

NexusLIMS: Leveraging Shared Microscopy Resources for Data Analysis with a Configurable Laboratory Information Management System



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August 6, 2020

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Any opinions expressed are my own, and not a statement on behalf of the U.S. Government.

FAIR Data Principles

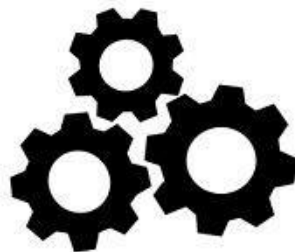
F_{indable}



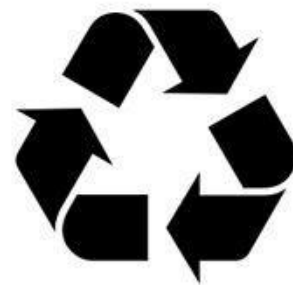
A_{ccessible}



I_{nteroperable}



R_{eusable}

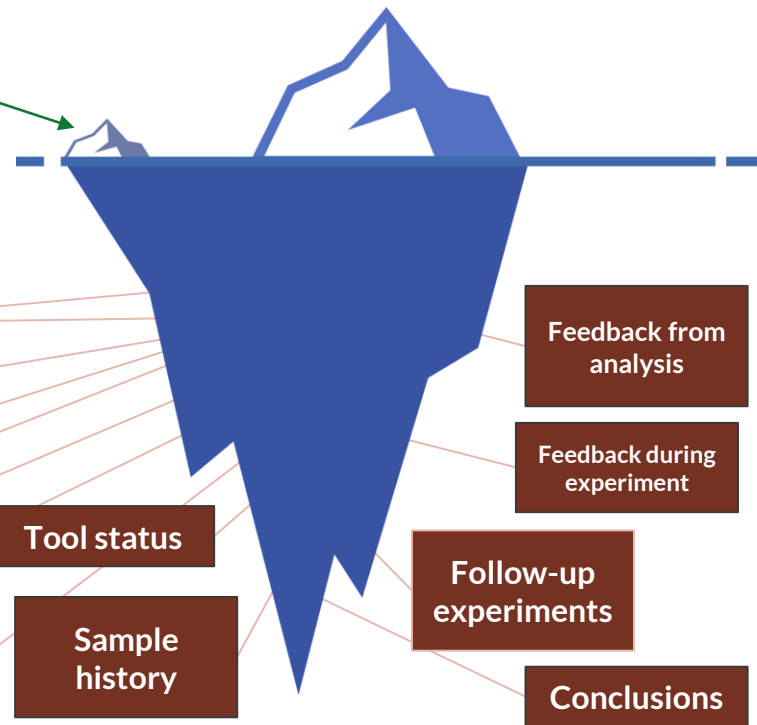


Wilkinson *et al.*, *Scientific Data*, 3, 160018, 2016 ([link](#))

Image: Sangya Pundir - [CC-BY-SA 4.0](#)

The challenge of contextual data

"Easy" metadata
(who, what, when, where)



The "Why"

