

Automatic translation of measurement data on materials data platform: M-DaC (Materials Data Conversion Tools)

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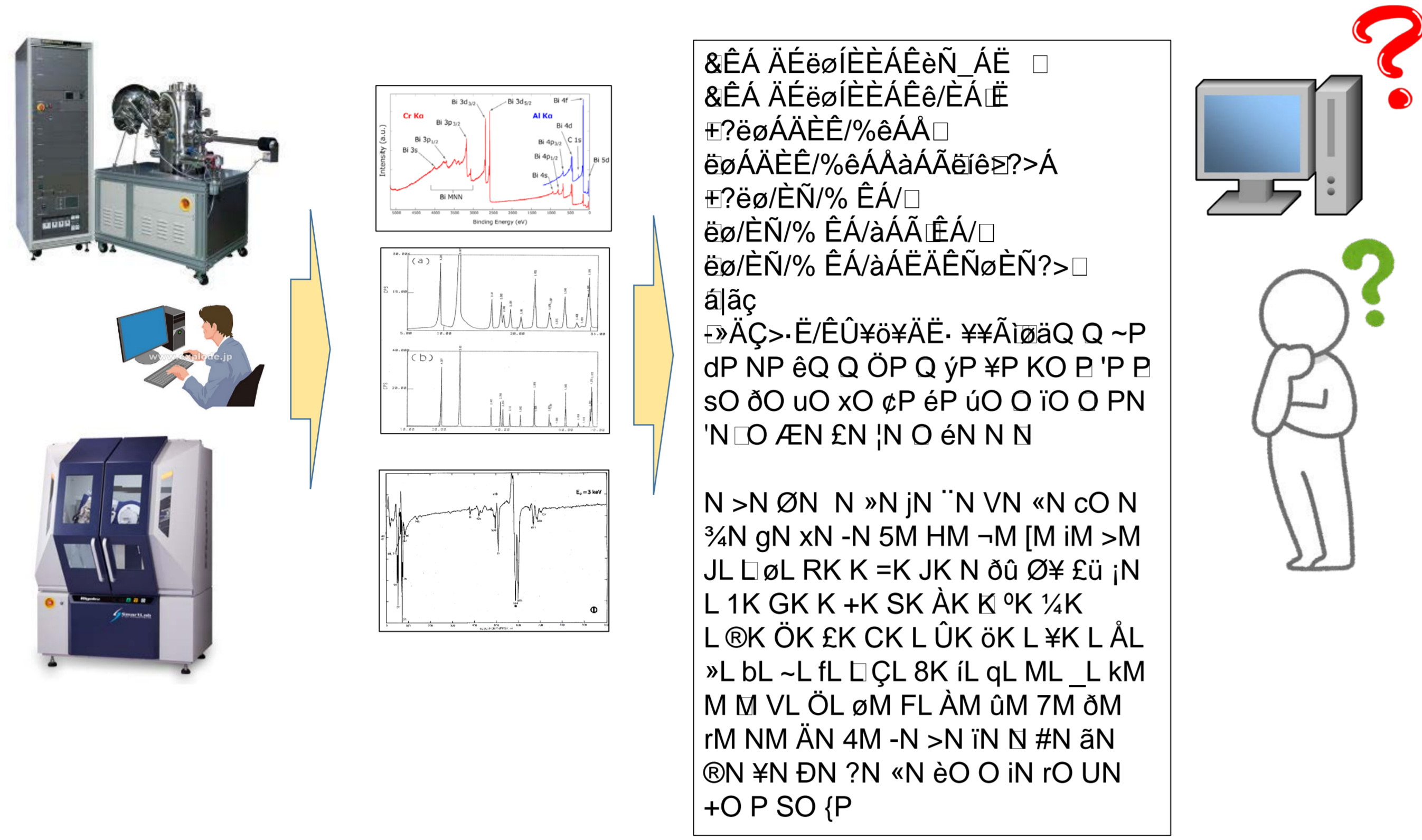
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Please visit <https://www.nims.go.jp/MaDIS/about/M-DaC.html>

Introduction

The conversion of measurement data from raw data to machine-readable data package is one of the key preparation techniques prior to informatics analysis.



