

#### 4CeeD Lecture Series Use of 4CeeD Services for Material Scientists

Lecture #2: 4CeeD for Collaboration and Data Processing March 23<sup>rd</sup>, 2023 **Robert Kaufman (rbkaufm2@Illinois.edu)**, Leah Espenhahn (leahe2@illinois.edu) Beitong Tian, and Prof. Klara Nahrstedt (Klara@Illinois.edu)



#### A timely and trusted curator and coordinator of scientific data







# **Lecture Series Learning Objectives**

- Lecture 1 (3/21): Overview of 4CeeD
- Lecture 2 (3/23): Workshop (Cont.) & Advanced Features
  - Reviewing 4CeeD Structure
  - Introducing Data Sharing and Extractors
  - Visualizing Trends with Jupyter
  - **Breakout**: Analyzing an Experiment with 4CeeD and Jupyter
- Lecture 3 (3/28): 4CeeD Backend Services
- Lecture 4 (3/30): SENSELET: Sensory Network Infrastructure for Scientific Lab Environments

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## **Lecture Series Learning Objectives**

- Lecture 2: Demonstration of 4CeeD
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  - **Breakout**: Analyzing an Experiment with 4CeeD and Jupyter





#### **4CeeD Review**



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# 4CeeD Review GUI Dashboard

Dashboard View of 4CeeD





# 4CeeD Review Dataset Page





# 4CeeD Review **Dataset Page**

TI-QCL (RBK) / 🗐 10. Base Zn Dif	=000-			Space containing the Dataset	an
🗐 10. Base Zn Diffusi	Dataset Metao	data			×
Created by Robert Kaufman Created on Aug 21, 2019 Access:  Space Default (Private)  Private	Select a template	:			
Public Process of diffusing Zn into the base region of	Select One			Ŧ	
Process (See detailed process on sheet in 211 1. Prepare tubes	Key:	Value	Units:		
<ol> <li>Flame off and dimple</li> <li>Load diffusant (Zn3As2); load sample</li> </ol>	Time	13	min	REMOVE	
<ol> <li>Seal off</li> <li>Heat in furnace</li> </ol>	Key:	Value	Units:		
-560C for 10-20 min	Tempearture	425	С	REMOVE	
-Test with GaAs dummy samples first (try ap	Key:	Value	Units:		
-steps 7-11 are not necessary it skipping zit di	Oxide Depth	12	um	REMOVE	
🕂 Add Files 🛃 Download All Files 🧃	Key:	Value	Units:		
	Oxide Layer	99	%	REMOVE	
Files Metadata Comments (0)	Key:	Value	Units:		
	Oxide Thick.	30	nm	REMOVE	
			)		
02-13-2020_TIC	ADD NEW			SUBMIT CLOSE	
image/png Feb 13, 2020					
1.8 MB			W		

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E Fabrication Development Dallesasse

Fabrication Development Space for Professor John Dallesasse Group: Creator: Patrick Su Viewers: Rob Kaufman, Kevin Pikul, John Carlson

n Delete Create Dataset Create Collections



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E Fabrication Rec... / L Manage Users

#### Manage Users of Space Fabrication Recipe Bank

Users Invites Requests (0)	
Owner: Patrick Su	Admin Admin Role
Admin Admin Role	Patrick Su (psu8@illinois.edu) [Local Account]      Select Users for this Level
Select Users for this Level	Collaborator
Admin Admin Role • Patrick Su (psu8@illinois.edu) [Local Account] ★ Select Users for this Level	A collaborator can add datasets and files to a space. They cannot delete anything except their own <ul> <li>Robert Kaufman (rbkaufm2@illinois.edu) [Local Account] ×</li> <li>Thomas O'Brien (tobrien3@illinois.edu) [Local Account] ×</li> <li>John Carlson (jcarls21@illinois.edu) [Local Account] ×</li> </ul>
Collaborator A collaborator can add datasets and files to a space. They cannot del	<ul> <li>Maanav Ganjoo (ganjoo2@illinois.edu) [Local Account] X</li> <li>Kevin Pikul (kpikul2@illinois.edu) [Local Account] X</li> </ul>
<ul> <li>Robert Kaufman (rbkaufm2@illinois.edu) [Local Account]</li> <li>Thomas O'Brien (tobrien3@illinois.edu) [Local Account]</li> <li>John Carlson (jcarls21@illinois.edu) [Local Account] X</li> <li>Maanav Ganjoo (ganjoo2@illinois.edu) [Local Account]</li> </ul>	Select Users for this Level
<ul> <li>Kevin Pikul (kpikul2@illinois.edu) [Local Account] X</li> <li>Select Users for this Level</li> </ul>	Collaborators

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#### **Effective Collaboration: Communication**



