MDCSAPI

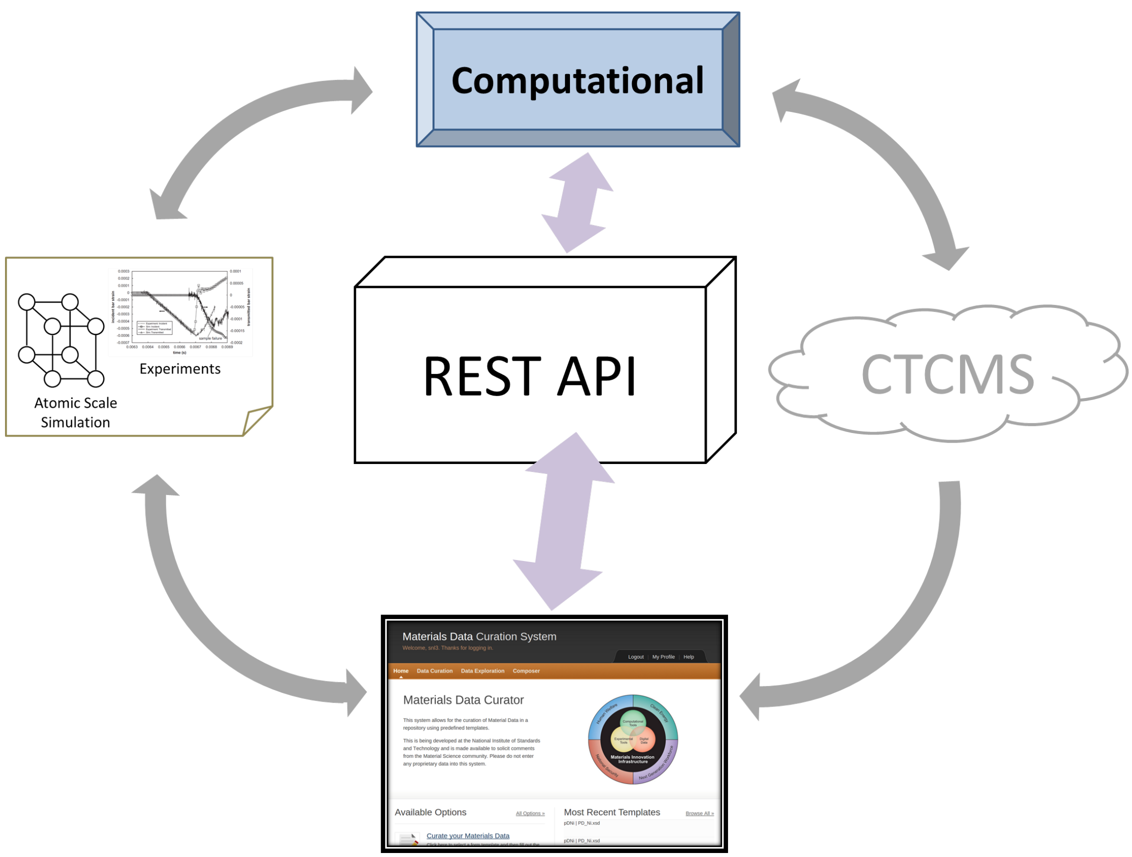
April 27, 2016

0.1 Representational State Transfer (REST) API

(1) This notebook works with Python 2.7.
(2) MDCS should be running on background.
(3) For more examples for REST api, check http://127.0.0.1:8000/docs/api.