Binary raw data read by using text editor

Examples of metadata and formatted numerical data (FND)

XPS metadata

ITEM (Eng)	ITEM (Jpn)	Units	Example value
Measurement Technique	測定手法	--	XPS
Measurement Instrument	測定装置	--	PHI Quanterta SXM
Experiment ID	測定内容識別ID	--	20170606
File Property	測定ファイル_属性	--	SPECTRUM
Xray Source	X線源	--	Al 1486.6 mono
Xray Power	X線パワー	W	103.08
Xray Beam Diameter	X線ビーム径	mm	100
Analysis source strength	入射プローブの強度	--	103.08W_HP
Analyzer Mode	分析器分光動作モード	--	FAT
Analyzer Work Function	分析器仕事関数	eV	4.25
Xray Analyzer Angle	照射X線_分析器間角度	deg	45
Analyzer Solid Angle	分析器取込立体角度	sr	0.38
Pass Energy	パスエネルギー値	eV	280

powder-XRD metadata

ITEM (Eng)	ITEM (Jpn)	Units	Example value
Operator identifier	測定者	--	English
Detector Pixel Size	検出器ピクセルサイズ	mm	0.075
Selected Detector Name	使用検出器名称	--	DteX250(H)
X-ray Target Material	X線ターゲットの材質	--	Cu
K_alpha1 Wavelength	K_alpha1の波長	Angstrom	1.540593
K_alpha2 Wavelength	K_alpha2の波長	Angstrom	1.544414
K_beta Wavelength	K_betaの波長	Angstrom	1.392246
Optics Attribute	光学系属性	--	DB
X-ray Tube Current	X線管電流	mA	30
X-ray Tube Voltage	X線管電圧	kV	40
Wavelength Type	波長タイプ	--	K_alpha
Data Point Number	データ点数	--	3501
Scan Axis	スキャン軸	--	Theta/2-Theta
Scan Starting DateTime	スキャン開始時刻	--	11/21/2017 08:32:31

