



PHYTON DRIVING LICENSE

Exam project

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Academic year: 2022 - 2023

School of Industrial and Information Engineering

PhD XXXVIIIth cycle — Materials Engineering



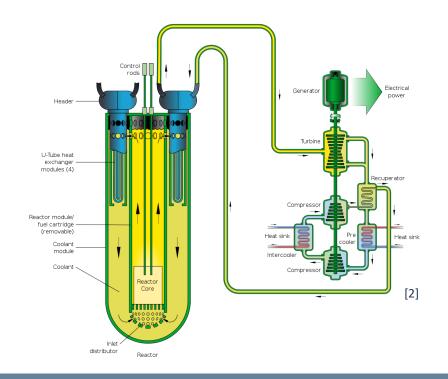
Next generation nuclear reactors

Materials challenges Troubleshooting solutions

Materials requirements Aim of the current PhD project

Fast Breeder Reactor (FBR) concepts

Lead-cooled fast reactor (LFR) technology





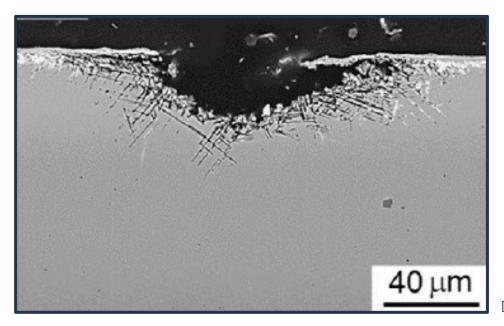
Next generation nuclear reactors

Materials challenges Troubleshooting solutions

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Heavy Liquid Metal (HLM) dissolution

Integrity of reactor's in-core steel parts





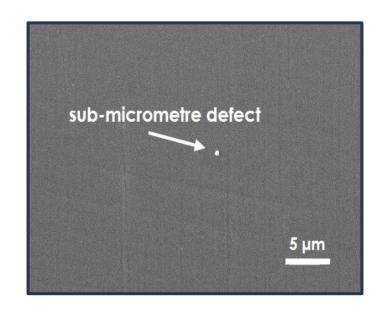
Next generation nuclear reactors

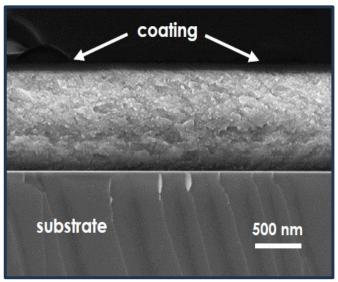
Materials challenges **Troubleshooting** solutions

Materials requirements Aim of the current PhD project

Ceramic protective barriers

PLD-grown a- Al_2O_3 coatings





Next generation nuclear reactors

Materials challenges Troubleshooting solutions

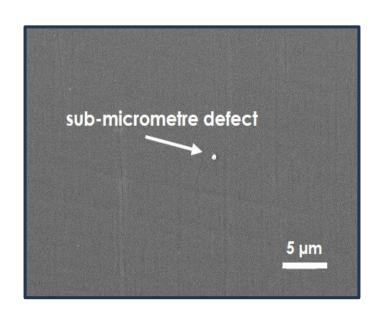
Materials requirements Aim of the current PhD project

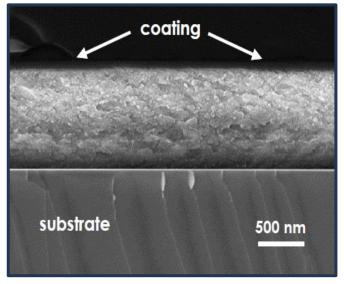
Preservation of the film's integrity

- Corrosion-damage exposure
- Radiation-damage exposure
- **Mechanical deformation**