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- Extractors automatically log pertinent information of uploaded data
- **Basic Example:** Image Thumbnails

#### Extractions

List extraction events

Submit file for extraction

Extractor	Start	End	Status
ncsa.image.preview	Thu Mar 18 00:54:10 GMT 2021	N/A	StatusMessage.start: Started processing
ncsa.image.preview	Thu Mar 18 00:54:10 GMT 2021	N/A	StatusMessage.processing: Downloading file.
ncsa.image.preview	Thu Mar 18 00:54:10 GMT 2021	N/A	StatusMessage.processing: Uploaded thumbnail of type png
ncsa.image.preview	Thu Mar 18 00:54:10 GMT 2021	N/A	StatusMessage.processing: Uploading file preview.
ncsa.image.preview	Thu Mar 18 00:54:10 GMT 2021	N/A	StatusMessage.processing: Uploaded preview of type png
ncsa.image.preview	Thu Mar 18 00:54:10 GMT 2021	N/A	DONE



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• A more useful example is with SEM metadata



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	ZNSEL003 / ZNSEL Extractor		Space containing the Dataset
	Created by Patrick Su All Right Created on Apr 01, 2020 Access:   Space Default (Private)  Private Public Add a description	hts Reserved Patrick Su	ZNSEL003         4 datasets   ★ Remove         Select a Space         Collections containing the Dataset
	🕇 Add Files 🛃 Download All Files ា Delete 👤 Collabo	prators	Select a collection    ADD  Tags
	Files Metadata Comments (0)		TAG
SEM Image Captures	07-17-2019_BCl3=7-5_Cl2=2-5         5_RIE=185W_ICP=375W_P7to         VIEpi_Sidewall_q05.tif         image/tiff         Apr 01, 2020         1.2 MB         𝔅 0 ≡ 0 🖛 0 mm	i_Ar=3- 2mT_10C_II- ★ Download ★Follow	
	O2-12-2020_GaAsBulk650um_2           7p5Cl2-2p5Ar-10mT-10C_q01.t           text/plain           Apr 01, 2020           949 B           №0 :≣ 0 ♥ 0 前	2mins-400ICP-185RIE-15BCI3- xt	Corresponding .txt of SEM capture conditions

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	Extracted Text File	Corresponding 4CeeD Metadata
[SemImageFile] InstructName=S-4800 SerialNumber=HI-9126-000 DataNumber=	6	Metadata     Extracted by http://clowder:9000/extractors/sem.extractor/2.0.0 on Mar 18, 2021
SampleName= Format=tif ImageName=02-12-2020_C Directory=D:\Image\Psu8 (F Date=02/12/2020 Time=11:31:14 Media=HD[DATA]	GaAsBulk650um_2mins-400ICP-185RIE-15BCl3-7p5Cl2-2p5 Patrick Su)\ZNSEL003\GaAs_Etch_Dev\	DSAr-10mT-10C_q01.tif Media: HD[DATA] SerialNumber: HI-9126-0006 Disceterus Dillmage/Deuß (Detrick Sul) ZNSEL 002) Origination, Calib)
DataSize=1280x960 PixelSize=22.04861		Magnification: 13000
SignalName=SE(M) AcceleratingVoltage=5000 V	Volt	DataDisplayCombine: 1
DecelerationVoltage=0 Volt		KeyWord2:
WorkingDistance=8000 um		KeyWord1:
EmissionCurrent=7400 nA LensMode=High		CalibrationScanSpeed: 25
PhotoSize=1000		SubMagnification: 0
		Format: tif
		Vacuum:
		Date: 02/24/2020
		DataSize: 2560x1920
		WorkingDistance: 6800 um
		Condencer1: 5000
		LensMode: High
		SubSignalName:
		EmissionCurrent: 7800 nA



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# 4CeeD Integrated Jupyter Notebook

- Access metadata from datasets
- Uses pandas DataFrames to store info
  - Quick table views
  - Create custom columns
  - Easy data retrieval and sorting
- Quick plotting and visualization through matplotlib

o tear p	
R	vieving datasets
	Fabrication Development Dallasius Group (Space)
	Classroom Demos (Space)
	4CeeD Demo: GaN Etch Recipe Optimization Figure 2 (Space)
	▼ datasets
	✓ GaN Etch Pressure 9 mTorr
	GaN Etch Pressure 7 mTorr
	GaN Etch Pressure 5 mTorr
	4CeeD Demo: GaN Etch Recipe Optimization Figure 1 (Space)
	TI-QCL 006B (Collection)
	TI-QCL 005-006 (Collection)
	Submit