Instrument setup

Purpose of experiment

Sample composition

Feedback from analysis

Reservation information

Sample prep information

Feedback during experiment

Tool status

User proposal

Background documents

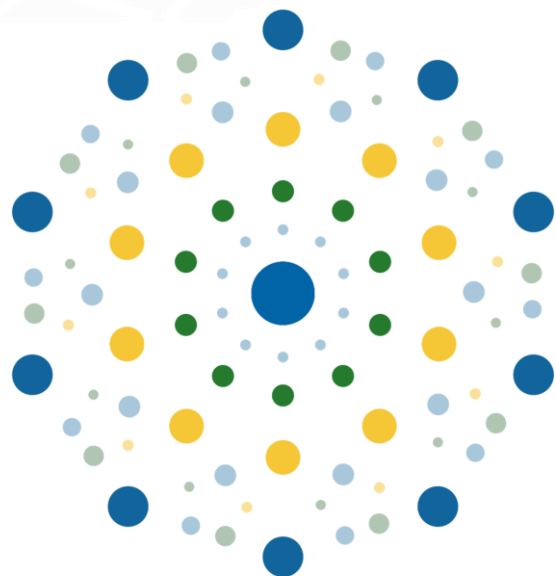
Instrument calibration

Sample history

Follow-up experiments

Conclusions

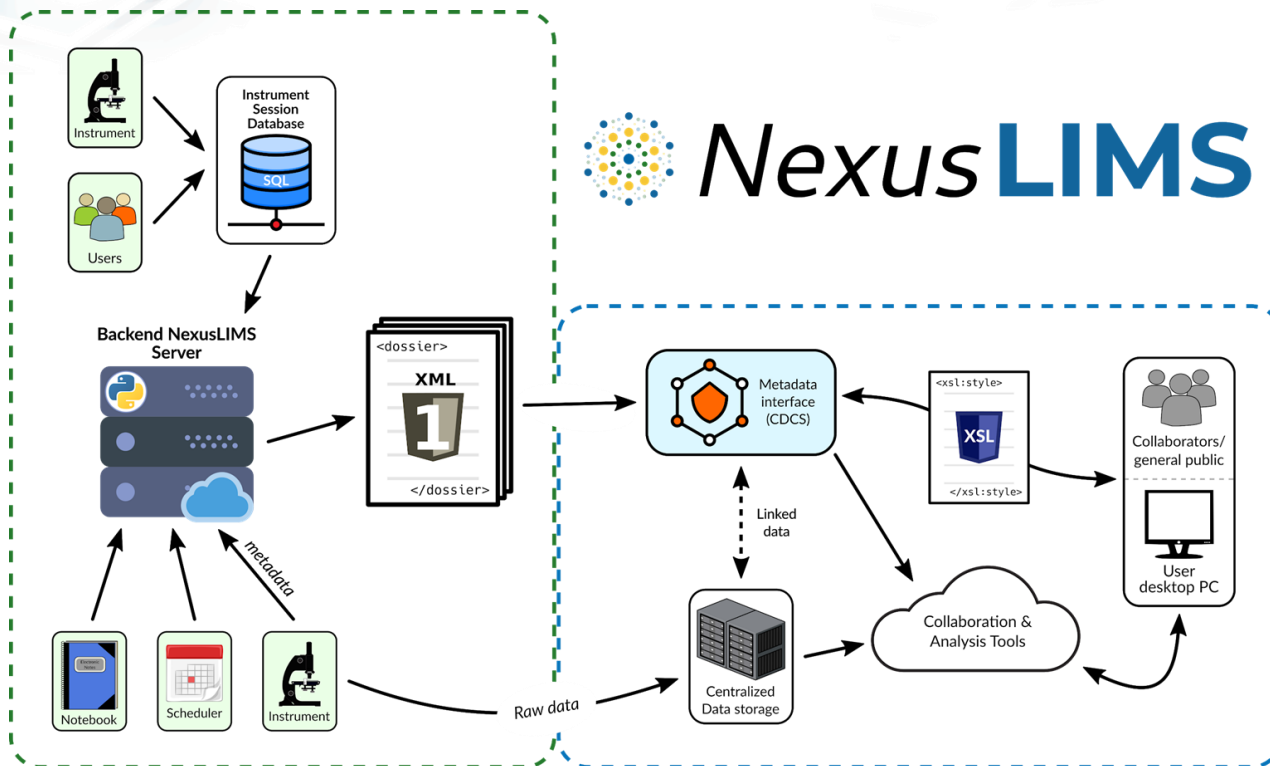
A LIMS for materials microscopy



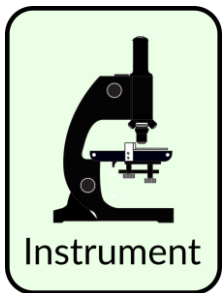
*Nexus***LIMS**

Laboratory
Information
Management
System

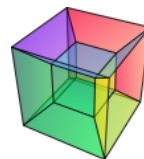
What does a LIMS for microscopy look like?