Focus of the project hereby presented







Next generation nuclear reactors

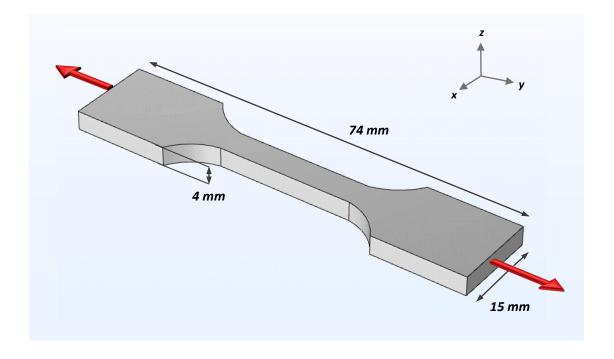
Materials challenges Troubleshooting solutions

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TENSILE TESTS experimental campaign

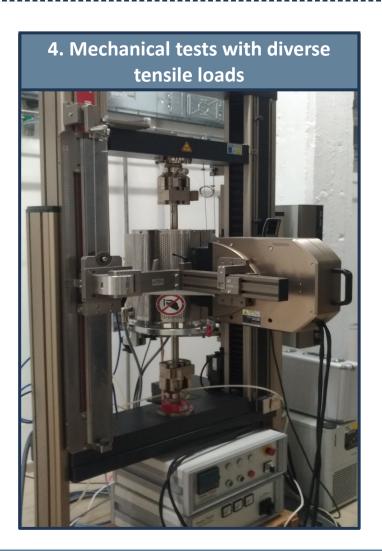


- Planar dog-bone geometry
- Externally **imposed strain/stress**
- Evaluate the coating's response upon mechanical deformations



Experimental analysis

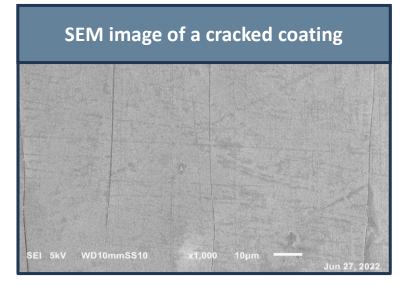
- **Generation** of dog-bone substrates from a cold-rolled AISI316 metal sheet
- Pre-deposition treatments (grinding, polishing, ultrasonic cleaning, ion gun cleaning)
- 3. Pulsed Laser Deposition of a- Al_2O_3 coatings with different thickness



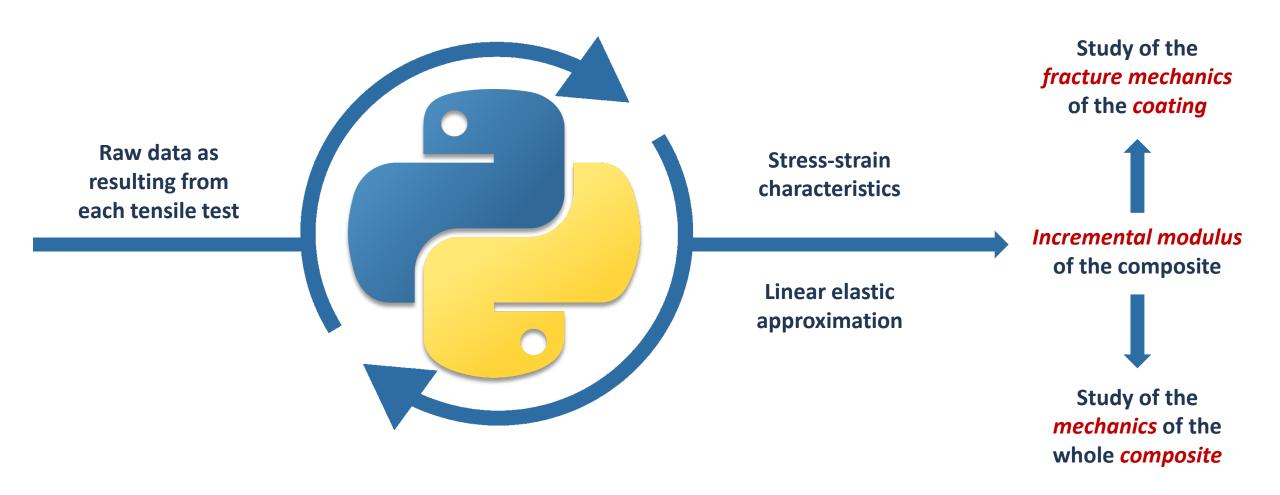
5. Ex-situ characterization and analysis