GaN Etch Pressure 7 mTorr	280.0	49.0	21.0	1000.0	150.0	7.0	25.0
GaN Etch Pressure 5 mTorr	300.0	49.0	21.0	1000.0	150.0	5.0	25.0
GaN Etch Pressure 3.5 mTorr	280.0	49.0	21.0	1000.0	150.0	3.5	25.0

Select Metadata to Read from 4Ceed

To [F], pydroad poad datacats matadata()

#### Plot Metadata



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## 4CeeD Integrated Jupyter Notebook

- Jupyter environment is hosted on 4CeeD servers
- Allows for remote access and processing of custom scripts





```
In [7]: resistances = [[] for x in range(trials)]
r_pads = []
avg_res = [0 for d in range(len(dist))]
for t in range(trials):
    for d in range(len(dist)):
        resistances[t] += [1/(stats.linregress(voltages[t][d], currents[t][d])[0
        avg_res[d] += resistances[t][d]/trials
        r_pads += [fitPlotSaveResistances(resistances[t],t+1)]
r_pads += [fitPlotSaveResistances(avg_res,0)]
```

print("Pad Resistance: "+str(r\_pads))

0.993471835645128 0.9876314375071126 0.9940794194313601 Pad Resistance: [1.0767903731516643e-05, 1.0060551297977721e-05, 1.041422751474 7174e-05]

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- py4ceed.enter\_key()
  - Prompts entry of API Key to access 4CeeD account
- py4ceed.read\_datasets\_metadata()
  - Opens GUI to select metadata info
- py4ceed.get\_metadata()
  - Returns selected metadata as a pandas DataFrame





#### • enter\_key()

	Create <del>-</del> Trash <del>-</del> Help-	-	Search	Q	Jupyter Hub	🕞 Logout	2,-
	Robert Kaufma	n				View Profile	
	rbkaufm2@illinois.edu		Link to	o hosted			
	User API Keys		Jup	byter			
	Create your personal API keys by	y providing a name for	the key and clicking the A	dd button. Key na	mes have to be un	ique per user.	
	Name	Кеу					
	m rbkaufm2_key	donistoite destata	er alla data barat				
Followed by 0 people Edit Profile	+ Add		Enter 4C	eed K	ey		1
		In [2]:	py4ceed.enter_	key()			
			User Key:				
			Submit				

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#### read\_datasets\_metadata()

Select Metadata to Read from 4Ceed

In [3]:	<pre>py4ceed.read_datasets_metadata()</pre>	▼4CeeD Demo: GaN Etch Recipe Optimization Figure 2 (Space)		
	Retrieving datasets			
	▶ Test Space (Space)	✓ datasets		
	▶ 4CeeD Demos (Space)	<ul> <li>GaN Etch Pressure 9 mTorr</li> <li>GaN Etch Pressure 7 mTorr</li> </ul>		
	▶ TIQCL007 (Space)	GaN Etch Pressure 5 mTorr		
	▶ SENSELET Data (Space)	GaN Etch Pressure 3.5 mTorr		
	▶ Growth Experiments (Space)	▶ 4CeeD Demo: GaN Etch Recipe Optimization Figure 1 (Space)		
	▶ collaborator role test space (Space)	<ul> <li>▶ rbs (Collection)</li> <li>▶ dm3 (Collection)</li> </ul>		
	▶ TI-QCL (RBK) (Space)			
		Submit		



#### get\_metadata()

#### Plot Metadata



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#### **Filter Metadata**





#### get\_metadata()



#### pandas.DataFrame

class pandas.DataFrame(data=None, index=None, columns=None, dtype=None, copy=False)

[source]

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Two-dimensional, size-mutable, potentially heterogeneous tabular data.

Data structure also contains labeled axes (rows and columns). Arithmetic operations align on both row and column labels. Can be thought of as a dict-like container for Series objects. The primary pandas data structure.



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# **Breakout: 4CeeD Jupyter Integration**

#### **Activity Objectives**

- Access the 4CeeD Jupyter server
- Extract stored 4CeeD metadata
- Quickly process that data in useful ways
- Save a snapshot of the notebook with the data

₩ 4CeeD 💭 Jupyter	Logout Control Panel	ln [11]:
Files         Running         Clusters           Select items to perform actions on them.	Upload New - 2	<pre>metadata_300ICP_3mT.plot(x='SF6_Flow', y='Etch_Rate') plt.show()</pre>
0 v hrivate	Name 🕹 Last Modified File size	
۵	seconds ago	0.8
	2 years ago	
MSE598JupyterDemo.ipynb	2 minutes ago 7.44 kB	
Deplot_metadata_tutorial.ipynb	9 months ago 60.4 kB	0.6
		0.5 -
		0.4 -
		0.3 -
		0.2 - Etch Rate
		0 10 20 30 40 50
		SF6_Flow





# **Questions?**







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