed during the experiment are *relatively* easily accessible trough ISIS data service.**
- **Some of the metadata, in particular the ones relative to the experimental set-up and the instruments are available from ISIS. Some of the metadata do not follow any standard…..**
- **The data can be visualised using free software (Mantid) made available from ISIS.**
- **Some of the information relative to the swords are available from the museum catalogue and previous archaeological paper.**
- **Results from data analysis have been published.**

Characterization of Sardinian bronze age swords of *Monte Sa Idda* type – data management

- **How people know that those Sardinian swords have been analysed with neutrons?**
- **It would be great if there was an open database of cultural heritage related objects, with an open search tools, containing information not only about the objects themselves but also on all the study performed on it…..**



Thank you for your attention!