XPS FND

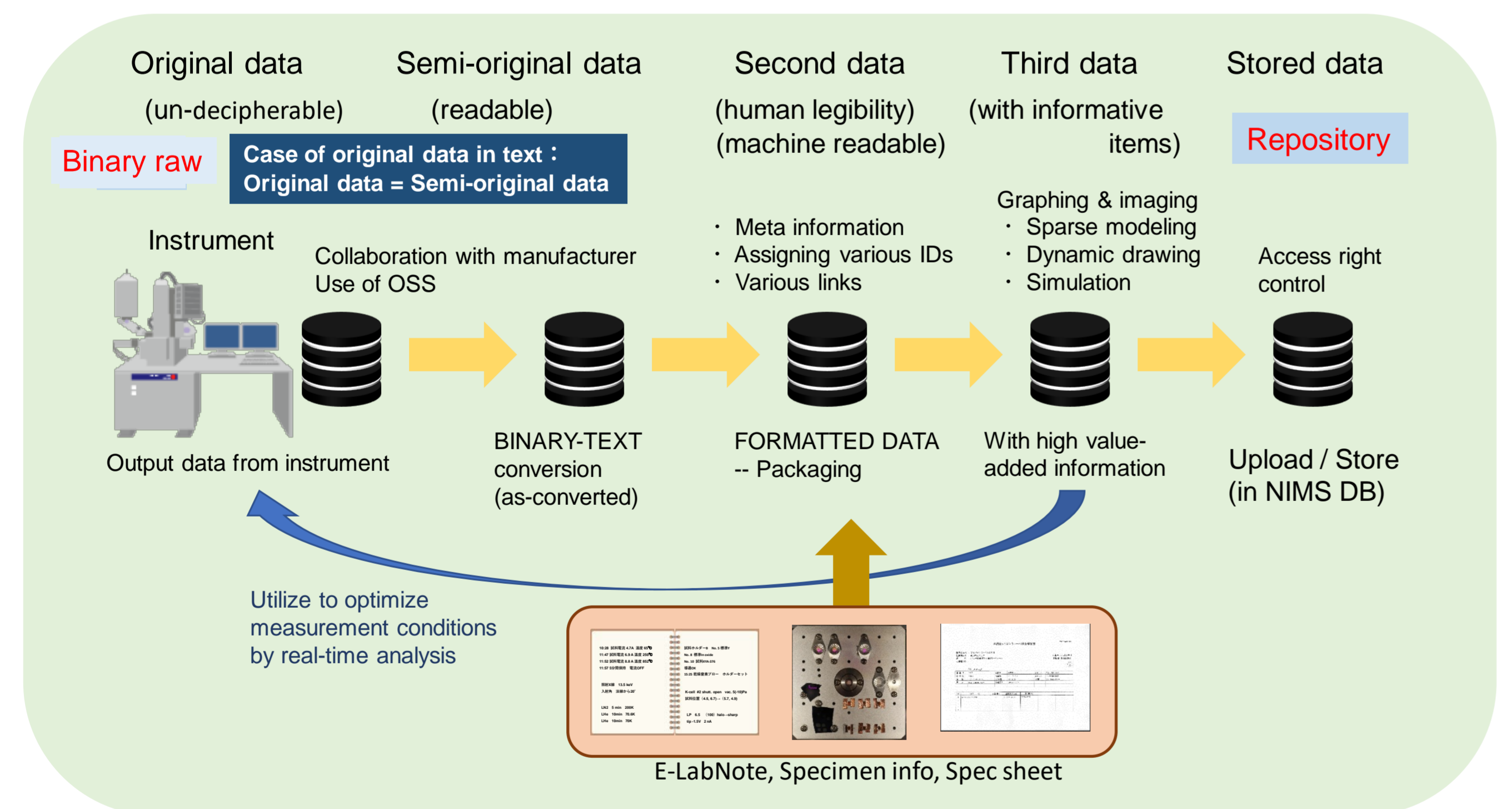
#title	#3 Cu foil	#x	Binding Energy	eV	reverse
#dimension	x	y			
#y	Intensity	cps			
#legend	Survey				
#acq_date	20170606				
#comment	SPECTRUM				
1380	333762.75				
1379.5	331214				
1379	324780.5				
.....				