In [1]:
```
from IPython.display import Image
Image("workflow.png", width=600)
```

Out[1]:



0.2 Import libraries for Python

In [2]:
```
# ---------------------------------------------- General Python library
import glob, os                               # Python standard library
```

```
import sys                                  # Python standard library
import time                                 # Python standard library
import unicodedata                          # Python standard library
import numpy as np                          # NEED to be installed

# -------------------------------------------- API
import json                                 # Python standard library
import requests                             # NEED to be installed

# -------------------------------------------- XML Schemas
import xml.dom.minidom                      # Python standard library
from xml.dom.minidom import parseString     # Python standard library
import collections                          # Python standard library

# https://pypi.python.org/pypi/xmltodict
import xmltodict                            # attached
# https://pypi.python.org/pypi/dicttoxml
import dicttoxml                            # attached

# -------------------------------------------- convert .XLSX to .XML files
# http://www.python-excel.org/
import xlrd                                 # NEED to be installed


# -------------------------------------------- Matplotlib for plotting
                                            # NEED to be installed
# http://matplotlib.org/
import matplotlib.pyplot as plt
import matplotlib.colorbar as clb
import matplotlib.patches as mpatches
import matplotlib.lines as mlines
import matplotlib.gridspec as gridspec
from matplotlib import ticker
from matplotlib.ticker import LogLocator
%matplotlib inline
```

0.3 Personal information at MDCS

In [3]:
```
# ---- setup information to sign in MDCS
USER = "admin"
PSWD = "admin"
MDCS_URL = "http://127.0.0.1:8000"
```

===
Database status of MDCS

0.3.1 (1) Counting the number of Schema

In [4]:
```
# url is needed in order to communicate with REST api
# to select ALL the schemas in the database, the url is
# "/rest/templates/select/all"
url = MDCS_URL + "/rest/templates/select/all"

# sending the request by url and pass the results to the Python list "allSchemas"
allSchemas = json.loads(requests.get(url, auth=(USER, PSWD)).text)
```

```
        # counting the number schemas of the list
        print "Number of Schemas: ",len(allSchemas)

        # print the details of the schema
        # schema/templet ID is the key to post/query data so it's printed out here
        for i in range(len(allSchemas)):
            print "Schema %s: %s" % (allSchemas[i]['title'],allSchemas[i]['id'])
```

```
Number of Schemas:  16
Schema DSC_s: 56ec3eff1ff0f311d9762c18
Schema mod_demo_diffusion0224: 56ce39e51ff0f30d02759a76
Schema interDiffusion: 56ce3e601ff0f30d02759f2b
Schema demoTEM: 56cea6871ff0f30e114e50af
Schema wsTEM: 56cf3f711ff0f30c3c623b12
Schema mod_demo_diffusion0225: 56cf62601ff0f30c3c62415f
Schema mod_demo_diffusion0225: 56cf63841ff0f30c3c6242d2
Schema mod_demo_diffusion0225: 56cf64821ff0f30c3c62440e
Schema mod_demo_diffusion0225: 56cf6dd61ff0f30c3c624757
Schema mod_demo_diffusion0225: 56cf6f331ff0f30c3c62483d
Schema diffu_SY2: 56cf71531ff0f30c3c624979
Schema thermalanalysis: 56e846471ff0f3119c9bbb3f
Schema thermalanalysis: 56e97cf61ff0f3100de42edc
Schema thermalanalysis: 56e97e741ff0f3100de42f7a
Schema interDiffusion: 5720e2511ff0f31620f6cafd
Schema interDiffusion: 5720e9701ff0f31620f6cb00
```

0.3.2 (2) Counting the number of XMLs

for schemas the url is "/rest/templates/select/all" for xml files the url is "/rest/explore/select/all"

```
In [5]: url = MDCS_URL + "/rest/explore/select/all"
        allXMLs = json.loads(requests.get(url, auth=(USER, PSWD)).text)

        print "Number of XMLs: ",len(allXMLs)
```

```
Number of XMLs:  211
```