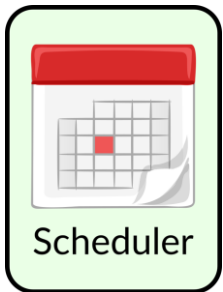
Harvesting and extracting experiment metadata



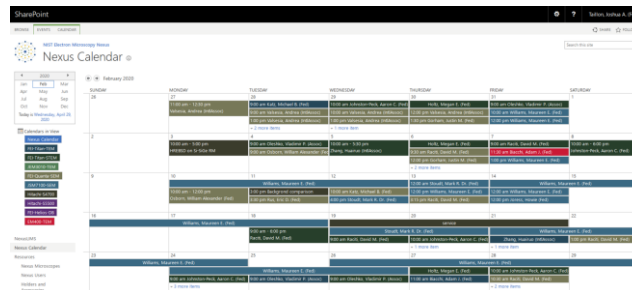
Instrument and
image/spectral
metadata from
central file
storage



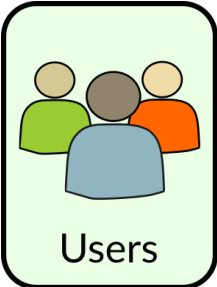
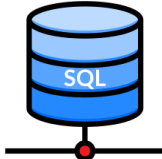
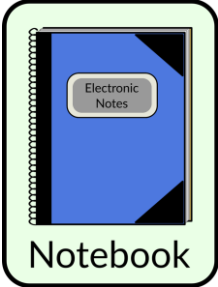
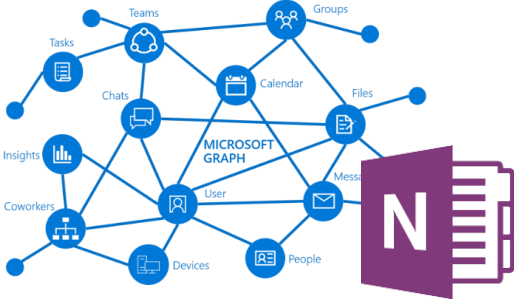
HyperSpy
multi-dimensional data analysis



User and session
information from
SharePoint
calendar



Harvesting and extracting experiment metadata

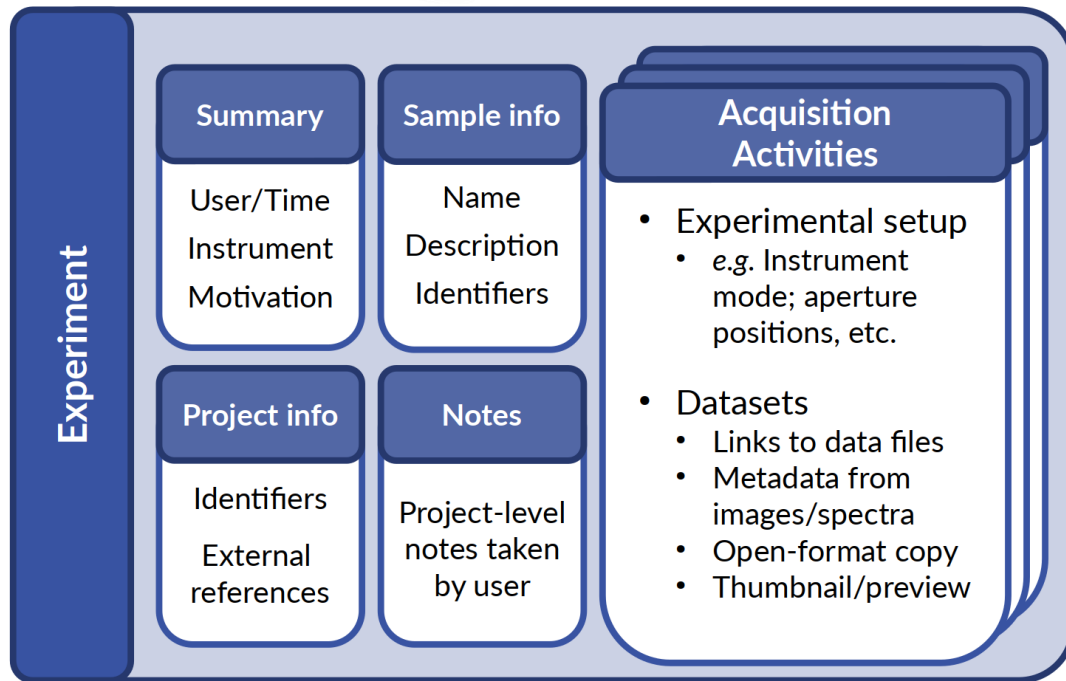
 <p>Users</p>	<p>User-triggered session information</p>	 <p>Instrument Session Database</p>
 <p>Notebook</p>	<p>Users' freeform and/or structured notes</p> <p><i>...to be implemented</i></p>	