Retrive the conditions (stress or strain) upon which the coating failed i.e., cracked or delaminated











General overview of the assignment

Sequence of the operations leading to the expected result:

- Creation of a **test script** for a random case study
- **Adjustment** of the previous script to all case studies
- Generation of re-elaborated scripts

Focus on:

- **DATABASE ANALYSIS**
- **MANIPULATION OF RAW DATA**
- PLOTS AND DIAGRAMS

Phyton libraries adopted for the purpose:

MatPlotLib

Graphics

NumPy/SciPy

Mathematics

Scikit-Learn/Statistics

Data analysis

Pandas

Data manipulation



Test script

Definition of useful **functions**

```
def engineering stress(load):
    A0 = 24
    return load*1000/A0
```

```
def median value(array):
    sum val = 0
   for i in range (0, array.shape[0]):
        sum_val += array[i]
   return sum val/array.shape[0]
```

```
def r2regression(valori_reali, valori_attesi):
    RSS = float(0)
    TSS = float(0)
    media = median value(valori reali)
   for i in range (0, valori reali.shape[0]):
        RSS += (valori reali[i] - valori attesi[i])**2
        TSS += (valori reali[i] - media)**2
    return round(float(1-RSS/TSS), 4)
```

```
def regression reliability(r2):
   if(r2>=0.95):
        return 'VERY GOOD'
    elif(r2<0.95 and r2>=0.90):
        return 'ADMISSIBLE'
    else:
        return 'NOT GOOD'
```

```
def engineering strain(extension):
    L0 = 15
    return extension/L0
```

 R^2 analytical definition: [3]

$$R^2 = 1 - rac{RSS}{TSS}$$
 $RSS = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$
 $TSS = \sum_{i=1}^n (y_i - \overline{y})^2$



Test script

- Definition of useful functions
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed

```
df = pd.DataFrame(pd.read_excel(r'C:\Users\Federico\Desktop\PhD\EXAMS\PHYTON DRIVING LICENSE\PROJECT_EXAM\RTdegC(2,0).xlsx',
                               sheet_name='8.3kN', usecols=[0,1,2,3]))
df = df.rename(columns={'time\n[s]':'Time (s)', 'crosshead\n[mm]':'Crosshead (mm)', 'extensometer\n[mm]':'Extensometer (mm)'
                       'load\n[kN]':'Load (kN)'})
df['Engineering strain (abs.)'] = engineering strain( df['Extensometer (mm)'] )
df['Engineering stress (MPa)'] = engineering_stress( df['Load (kN)'] )
del df["Crosshead (mm)"] # crosshead data are useless and can be removed from the DataFrame
df.style.set_properties(**{'text-align': 'center'}) #centering the text
display(df)
```



	Time (s)	Extensometer (mm)	Load (kN)	Engineering strain (abs.)	Engineering stress (MPa)
0	0.0000	0.000000e+00	0.364120	0.000000e+00	15.171654
1	0.0200	-4.717588e-07	0.364118	-3.145059e-08	15.171579
2	0.0400	-9.435175e-07	0.364116	-6.290117e-08	15.171508
3	0.0600	-1.415276e-06	0.364114	-9.435173e-08	15.171433
4	0.0800	-1.887035e-06	0.364113	-1.258023e-07	15.171363
1954	39.0800	2.212456e-01	7.747406	1.474971e-02	322.808583
1955	39.1000	2.212485e-01	7.747242	1.474990e-02	322.801750
1956	39.1200	2.212513e-01	7.747077	1.475009e-02	322.794875
1957	39.1400	2.212542e-01	7.746913	1.475028e-02	322.788042
1958	39.1402	2.212542e-01	7.746912	1.475028e-02	322.788000
←					
		Raw data		Processe	<mark>ed data</mark>