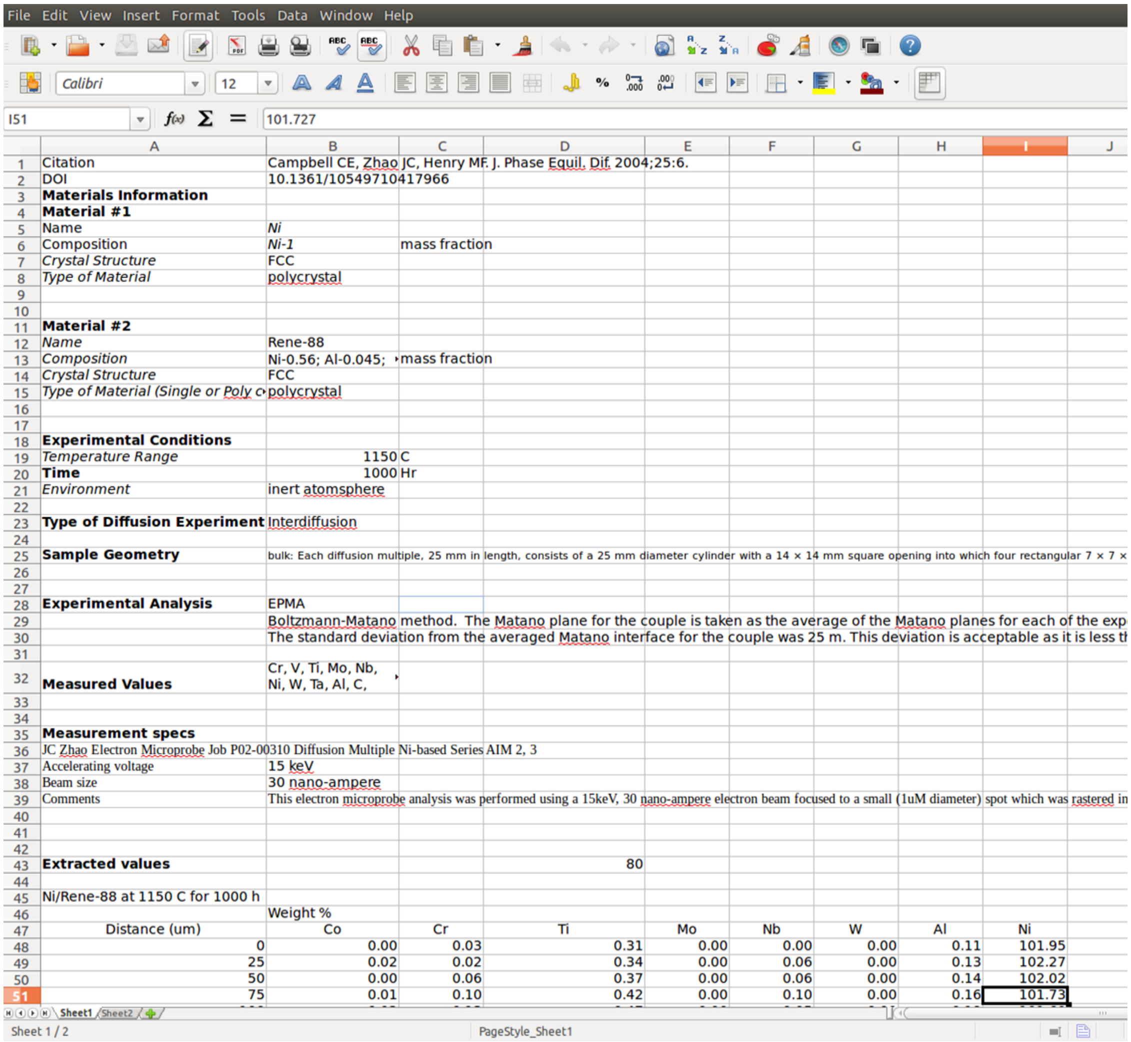
===
Case Study - diffusion couple experiment

0.3.3 Problem Statement:

A spreadsheet of diffusion couple data need to be stored.

```
In [6]: Image("xlsx.png", width=600)
```

```
Out[6]:
```