How do we actually do it?

- nexusLIMS Python package:
 - Session logger: A portable Windows application that runs on the individual microscope PCs; logs simple information to a database about when an Experiment has occurred
 - Harvesters: Connect to external sources to collect session metadata (such as the SharePoint reservation system)
 - Extractors: Inspect data files saved on disk to pull out relevant metadata contained - also preview generation
 - Record builder: The “heart” of the NexusLIMS back-end; orchestrates creation of a new record and its insertion into the NexusLIMS CDCS instance

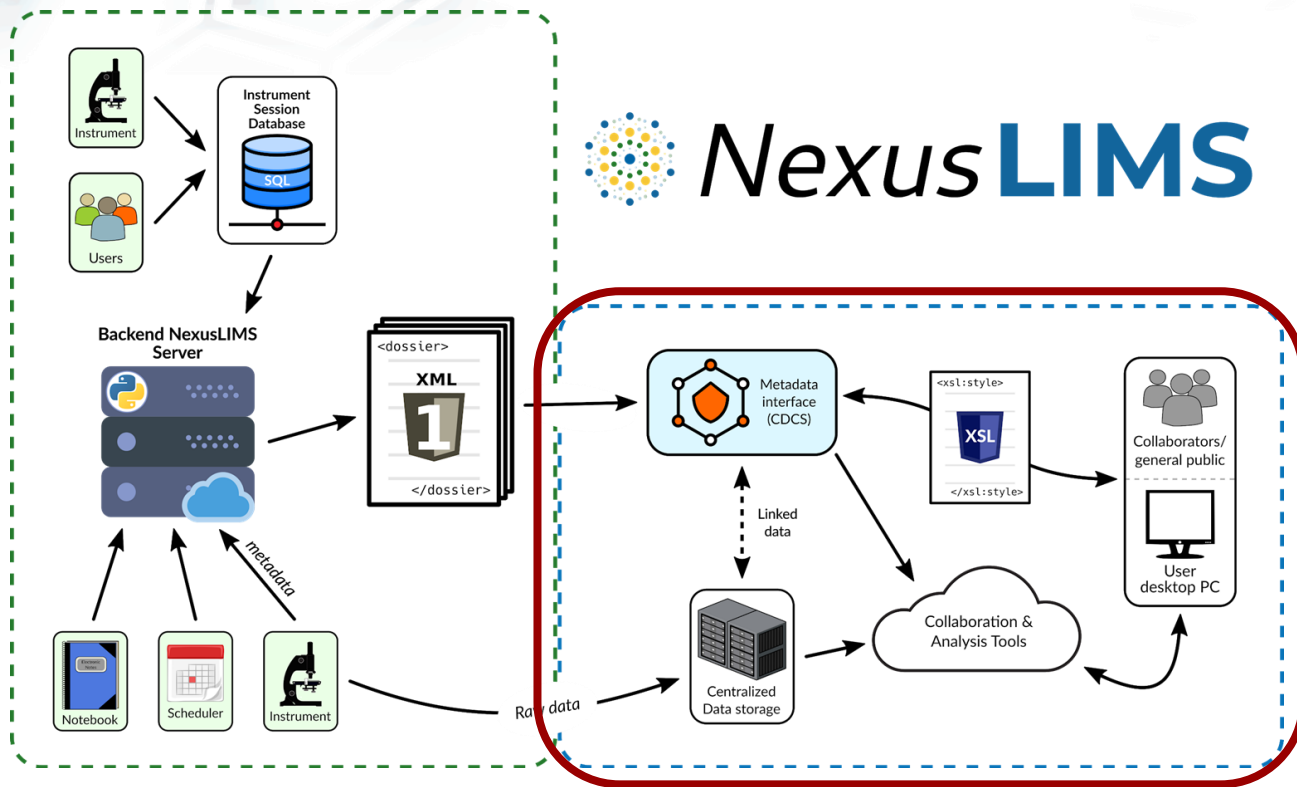
Building a schema for materials microscopy