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**

```
X = df['Engineering strain (abs.)']
Y = df['Engineering stress (MPa)']
interpolation function = interp1d(X, Y, kind = 'linear')
interpolation points = np.linspace(0, df.iloc[-1]['Engineering strain (abs.)'], Y.shape[0])
interpolated value = interpolation function(interpolation points)
```

The entire strain and stress columns of the DataFrame are collected into an array-like parameter (X and Y, respectively)

The "interp1d" class generates the interpolation function

The "linspace" class creates the interpolation points by specifying evenly spaced numbers over a specified interval (the entire strain column of the DataFrame)



The **interpolated value** is obtained by computing the interpolation function all over the prescribed interpolation points

Test script

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**

```
X1 = X[:1100].values.reshape(-1,1)
Y1 = Y[:1100].values.reshape(-1,1)
regressor = LinearRegression(fit intercept = False).fit(X1, Y1)
# print(regressor.intercept ) --> to verify that the straight line effectively passes through the origin
y estimated = regressor.predict(X1)
incremental modulus = int(regressor.coef /1000)
```

The entire strain and stress columns of the DataFrame are collected into a reshaped matrixlike parameter (X1 and Y1 respectively)

The "LinearRegression" class fits the x- and y- data (X1 and Y1, respectively) generating a straight line passing through the origin (specified by the "fit intercept" parameter)



The **estimated y-value** as resulting from the linear regression is obtained by way of the "predict" method, applied to all the x-values (X1, in this case)

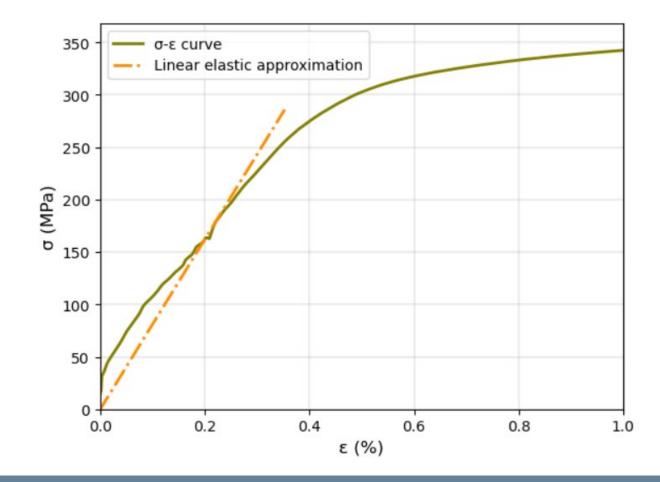


The **incremental modulus** is the slope of the linear regression straight line passing through the origin (divided by 1000 to have the result in GPa)



- Definition of useful functions
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results

"pyplot" class is used to display the stress-strain curve and the linear elastic approximation



Test script

- Definition of useful **functions**
- Raw data import from an excel file
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- **Linear interpolation**
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- **Graphical analysis** of the results
- Determination of the **numerical results**

```
--> The R<sup>2</sup> value of the linear regression computed analytically is: ~ 0.9111
--> The R<sup>2</sup> value of the linear regression computed with r2_score is: ~ 0.9111
--> The regression reliability is: ADMISSIBLE
--> The elastic modulus in the linear elastic region is: ~ 81 GPa
```

The R^2 value of the linear regression has been computed analytically by calling the "r2regression" function and with a specific class belonging to the scikit-learn library

A function determines the goodness of the linear elastic approximation performed so far

The incremental (elastic) modulus is returned as an integer, whose magnitude is in GPa

