Metadata Schemas for FAIR* Data in Materials Science: Scanning Electron Microscopy (SEM) Use Case

A detailed and practical schema developed in cooperation with materials scientists

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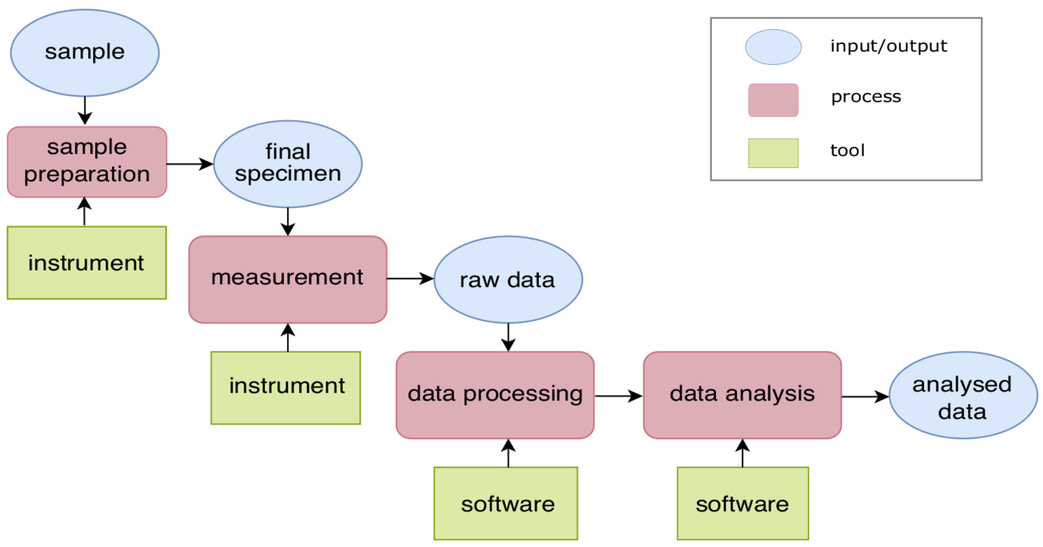
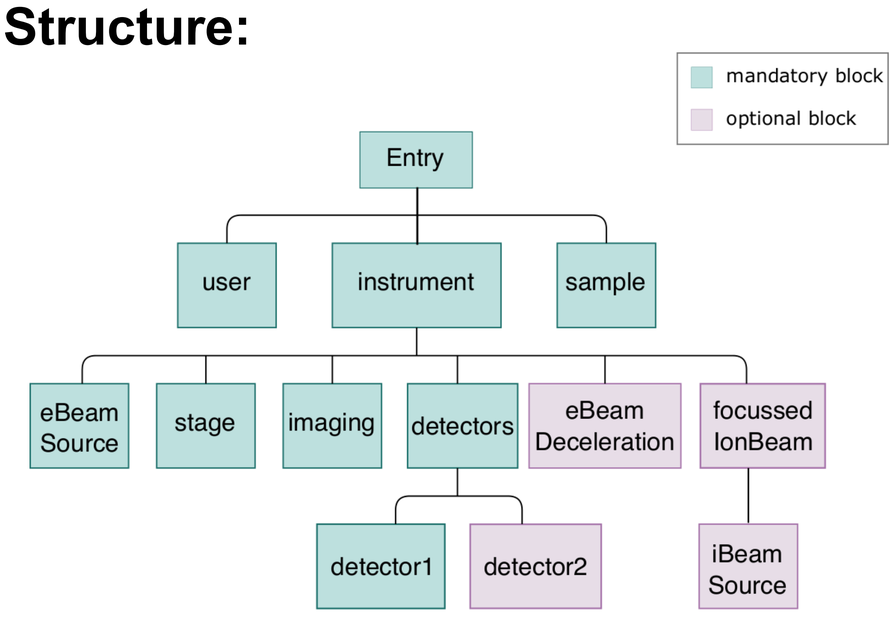
Motivation:

- referencing in space and/or time needed for correlative characterisation
- Traceability required from sample preparation to data analysis for proper results and repeatability

Workflow of obtaining data:

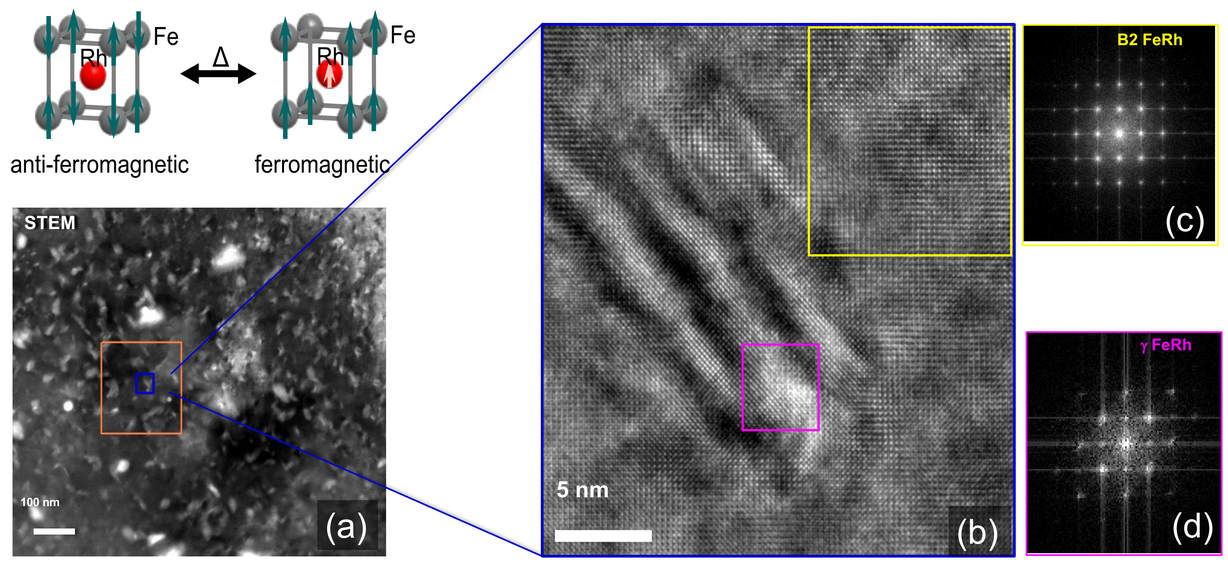


Structure:



Advantages:

- Modular and adaptable
- Easy-to-use, through controlled lists and limited number of mandatory fields
- Bridges gap between low-level schemas and high-level ontologies



Prototype of a thin-film memory device based on the influence of precipitates on the magnetic behavior of an Fe-Rh alloy. An anti-ferromagnetic region is formed at the interface of the precipitates with the rest of the alloy (in ferromagnetic B2 phase). Correlative characterisation using Scanning Transmission Electron Microscopy (STEM), High Resolution Transmission Electron Microscopy (HRTEM) and Fast Fourier Transform (FFT) processing helps to identify the zones with different magnetic behaviours. (a) STEM image of a sample of Fe-Rh alloy, (b) HRTEM image corresponding to a small portion of the STEM image, (c) FFT diffractogram showing the ferromagnetic B2 phase, and (d) FFT diffractogram showing the rhodium-rich γ phase precipitate.

The instrument settings and reference coordinates, along with the information about the sample and the parameters used for FFT processing need to be recorded accurately, for proper inference of results, necessitating the need of an extensive metadata schema.

SEM Schema Implementation (XSD)

-available on GitHub†

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  ▼<chamberPressure>
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     <unit>mbar</unit>
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  ▼<eBeamSource>
   ▼<accelerationVoltage>
      <value>5</value>
      <unit>kV</unit>
    </accelerationVoltage>
   </eBeamSource>
  ▼<stage>
   ▼<tiltAngle>
      <value>54</value>
      <unit>degree</unit>
    </tiltAngle>
   ▼<eBeamWorkingDistance>
      <value>5.1</value>
      <unit>mm</unit>
    </eBeamWorkingDistance>
  </stage>
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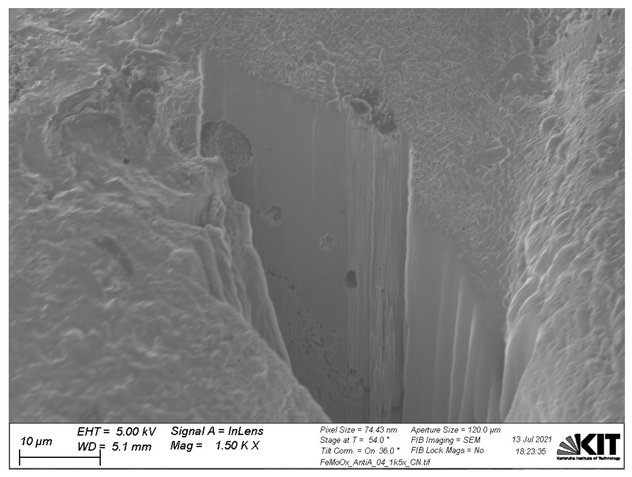

Snippet of an xml file describing the SEM image on the right obtained from an FeMoOx pellet, recorded according to the newly developed SEM schema.

Conclusions:

- The entire workflow of obtaining data from the sample to the results are documented in the schema
- Given the same specimen and tools, the results can be reproduced with the schema
- FAIR principles can be met with the help of the Schema

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* Findable Accessible Interoperable Reusable

† https://github.com/kit-data-manager/Metadata-Schemas-for-Materials-Science