- **Data is most useful when intelligently structured**
 - Allows browsing, querying, transforming, validating, etc.
- **Structure should be tailored to context**
 - What information could a researcher/manager/auditor want to see?
- **A “record” represents an individual experimental session on microscope**



J.. Taillon, et al., *Microscopy and Microanalysis*, vol. 25, no. S2, pp. 140–141, 2019.

What does a LIMS for microscopy look like?



For more details on CDCS,
please visit:

<https://go.usa.gov/xfKXX>



Welcome to NexusLIMS!

This laboratory information management system (LIMS) allows for the automated creation and curation of microscopy experimental records using the schema co-developed by ODI and the MML Electron Microscopy Nexus Facility. Experimental records are automatically harvested from multiple data sources to facilitate browsing and searching of data collected from the varied instruments in the Nexus Facility.

To learn more about how NexusLIMS operates and is developed, please visit the [documentation page](#), or to get started, please click the link below to start browsing experimental records:



Browse and Search Records

Click here to explore the NexusLIMS record repository





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Querying the database

STEM ✕

Search

Tools ▾

Found 11 Results:



 **4D STEM for our collaborators**  30 data files in 6 activities  30 dm3

Taillon, Joshua A. (Fed) - March 12, 2020

Motivation: to see if we can see any signs of modulation in 4d stem

 **Martensite search**  27 data files in 2 activities  27 dm3

Katz, Michael B. (Fed) - November 13, 2018

Motivation: Trying to find us some martensite!

 **STEM Condition Experiments**  52 data files in 4 activities  52 dm3

Holtz, Megan E. (Fed) - March 10, 2020


Motivation: to map atomic coordinates using 4d STEM to compare to atomic resolution STEM

 **Looking for Twins in Additive Manufacturing Sample**  22 data files in 3 activities  35 dm3

Taillon, Joshua A. (Fed) - March 10, 2020

Motivation: Checking AM samples to see if twinning is still occurring

Querying the database

 🔍 Browse and Search Records 📅 Sharepoint Calendar 🔗 Tutorial Help ▾ admin ▾

Search

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 **Martensite search** FEI Titan TEM 27 data files in 2 activities 🔗 27 dm3

Katz, Michael B. (Fed) - November 13, 2018

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 **STEM Condition Experiments** FEI Titan STEM 52 data files in 4 activities 🔗 52 dm3

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 **Looking for Twins in Additive Manufacturing Sample** FEI Titan TEM 22 data files in 3 activities 🔗 35 dm3

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Browsing and previewing (meta)data

 **NexusLIMS**

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[Sharepoint Calendar](#)

[Tutorial](#)

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Explore record:

Activity 1

STEM Imaging

Activity 2

STEM Imaging

Activity 3

STEM Imaging

Activity 4

STEM Imaging

Activity 5

STEM Imaging

 **4D STEM for our collaborators**

FEI Titan STEM

30 data files in 6 activities

 30

dm3

Taillon, Joshua A. (Fed) - March 12, 2020

Motivation: to see if we can see any signs of modulation in 4d stem

Session Summary

Date:

2020-03-12

Start Time:

00:00:00

End Time:

23:59:00

Session ID:

191

Sample name:

KBTFNF

Sample ID:

3fcd58eb-9320-4007-8dcc-3ae61c695b37

Project Information

Name:

4D Fast Camera Research

ID:

642.02.0837

Division:

641

Group:

02








08_rot00_HAADF_2,55Mx_2048px_8us



Dataset 27 of 30

Activity 6 of 6


Browsing and previewing (meta)data



 **NexusLIMS**  Browse and Search Records  Sharepoint Calendar  Tutorial  Help  admin 

« Page 1 of 2 »

Explore record:


- Activity 1
STEM Imaging
- Activity 2
STEM Imaging
- Activity 3
STEM Imaging
- Activity 4
STEM Imaging
- Activity 5
STEM Imaging

 **4D STEM for our collaborators**


FEI Titan STEM 30 data files in 6 activities  30  dm3

Taillon, Joshua A. (Fed) - March 12, 2020




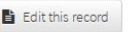
Motivation: to see if we can see any signs of modulation in 4d stem

Session Summary 

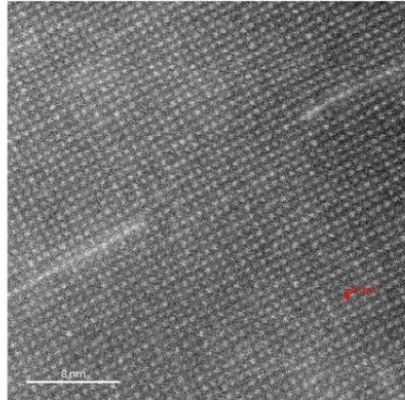
Date: 2020-03-12
Start Time: 00:00:00
End Time: 23:59:00
Session ID: 191
Sample name: KBTBNF
Sample ID: 3fcd58eb-9320-4007-8dcc-3ae61c695b37

Project Information 


Name: 4D Fast Camera Research
ID: 642.02.0837
Division: 641
Group: 02


08_rot00_HAADF_2,55Mx_2048px_8us





8 nm


Dataset 27 of 30
Activity 6 of 6 

Browsing and previewing (meta)data


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 Browse and Search Records

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Explore record:


Activity 1
STEM Imaging


Activity 2
STEM Imaging

Activity 3
STEM Imaging

Activity 4
STEM Imaging

Activity 5
STEM Imaging

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Sample name: KBTBNF

Sample ID: ⓘ 3fcd58eb-9320-4007-8dcc-3ae61c695b37

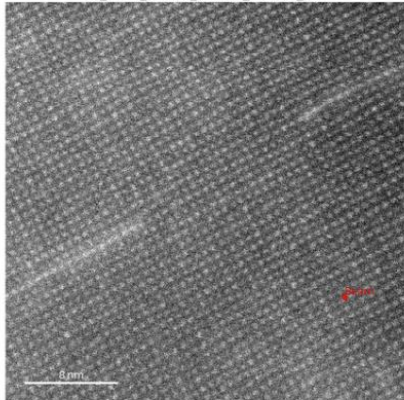
Project Information ⓘ

Name: 4D Fast Camera Research

ID: 642.02.0837

Division: 641

Group: 02




08_rot00_HAADF_2,55Mx_2048px_8us

Dataset 27 of 30

Activity 6 of 6 ⓘ

Browsing and previewing (meta)data

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Page 1 of 2

Explore record:


[Activity 1](#)
STEM Imaging



[Activity 2](#)
STEM Imaging

[Activity 3](#)
STEM Imaging

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STEM Imaging

[Activity 5](#)
STEM Imaging

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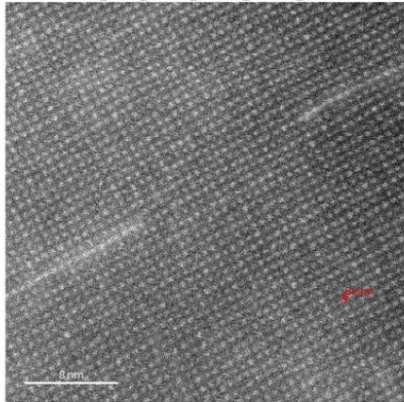
Date: 2020-03-12
Start Time: 00:00:00
End Time: 23:59:00
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Project Information