File Edit View Insert Format Tools Data Window Help

I51 | 101.727

	A	B	C	D	E	F	G	H	I	J
1	Citation	Campbell CE, Zhao JC, Henry MF. J. Phase Equil. Dif. 2004;25:6.								
2	DOI	10.1361/10549710417966								
3	**Materials Information**									
4	**Material #1**									
5	Name	*Ni*								
6	Composition	*Ni-1*	mass fraction							
7	*Crystal Structure*	FCC								
8	*Type of Material*	polycrystal								
9										
10										
11	**Material #2**									
12	*Name*	Rene-88								
13	*Composition*	Ni-0.56; Al-0.045;	mass fraction							
14	*Crystal Structure*	FCC								
15	*Type of Material (Single or Poly c*	polycrystal								
16										
17										
18	**Experimental Conditions**									
19	*Temperature Range*	1150	C							
20	**Time**	1000	Hr							
21	*Environment*	inert atomsphere								
22										
23	**Type of Diffusion Experiment**	Interdiffusion								
24										
25	**Sample Geometry**	bulk: Each diffusion multiple, 25 mm in length, consists of a 25 mm diameter cylinder with a 14 × 14 mm square opening into which four rectangular 7 × 7 ×								
26										
27										
28	**Experimental Analysis**	EPMA								
29		Boltzmann-Matano method. The Matano plane for the couple is taken as the average of the Matano planes for each of the exp								
30		The standard deviation from the averaged Matano interface for the couple was 25 m. This deviation is acceptable as it is less th								
31										
32	**Measured Values**	Cr, V, Ti, Mo, Nb, Ni, W, Ta, Al, C,								
33										
34										
35	**Measurement specs**									
36	JC Zhao Electron Microprobe Job P02-00310 Diffusion Multiple Ni-based Series AIM 2, 3									
37	Accelerating voltage	15 keV								
38	Beam size	30 nano-ampere								
39	Comments	This electron microprobe analysis was performed using a 15keV, 30 nano-ampere electron beam focused to a small (1uM diameter) spot which was rastered in								
40										
41										
42										
43	**Extracted values**			80						
44										
45	Ni/Rene-88 at 1150 C for 1000 h									
46		Weight %								
47	Distance (um)	Co	Cr	Ti	Mo	Nb	W	Al	Ni	
48	0	0.00	0.03	0.31	0.00	0.00	0.00	0.11	101.95	
49	25	0.02	0.02	0.34	0.00	0.06	0.00	0.13	102.27	
50	50	0.00	0.06	0.37	0.00	0.06	0.00	0.14	102.02	
51	75	0.01	0.10	0.42	0.00	0.10	0.00	0.16	101.73	

Sheet1 Sheet2

Sheet 1 / 2 PageStyle_Sheet1

0.3.4 Solution:

data preparation (a) design a schema (Interdiffusion3-LT.xsd) for this spreadsheet (b) load data using xmltodict in Python (c) write data to interdiffusion.xml file using dicttoxml library REST api (d) push Interdiffusion3-LT.xsd to MDCS (e) post interdiffusion.xml to MDCS (f) query and visualize the data under this schema

0.3.5 The schema for diffusion couple

print out the pre-designed schema

```
In [ ]: #%pycat Interdiffusion3-LT.xsd
```

0.4 XMLs preparation from .xlsx file

0.4.1 open file –> get table name –> load data by table name

get files

In [7]:
```
# glob.glob is included in default Python library for
# communicating with the file system
xlsx_files = glob.glob("xlsx/Ni-R88*.xlsx")
print xlsx_files
```

```
['xlsx/Ni-R88-Campbell.xlsx']
```

Open the first file and read the name(s) of the sheet(s) to "xlfile"

In [8]:
```
# xlrd is the library used to read xlsx file
# https://secure.simplistix.co.uk/svn/xlrd/trunk/xlrd/doc/xlrd.html?p=4966
xlfile = xlrd.open_workbook(xlsx_files[0])

sheet_name = []
# find out the names of the spreadsheets of the first file
sheet_name = xlfile.sheet_names()

print ("Number of the sheet in the file: ",
       len(sheet_name),"; Name: ", sheet_name)
```

```
('Number of the sheet in the file: ', 2, '; Name: ', [u'Sheet1', u'Sheet2'])
```