An additional library ("colorama") is used to display colored text

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed

Adjustment of the test script to analyse 2 μm-thick coatings tensile tested at 25°C

```
# create the general dictionary
data = pd.read excel(r'C:\Users\Federico\Desktop\PhD\EXAMS\PHYTON DRIVING LICENSE\PROJECT EXAM\RTdegC(2,0).xlsx'
                     sheet name=[1,2,3,4], usecols=[0,1,2,3])
# create the 1st DataFrame from the general dictionary
df1 = pd.DataFrame.from_dict(data[1], orient='columns')
df1 = df1.rename(columns={'time\n[s]':'Time (s)', 'crosshead\n[mm]':'Crosshead (mm)',
                           'extensometer\n \nm]':'Extensometer (mm)','load\n[kN]':'Load (kN)'})
df1['Engineering strain (abs.)'] = engineering_strain( df1['Extensometer (mm)'] )
df1['Engineering stress (MPa)'] = engineering stress( df1['Load (kN)'] )
del df1["Crosshead (mm)"]
display(df1)
```

If multiple sheets are imported contemporarily, the Pandas library creates a general dictionary



Each sheet corresponds to a diverse tensile load (experimental condition)

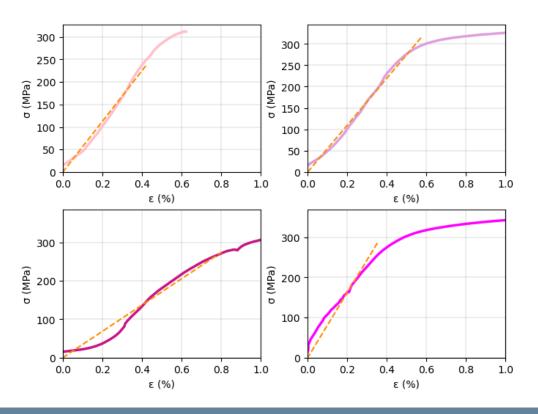


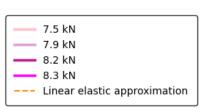
Every DataFrame must be extracted from the dictionary singularly

Adjustment of the test script to analyse 2 μm-thick coatings tensile tested at 25°C

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results

"pyplot" class (subplot method) is used to display the stress-strain curve and the linear elastic approximation for every tensile load applied by the tensile machinery





- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results
- Determination of the **numerical results**

Adjustment of the test script to analyse 2 μm–thick coatings tensile tested at 25°C

```
# generation of 4 different lists of results
pulling force = ['7.5', '7.9', '8.2', '8.3']
r2 results = [r2 score(Y1 1, y estimated1), r2 score(Y2 2, y estimated2), r2 score(Y3 3, y estimated3),
              r2 score(Y4 4, y estimated4)]
r2 reliability = [regression reliability(r2 score(Y1 1, y estimated1)),
                  regression reliability(r2 score(Y2 2, y estimated2)),
                  regression reliability(r2 score(Y3 3, y estimated3)),
                  regression reliability(r2 score(Y4 4, y estimated4))]
incremental moduli = [incremental modulus1, incremental modulus2, incremental modulus3, incremental modulus4]
# creation of the corresponding DataFrame (N.B: each list is added to the DataFrame by way of the "zip" function)
df results = pd.DataFrame(list(zip(pulling force, r2 results, r2 reliability, incremental moduli)),
                          columns =['Load (kN)', 'R\u00b2 value', 'Linear regression reliability',
                                    'Approximate incremental modulus (GPa)'])
# visualization of the final results
display(df results.style.set properties(**{'text-align': 'center'}))
```

Numerical results are saved into appropriate lists (arrays)



A DataFrame collecting the results is then generated by adding each list one next the other

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results
- Determination of the **numerical results**

Adjustment of the test script to analyse 2 μm–thick coatings tensile tested at 25°C