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ID: 642.02.0837
Division: 641
Group: 02


[Back to previous](#) [Download files](#) [Download XML](#) [Edit this record](#)

08_rot00_HAADF_2,55Mx_2048px_8us



Dataset 27 of 30
Activity 6 of 6

Browsing and previewing (meta)data

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« Page 1 of 2 »

Explore record:

Activity 1

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STEM Imaging

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FEI Titan STEM

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dm3

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641

Group:

02

08_rot00_HAADF_2,55Mx_2048px_8us



Dataset 27 of 30

Activity 6 of 6

Browsing and previewing (meta)data

Sharepoint Calendar Tutorial Help admin

Back to previous Download files Download XML Edit this record

Complete filelisting for:
4D STEM for our collaborators - March 12, 2020
Root path: /643Titan/meh11/20200312_KBT_BNF_Merlin/
Search: []
Select all Select none Download all as .zip Download selected as .zip
Copy CSV Excel Print
Total size of all datasets: 794.1 MiB.

Dataset Name	Path	Size	Type	Meta	D/L
<input type="checkbox"/> 01_HAADF_210kX_0,4mrad_100mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 02_HAADF_210kX_0,4mrad_100mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 03_HAADF_300kX_0,4mrad_100mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 04_HAADF_300kX_0,4mrad_100mm.dm3	/	182.5 KiB	Image		
<input type="checkbox"/> 05_HAADF_420kX_0,4mrad_100mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 06_HAADF_300kX_0,4mrad_100mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 07_HAADF_600kX_0,4mrad_100mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 08_HAADF_300kX_0,4mrad_77mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 09_HAADF_1,7MX_0,4mrad_77mm.dm3	/	183.2 KiB	Image		
<input type="checkbox"/> 10_HAADF_850kX_0,4mrad_77mm.dm3	/	183.2 KiB	Image		

Showing 1 to 10 of 30 datasets

08_rot00_HAADF_2,55Mx_2048px_8us

Dataset 27 of 30
Activity 6 of 6

Browsing and previewing (meta)data

Experiment activity 1



Activity contents: *STEM Imaging*

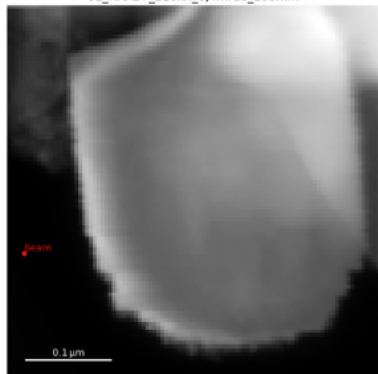
3 data files



3

dm3

01_HAADF_210kX_0,4mrad_100mm



Dataset Name [?]	Creation Time	Type [?]	Role [?]	Meta	D/L
01_HAADF_210kX_0,4mrad_100mm.dm3	2020-03-12T10:55:44.137411	Image	Experimental		
02_HAADF_210kX_0,4mrad_100mm.dm3	2020-03-12T10:58:31.069478	Image	Experimental		
03_HAADF_300kX_0,4mrad_100mm.dm3	2020-03-12T11:01:19.258538	Image	Experimental		

Browsing and previewing (meta)data

Experiment activity 1

Activity contents: *STEM Imaging*

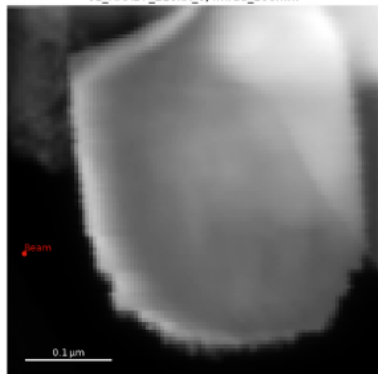
3 data files



3

dm3

01_HAADF_210kX_0,4mrad_100mm



Experiment activity 1

Activity contents: *STEM Imaging*










Search:

« 1 2 »

Setup Parameter	Value
Start time	10:55:44.137411
Acquisition Device	DigiScan
Cs(mm)	1.0
Data Dimensions	(100, 100)
Data Type	STEM Imaging
Detector	GIF CCD
GMS Version	2.32.888.0
Illumination Mode	STEM MICROPROBE
Imaging Mode	DIFFRACTION
Instrument ID	FEI-Titan-STEM-630901

Browsing and previewing (meta)data

```
- nx_meta: {  
  Acquisition Device: "DigiScan",  
  Creation Time: "2020-03-12T10:55:44.137411",  
  Cs(mm): 1,  
  Data Dimensions: "(100, 100)",  
  Data Type: "STEM_Imaging",  
  DatasetType: "Image",  
  Detector: "GIF CCD",  
  Field of View (μm): 0.6287767790097984,  
  GMS Version: "2.32.888.0",  
  Illumination Mode: "STEM MICROPROBE",  
  Imaging Mode: "DIFFRACTION",  
  Indicated Magnification: 210000,  
  Instrument ID: "FEI-Titan-STEM-630901",  
  Microscope: "Titan80-300_D3094",  
  Name: "FEI Tecnai Remote",  
  Operation Mode: "SCANNING",  
  Operator: "JoshuaTaillon",  
  STEM Camera Length: 100,  
  Specimen: "STEM",  
- Stage Position: {  
  X: 38.2395,  
  Y: -13.3358,  
  Z: -23.6052,  
  α: -1.7284933467727162,  
  β: 3.574998810608528  
},  
  Voltage: 300000,
```

Dataset Name ?	Creation Time	Type ?	Role ?	Meta	D/L
01_HAADF_210kX_0.4mrad_100mm.dm3	2020-03-12T10:55:44.137411	Image	Experimental	 	
02_HAADF_210kX_0.4mrad_100mm.dm3	2020-03-12T10:58:31.069478	Image	Experimental	 	
03_HAADF_300kX_0.4mrad_100mm.dm3	2020-03-12T11:01:19.258538	Image	Experimental	 	

Data management without the effort

- NexusLIMS implementation in current use by over 50 research staff
- Key pieces:
 - Networked instruments
 - Centralized storage
 - Metadata schema
 - Leveraging existing tools (CDCS)
- Final step: Data publication
 - <https://data.nist.gov>



What's next? / When can I use it?

- **Integration/federation with other repositories**
 - Sample, instrumentation, etc.
- **Bindings for “cloud” processing**
 - Import data directly from (for example) Jupyter notebooks
- **Still in internal use/testing**
 - Will soon be released at <https://github.com/usnistgov>
 - Full publication in coming months

Acknowledgements

HyperSpy development team:

Francisco de la Peña
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Tomas Ostasevicius
Mike Sarahan
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Vadim Migunov
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Stefano Mazzucco
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Eric R. Hoglund
Daniel Lundeby
Luiz Fernando Zagonel

Eric Prestat
Pierre Burdet
Magnus Nord
Katherine E. MacArthur
Duncan N. Johnstone
Jonas Lähnemann
Alberto Eljarrat
Thomas Aarholt
Michael Walls
Florian Winkler
Ben Martineau
Robert McLeod
Ivo Alxneit
Trond Henninen
Andreas Garmannslund

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June Lau - NIST MSE Division
Gretchen Greene - NIST ODI
Ray Plante - NIST ODI
Marcus Newrock - NIST ODI
Thomas Bina (Penn. State University)
Rachel Devers (University of Maryland)
Sarita Upreti (Montgomery College)

Data guinea pigs/ trial users:

Mike Katz
Vladimir Oleshko
Andy Herzing/Megan Holtz

CDCS team:

Ben Long
Guillaume Amaral
Adrien Catel
Philippe Dessauw
Xavier Schmitt

Thank you!

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