Read data to the Python list "sheet_content"

In [9]:
```
sheet_content = []

# only read the first sheet
for sh in range(1):
    # xlfile.sheet_by_name is the function read the sheet by it's "name"
    sheet_content.append(xlfile.sheet_by_name(sheet_name[sh]))

    # information of the sheet: how many rows and columns
    print "Number of rows:",sheet_content[0].nrows
    print "Number of columns:",sheet_content[0].ncols
```

```
Number of rows: 128
Number of columns: 18
```

Print out the content of the file

In [ ]:
```
#for no_row in range(sheet_content[0].nrows):
#    print sheet_content[0].row_values(no_row)
```

0.4.2 Write the content from .XLSX to .XML

Using dictoxml to write the xml file, the data need to be prepared as Python dictionary. While the sheet is too large, iPython notebook can not handle the writting in one execution. Run the following cell twice.

In [10]:
```
#-------------------------------define the lists for the schma structure
diffusionData = []
experimenttype = []
material = []
experimentalConditions = []
measurementspecs = ''
measurementDescription = ''
measuredvalues = []
reference = ''
```

```python
citation = []
doi = ''
row_value = []
time_type = []
time=''
temperature_type = []
temperature=''
env=''

# scan through the sheet and write the information in each block
# (refer to the note) to the schema module
for no_row in range(sheet_content[0].nrows):
    # the number type belongs to block #6, so it's not handled here
    if(type(sheet_content[0].row_values(no_row)[0]) is float):
        continue

# -- material (block #2)
    # #2 block includes the material information
    if(sheet_content[0].row_values(no_row)[0][:10]=='Material #'):

        # 'MaterialName' is the xml tag for the name of material
        # sheet_content[0]       -- first table
        # row_values(no_row+1)  -- row number no_row+1
        # [1]                    -- second value
        material.append({'MaterialName':
                         sheet_content[0].row_values(no_row+1)[1]})

        # 'CrystalStructure', the tag for crystal structure
        material.append({'CrystalStructure':
                         sheet_content[0].row_values(no_row+3)[1]})

        # separate the string by ';'
        element_list=sheet_content[0].row_values(no_row+2)[1].split(';')
        for ele in range(len(element_list)):
            # separate the string by '-'
            element=str(element_list[ele]).split('-')
            # the minimum and maximum of the composition
            comprange = []
            comprange.append(({'min':element[1]},{'max':element[1]}))
            # 'element'-'CompositionRange' (comprange)-'quantityunit'
            comp = []
            comp.append(({'element':element[0].strip(' ')},
                         {'CompositionRange':comprange},
                         {'quantityUnit':
                          sheet_content[0].row_values(no_row+2)[2]}))
            material.append({'Composition':comp})

        material.append({'materialForm':
                         sheet_content[0].row_values(no_row+4)[1]})

# --exp conditions (block #3)
    if(sheet_content[0].row_values(no_row)[0][:11]=='Temperature'):
        temperature=sheet_content[0].row_values(no_row)[1]
        temperature_unit=sheet_content[0].row_values(no_row)[2]
```

```
    if(sheet_content[0].row_values(no_row)[0][:4]=='Time'):
        time=sheet_content[0].row_values(no_row)[1]
        time_unit=sheet_content[0].row_values(no_row)[2]
    if(sheet_content[0].row_values(no_row)[0][:11]=='Environment'):
        env=sheet_content[0].row_values(no_row)[1]

# --measurement specs (block #4)
    if(sheet_content[0].row_values(no_row)[0][:17]=='Measurement specs'):
        measurementspecs=(str(sheet_content[0].row_values(no_row+1)[0])
                        +str(sheet_content[0].row_values(no_row+2)[0])
                        +str(sheet_content[0].row_values(no_row+2)[1])
                        +str(sheet_content[0].row_values(no_row+3)[0])