powder-XRD FND

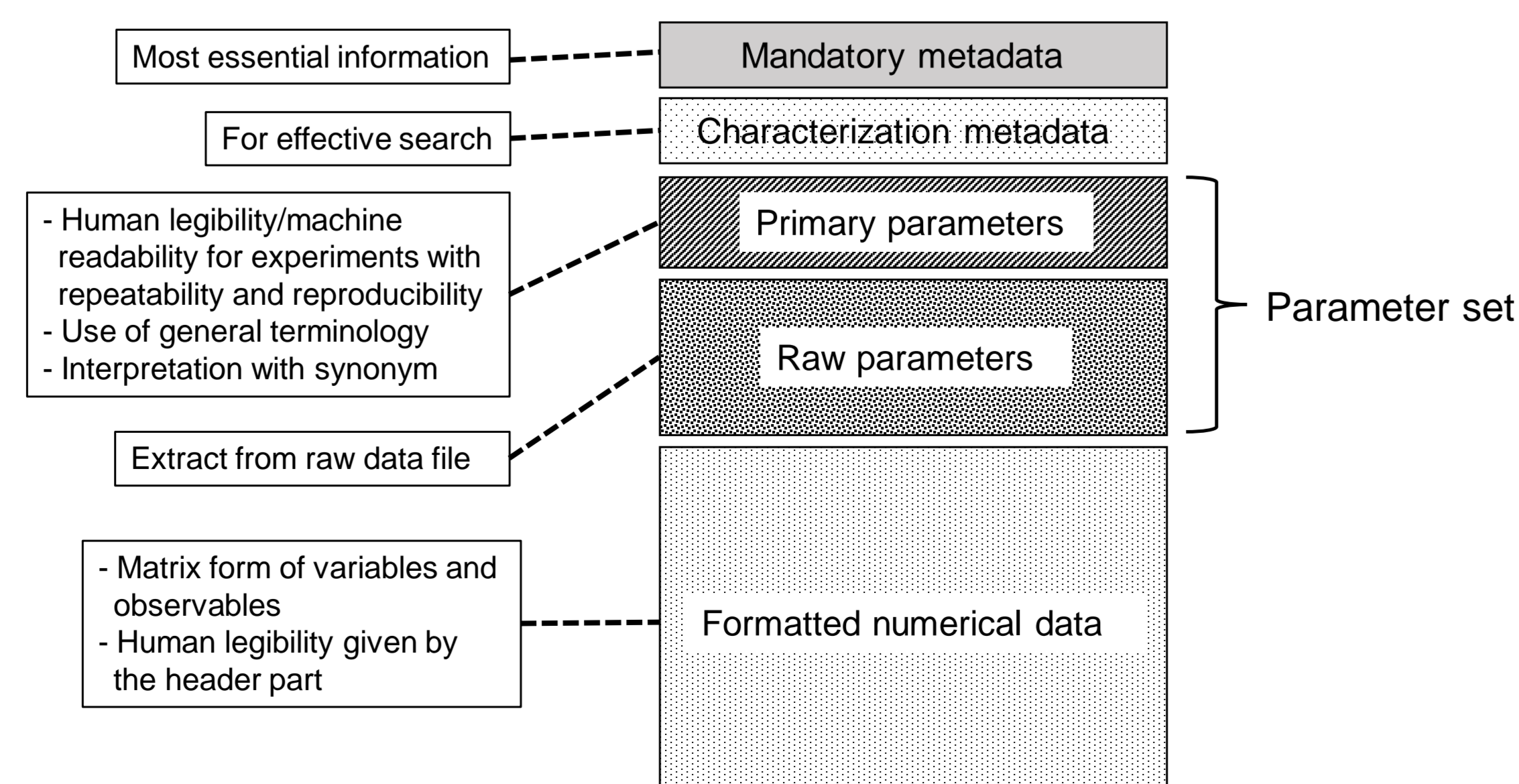
#title	SL3.ras	#x	2Theta-Theta	deg	y
#dimension	x	y			
#y	Intensity	counts			
#legend	Cu K_alpha				
#acq_date	11/21/2017 08:37:42				
25	13				
25.01	7				
25.02	12				
.....				

Conversion flow

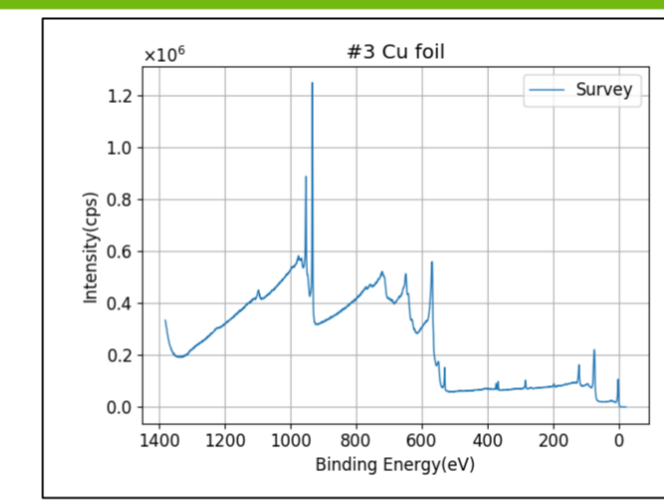
- (1) to convert binary or binary-text mixed raw data to plain text data
- (2) to retrieve measurement parameters and to create metadata set
- (3) to exchange primary parameter terms to general vocabularies
- (4) to reconstruct numerical value array to machine readable one