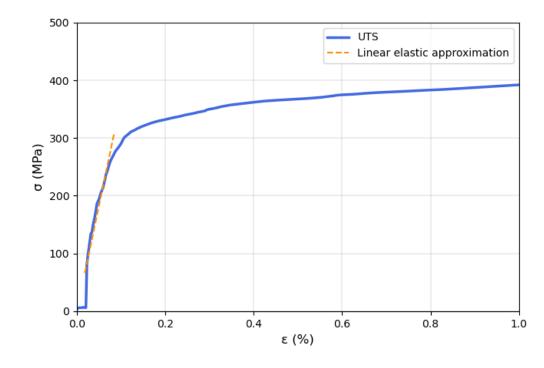
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pulling force = ['7.5', '7.9', '8.2', '8.3']
r2 results = [r2 score(Y1 1, y estimated1), r2 score(Y2 2, y estimated2), r2 score(Y3 3, y estimated3),
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                  regression reliability(r2 score(Y2 2, y estimated2)),
                  regression reliability(r2 score(Y3 3, y estimated3)),
                  regression reliability(r2 score(Y4 4, y estimated4))]
incremental moduli = [incremental modulus1, incremental modulus2, incremental modulus3, incremental modulus4]
# creation of the corresponding DataFrame (N.B: each list is added to the DataFrame by way of the "zip" function)
df results = pd.DataFrame(list(zip(pulling force, r2 results, r2 reliability, incremental moduli)),
                          columns =['Load (kN)', 'R\u00b2 value', 'Linear regression reliability',
                                    'Approximate incremental modulus (GPa)'])
# visualization of the final results
display(df results.style.set properties(**{'text-align': 'center'}))
```

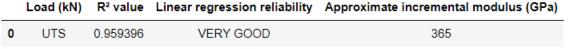
	Load (kN)	R² value	Linear regression reliability	Approximate incremental modulus (GPa)
0	7.5	0.982522	VERY GOOD	56
1	7.9	0.991223	VERY GOOD	54
2	8.2	0.963955	VERY GOOD	34
3	8.3	0.911062	ADMISSIBLE	81

Adjustment of the test script to analyse 3 μm-thick coatings tensile tested at 25°C

- Definition of useful functions
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results
- Determination of the numerical results

"pyplot" class is used to display the stress-strain curve and the linear elastic approximation





Adjustment of the test script to analyse 250 nm-thick coatings tensile tested at 25°C

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed

```
# create the general dictionary
data = pd.read excel(r'C:\Users\Federico\Desktop\PhD\EXAMS\PHYTON DRIVING LICENSE\PROJECT EXAM\RTdegC(0,25).xlsx
                       sheet_name=[1,2], usecols=[0,1,2,3])
# create the 1st DataFrame from the general dictionary
df1 = pd.DataFrame.from_dict(data[1], orient='columns')
df1 = df1.rename(columns={'time\n[s]':'Time (s)', 'crosshead\n[mm]':'Crosshead (mm)',
                             'extensometer\n[nm]':'Extensometer (mm)','load\n[kN]':'Load (kN)'})
df1['Engineering strain (abs.)'] = engineering_strain( df1['Extensometer (mm)'] )
df1['Engineering stress (MPa)'] = engineering stress( df1['Load (kN)'] )
del df1["Crosshead (mm)"]
display(df1)
```

If multiple sheets are imported contemporarily, the Pandas library creates a general dictionary



Each sheet corresponds to a diverse tensile load (experimental condition)

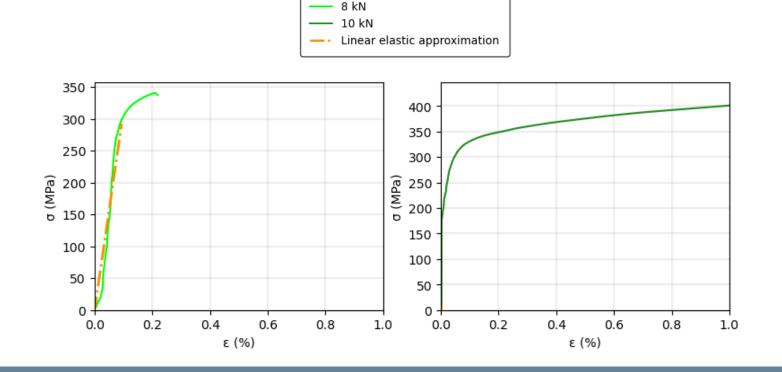


Every DataFrame must be extracted from the dictionary singularly

Adjustment of the test script to analyse 250 nm-thick coatings tensile tested at 25°C

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results

"pyplot" class (subplot method) is used to display the stress-strain curve and the linear elastic approximation for every tensile load applied by the tensile machinery



- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed
- **Linear interpolation**
- **Linear regression**
- **Graphical analysis** of the results
- Determination of the **numerical results**

Adjustment of the test script to analyse 250 nm–thick coatings tensile tested at 25°C