                        +str(sheet_content[0].row_values(no_row+3)[1])
                        +str(sheet_content[0].row_values(no_row+4)[0])
                        +str(sheet_content[0].row_values(no_row+4)[1]))
        #print measurementspecs


    if(sheet_content[0].row_values(no_row)[0][:16]=='Extracted values'):
# --measured value (block #5)
        measurementDescription=sheet_content[0].row_values(no_row+2)[0]

        non_empty_col = len(filter(None, sheet_content[0].row_values(no_row+4)))
        non_empty_row = sheet_content[0].nrows - (no_row+5)

        for non_empty_row in range(no_row+5,sheet_content[0].nrows):
            if(type(sheet_content[0].row_values(non_empty_row)[0]) is not float):
                break

# --measured value (block #6)
        non_empty_row-=(no_row+4)
        for tab_row in range(no_row+5,no_row+5+non_empty_row,1):
            for tab_col in range(non_empty_col):
                row_value.append({'quantity':
                                  sheet_content[0].row_values(no_row+4)[tab_col]})
                row_value.append({'value':
                                  sheet_content[0].row_values(tab_row)[tab_col]})
                #measuredvalues.append({'measuredValues':row_value})

# -- reference (block #1)
    if(sheet_content[0].row_values(no_row)[0][:8]=='Citation'):
        reference=sheet_content[0].row_values(no_row)[1]
    if(sheet_content[0].row_values(no_row)[0][:4]=='DOI'):
        doi=sheet_content[0].row_values(no_row)[1]

# summarize some types
temperature_type.append(({'value':temperature},
                         {'unit':temperature_unit}))
time_type.append(({'value':time},{'unit':time_unit}))
experimentalConditions.append(({'time':time_type},
                               {'temperature':temperature_type},
                               {'environment':env}))
```

```
# assemble the blocks #1-#6
diffusionData.append(('experimentalDetails',
             ({'material':material},                             # 2
              {'experimentalConditions':experimentalConditions}, # 3
              {'measurementSpec':measurementspecs},              # 4
              {'measurementDescription':measurementDescription}, # 5
              {'measuredValues':row_value})))                    # 6
diffusionData.append(('citation',
                    ({'reference':reference},{'doi':doi})))      # 1

# organize the Python dictionary
# https://docs.python.org/2/library/collections.html#collections.OrderedDict
diffusionData = collections.OrderedDict(diffusionData)

# using dicttoxml library to convert dictionary to xml
# the root of xml is 'interDiffusion'
# type attribute is the type in tag; eq <doi type='str'>xxxxx</doi>
diffusionDataxml = dicttoxml.dicttoxml(diffusionData,
                                       custom_root='interDiffusion',
                                       attr_type=False)

# write information to interdiffusion.xml
filename = str('data/interdiffusion.xml')
interdiffusionschema = open(filename, 'w')
interdiffusionschema.write("%s\n" %
            (parseString(diffusionDataxml).toprettyxml()))
interdiffusionschema.close()
```

Check the outputs

In [ ]:
```
#%pycat data/interdiffusion.xml
```

0.5 Push schema to MDCS

This schema is designed previously using Oxygen In this cell, we push this schema to MDCS and get the schema ID

In [12]:
```
file = open('Interdiffusion3-LT.xsd','r')
templateContent = file.read()

# calling the function by the url for pushing schema
url = MDCS_URL + "/rest/templates/add"

# to push schema you need to define
# (1)"title" of the schema  (2)"filename" of the schema in MDCS
# (3)"content" of the schema
push_data = {"title":"interDiffusion",
        "filename": "interDiffusionschema.xsd",
        "content": templateContent}

# post it
pSchema = json.loads(requests.post(url, push_data,
                                   auth=(USER, PSWD)).text)

# get schema/templet ID
```

```
templateId = pSchema['_id']['$oid']

print "Schema ID:",templateId
```

```
Schema ID: 5720ed2e1ff0f31620f6cb03
```