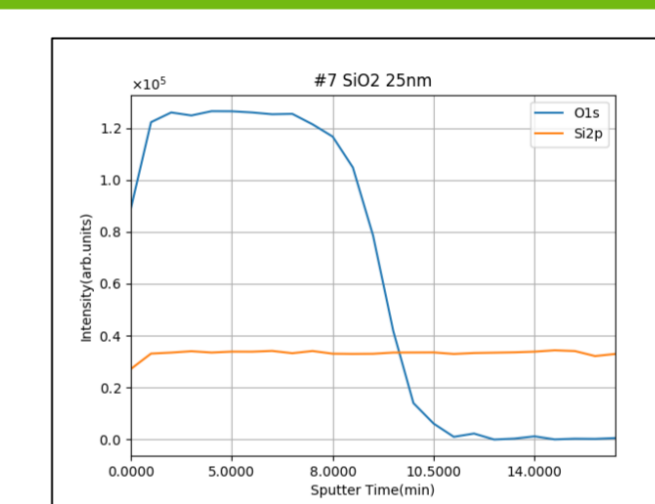
Configuration of converted data package



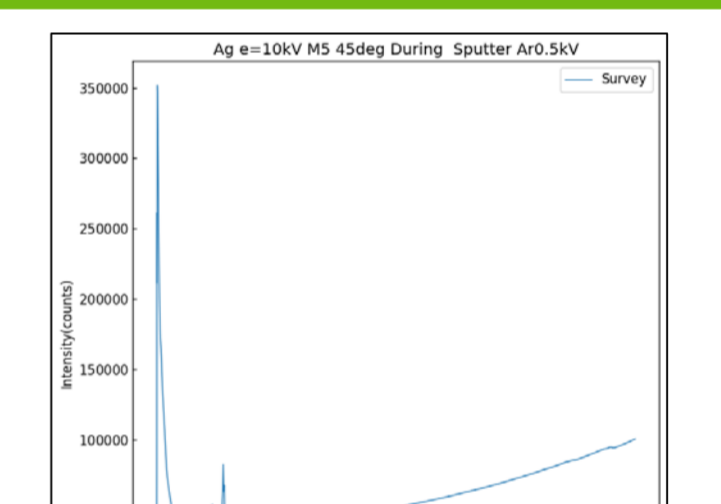
Examples of visualized data



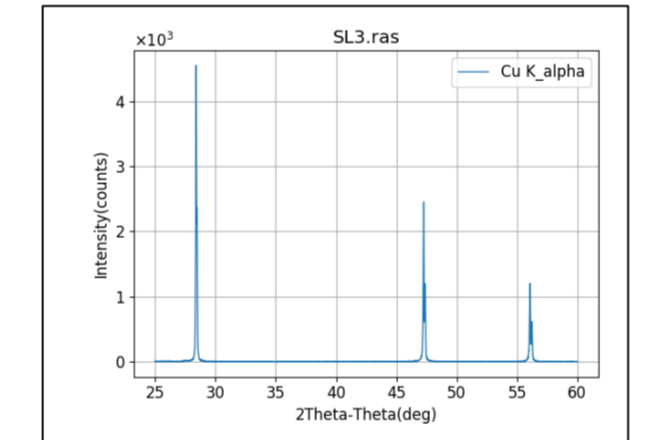
XPS spectrum



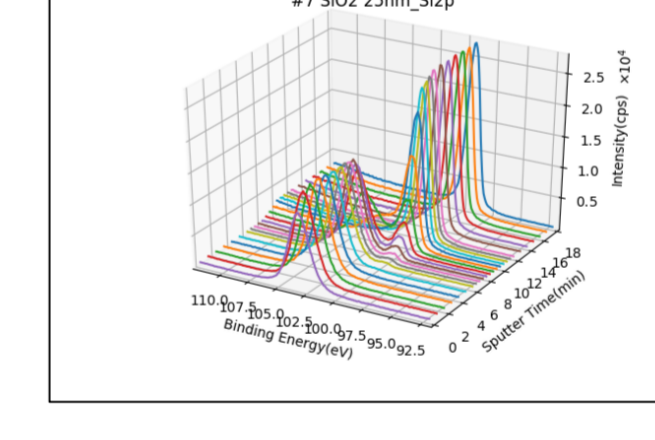
XPS depth profile



AES spectrum



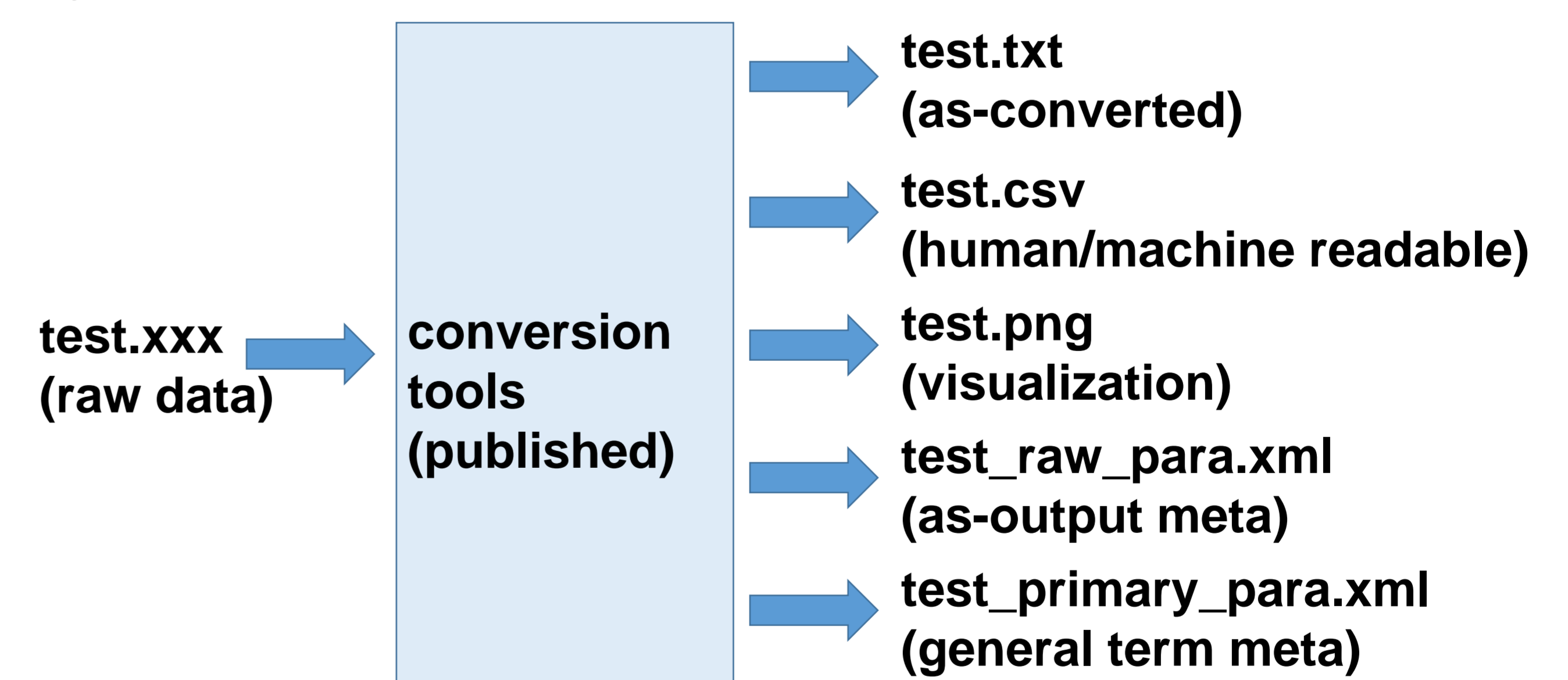
powder XRD pattern



XPS depth profile

Summary of output data files

ULVAC-PHI: SmartSoft-XPS JEOL: AES software
Rigaku: SmatLab software



Collaboration companies (in alphabetical order)

JEOL Ltd. 日本電子株式会社
Rigaku Corporation 株式会社リガク
Riken Keiki Co., Ltd. 理研計器株式会社
ULVAC-PHI, Inc. アルバック・ファイ株式会社