```
# generation of 4 different lists of results
pulling force = ['8', '10']
r2 results = [r2 score(Y1 1, y estimated1), r2 score(Y2 2, y estimated2), r2 score(Y3 3, y estimated3),
              r2 score(Y4 4, y estimated4)]
r2 reliability = [regression reliability(r2 score(Y1 1, y estimated1)),
                  regression reliability(r2 score(Y2 2, y estimated2)),
                  regression reliability(r2 score(Y3 3, y estimated3)),
                  regression reliability(r2 score(Y4 4, y estimated4))]
incremental moduli = [incremental modulus1, incremental modulus2, incremental modulus3, incremental modulus4]
# creation of the corresponding DataFrame (N.B: each list is added to the DataFrame by way of the "zip" function)
df results = pd.DataFrame(list(zip(pulling force, r2 results, r2 reliability, incremental moduli)),
                          columns =['Load (kN)', 'R\u00b2 value', 'Linear regression reliability',
                                    'Approximate incremental modulus (GPa)'])
# visualization of the final results
display(df results.style.set properties(**{'text-align': 'center'}))
```

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A DataFrame collecting the results is then generated by adding each list one next the other

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Adjustment of the test script to analyse 250 nm–thick coatings tensile tested at 25°C

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incremental moduli = [incremental modulus1, incremental modulus2, incremental modulus3, incremental modulus4]
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df results = pd.DataFrame(list(zip(pulling force, r2 results, r2 reliability, incremental moduli)),
                          columns =['Load (kN)', 'R\u00b2 value', 'Linear regression reliability',
                                    'Approximate incremental modulus (GPa)'])
# visualization of the final results
display(df results.style.set properties(**{'text-align': 'center'}))
```

	Load (kN)	R² value	Linear regression reliability	Approximate incremental modulus (GPa)	_
0	8	0.932999	ADMISSIBLE	311	
1	10	-138.525595	NOT GOOD	289	!!!

The linear regression is not always possible and may run into errors in fitting the linear elastic regime

Adjustment of the test script to analyse 500 nm-thick coatings tensile tested at 25°C

- Definition of useful **functions**
- Raw data import from an excel file
- Creation of a **DataFrame** containing the data to be analyzed

```
# create the general dictionary
data = pd.read_excel(r'C:\Users\Federico\Desktop\PhD\EXAMS\PHYTON DRIVING LICENSE\PROJECT_EXAM\RTdegC(0,50).xlsx
                       sheet name=[1,2,3,4], usecols=[0,1,2,3])
# create the 1st DataFrame from the general dictionary
df1 = pd.DataFrame.from_dict(data[1], orient='columns')
df1 = df1.rename(columns={'time\n[s]':'Time (s)', 'crosshead\n[mm]':'Crosshead (mm)',
                             'extensometer\n[nm]':'Extensometer (mm)','load\n[kN]':'Load (kN)'})
df1['Engineering strain (abs.)'] = engineering_strain( df1['Extensometer (mm)'] )
df1['Engineering stress (MPa)'] = engineering stress( df1['Load (kN)'] )
del df1["Crosshead (mm)"]
display(df1)
```

If multiple sheets are imported contemporarily, the Pandas library creates a general dictionary