0.6 Post data

find out the path of the .xml file

```
In [13]: push_files = glob.glob("data/interdiffusion*.xml")

         print "Number of .XML to post",len(push_files)
```

```
Number of .XML to post 1
```

post xml to MDCS

```
In [14]: import time

         # claim the URL path for posting
         url = MDCS_URL + "/rest/curate"

         # sequentially
         # open and post .xml file(s)
         for pfile in push_files:
             opfile = open(pfile,'r')
             fileContent = opfile.read()

             # api function
             # define (1) "title" of the xml  (2) which "schema"
             # you want to push to  (3) the "content" of xml
             data_to_send = {"title": "diffusion"+str(time.time())
                                           +str(time.clock())+".xml",
                             "schema":templateId,"content":fileContent}

             # post the data using request library
             r = requests.post(url, data_to_send, auth=(USER, PSWD))
```

0.7 Query and plot the results

define the plot function for this specific case

0.8 Setup plot function

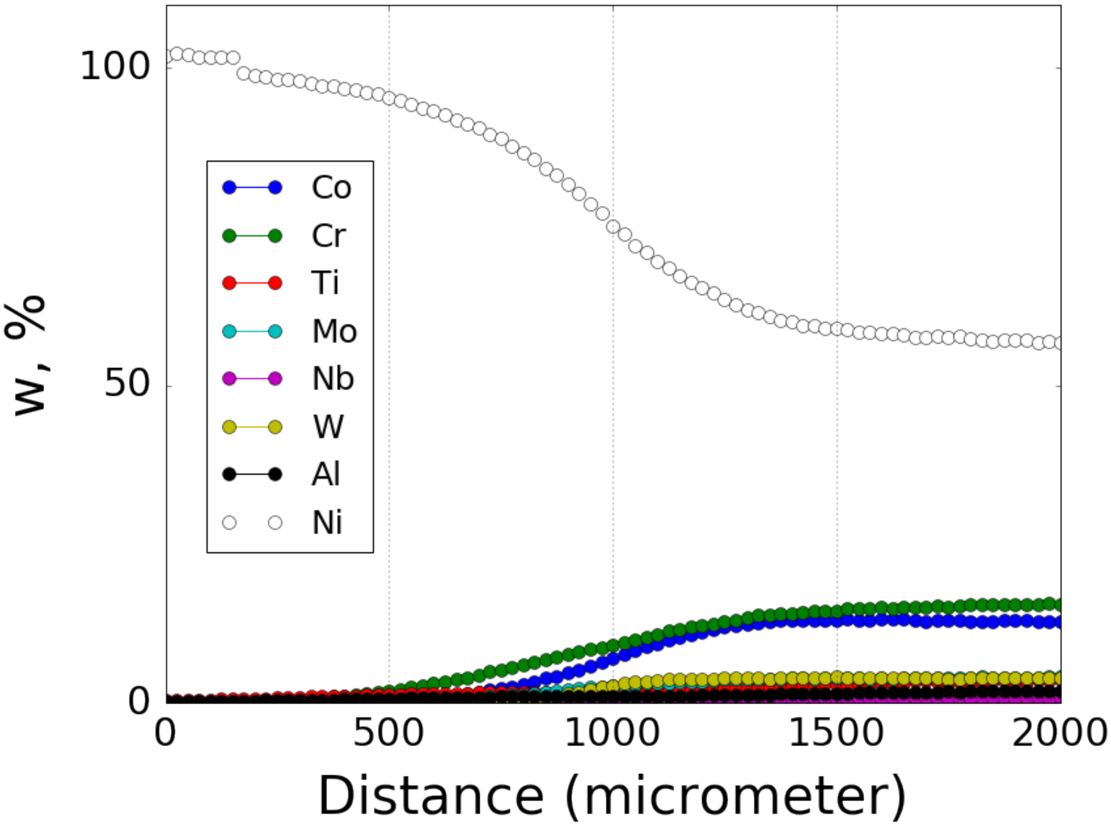
```
In [15]: def plot(samNo,samContent):
             fig, ax = plt.subplots(figsize=(12, 9))

             # -------------- parameters for plots
             titlesize=35
             labelsize=25
             labelpad=15
             pad=5
             p_alpha = 0.5
             vsize = 10
             flabsize = 40
```

```python
fticksize = 30
# --------------

content = []
x = []
y = []

for i in range(samNo):
    # the query results in xml format are stored as
    # Python list "samContent"
    # use xmltodict library to convert xml format to
    # Python dictionary
    # 'content' is the standard head from request
    # toprettyxml makes the output in organized shape
    content = (xmltodict.parse(xml.dom.minidom
                    .parseString(samContent[i]['content']).toprettyxml()))

    # according to the schema defined before,
    # the physical quantities are stored in the path of
    # 'interDiffusion'-->'experimentalDetails'
    #     -->'measuredValues'-->'quantity'
    # the measuerd values are
    # 'interDiffusion'-->'experimentalDetails'
    #     -->'measuredValues'-->'value'
    x.append(content['interDiffusion']['experimentalDetails']
             ['measuredValues']['quantity'])
    y.append(content['interDiffusion']['experimentalDetails']
             ['measuredValues']['value'])

# x and y are the long python lists
# numpy .reshape recovers them to a numerical table for plotting
x = np.asarray(x).reshape(-1,non_empty_col)
y = np.asarray(y).reshape(-1,non_empty_col)

ax.plot(y[:,0],y[:,1],'o-', ms=vsize, c='b', label=x[0,1])
ax.plot(y[:,0],y[:,2],'o-', ms=vsize, c='g', label=x[0,2])
ax.plot(y[:,0],y[:,3],'o-', ms=vsize, c='r', label=x[0,3])
ax.plot(y[:,0],y[:,4],'o-', ms=vsize, c='c', label=x[0,4])
ax.plot(y[:,0],y[:,5],'o-', ms=vsize, c='m', label=x[0,5])
ax.plot(y[:,0],y[:,6],'o-', ms=vsize, c='y', label=x[0,6])
ax.plot(y[:,0],y[:,7],'o-', ms=vsize, c='k', label=x[0,7])
ax.plot(y[:,0],y[:,8],'o-', ms=vsize, c='w', label=x[0,8])

ax.set_xlabel(x[0,0], fontsize=flabsize, labelpad=15)
ax.set_ylabel('w, %', fontsize=flabsize, labelpad=15)

ax.tick_params(axis='x', labelsize=fticksize, pad = 10, colors='black')
ax.tick_params(axis='y', labelsize=fticksize, pad = 10, colors='black')

ax.xaxis.grid(True)

ax.set_xlim(0,2000)
ax.set_ylim(0,110)
```

```
    ax.locator_params(axis = 'x', nbins = 4)
    ax.locator_params(axis = 'y', nbins = 3)

    handles, labels = ax.get_legend_handles_labels()

    ax.legend(handles, labels, bbox_to_anchor=(0.25, 0.8), fontsize=25)

    fig.tight_layout()
    plt.show()

    return (x,y)
```

0.9 query by schema/templateId

In [16]:
```
X = []
Y = []

# the url for query
url = MDCS_URL + "/rest/explore/query-by-example"

# assign the templet ID to the query function
#templateId = "560967af1ff0f30c8c26e73e"

# request data from MDCS
# use the python dictionary to send the "query" condition
# 'schema':templateId in this case
req_data = {"query": str({'schema':templateId})}

# get results to qres
qres = json.loads(requests.post(url,req_data,auth=(USER, PSWD)).text)

# plot the results using plot function defined in previous cell
X, Y = plot(len(qres),qres)
```



100
50
0
w, %
Co
Cr
Ti
Mo
Nb
W
Al
Ni
0
500
1000
1500
2000
Distance (micrometer)


```
In [ ]:
```