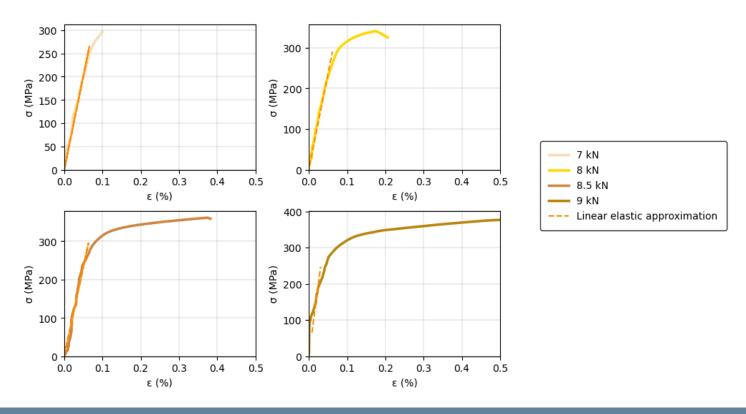
Each sheet corresponds to a diverse tensile load (experimental condition)



Every DataFrame must be extracted from the dictionary singularly

- Definition of useful functions
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- **Linear regression**
- **Graphical analysis** of the results

"pyplot" class (subplot method) is used to display the stress-strain curve and the linear elastic approximation for every tensile load applied by the tensile machinery



- Definition of useful **functions**
- Raw data import from an excel file
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- Determination of the **numerical results**

Adjustment of the test script to analyse 500 nm–thick coatings tensile tested at 25°C

```
# generation of 4 different lists of results
pulling force = ['7', '8', '8.5', '9']
r2 results = [r2 score(Y1 1, y estimated1), r2 score(Y2 2, y estimated2), r2 score(Y3 3, y estimated3),
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r2 reliability = [regression reliability(r2 score(Y1 1, y estimated1)),
                  regression reliability(r2 score(Y2 2, y estimated2)),
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incremental moduli = [incremental modulus1, incremental modulus2, incremental modulus3, incremental modulus4]
# creation of the corresponding DataFrame (N.B: each list is added to the DataFrame by way of the "zip" function)
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                          columns =['Load (kN)', 'R\u00b2 value', 'Linear regression reliability',
                                    'Approximate incremental modulus (GPa)'])
# visualization of the final results
display(df results.style.set properties(**{'text-align': 'center'}))
```

Numerical results are saved into appropriate lists (arrays)



A DataFrame collecting the results is then generated by adding each list one next the other

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              r2 score(Y4 4, y estimated4)]
r2 reliability = [regression reliability(r2 score(Y1 1, y estimated1)),
                  regression reliability(r2 score(Y2 2, y estimated2)),
                  regression reliability(r2 score(Y3 3, y estimated3)),
                  regression reliability(r2 score(Y4 4, y estimated4))]
incremental moduli = [incremental modulus1, incremental modulus2, incremental modulus3, incremental modulus4]
# creation of the corresponding DataFrame (N.B: each list is added to the DataFrame by way of the "zip" function)
df results = pd.DataFrame(list(zip(pulling force, r2 results, r2 reliability, incremental moduli)),
                          columns =['Load (kN)', 'R\u00b2 value', 'Linear regression reliability',
                                    'Approximate incremental modulus (GPa)'])
# visualization of the final results
display(df results.style.set properties(**{'text-align': 'center'}))
```

	Load (kN)	R² value	Linear regression reliability	Approximate incremental modulus (GPa)
0	7	0.984558	VERY GOOD	403
1	8	0.983680	VERY GOOD	472
2	8.5	0.968531	VERY GOOD	466
3	9	0.369303	NOT GOOD	804





- Results obtained with Phyton are in line with the MS Excel[™] ones computed in a previous analysis
- Phyton is an **efficient** and **ready-to-use** programming language
- The broad range of libraries permits to cover every aspect of data processing and graphical analysis
- Phyton permits to manage huge quantity of data with negligible computational times
- A large community and a thorough online documentation can easily **support** programmers





THANK YOU FOR YOUR KIND ATTENTION

School of Industrial and Information Engineering

PhD XXXVIIIth cycle — Materials Engineering