Laboratório Nacional de Ciência
e Tecnologia do Bioetanol

TUTORIAL

CRAFS

O CTBE integra o Centro Nacional de Pesquisa em Energia e Materiais (CNPEM) mantido pelo MCT
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Ministério da
Ciência e Tecnologia
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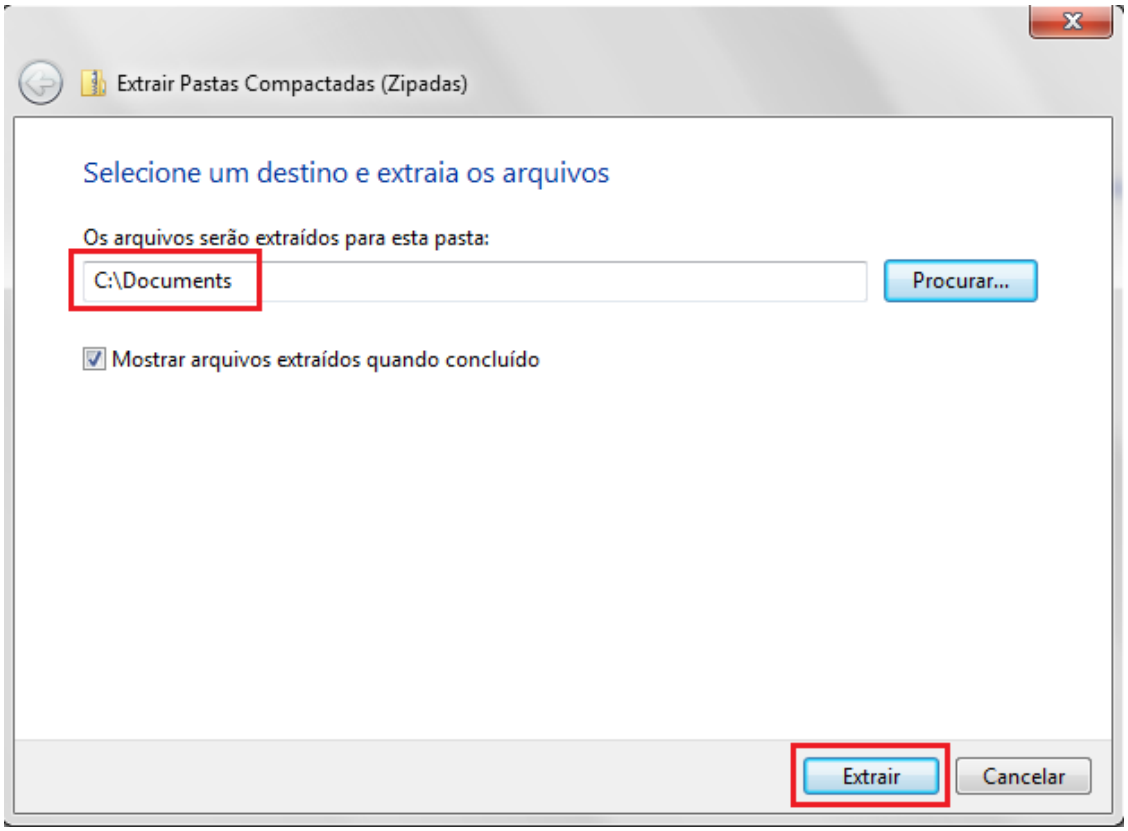
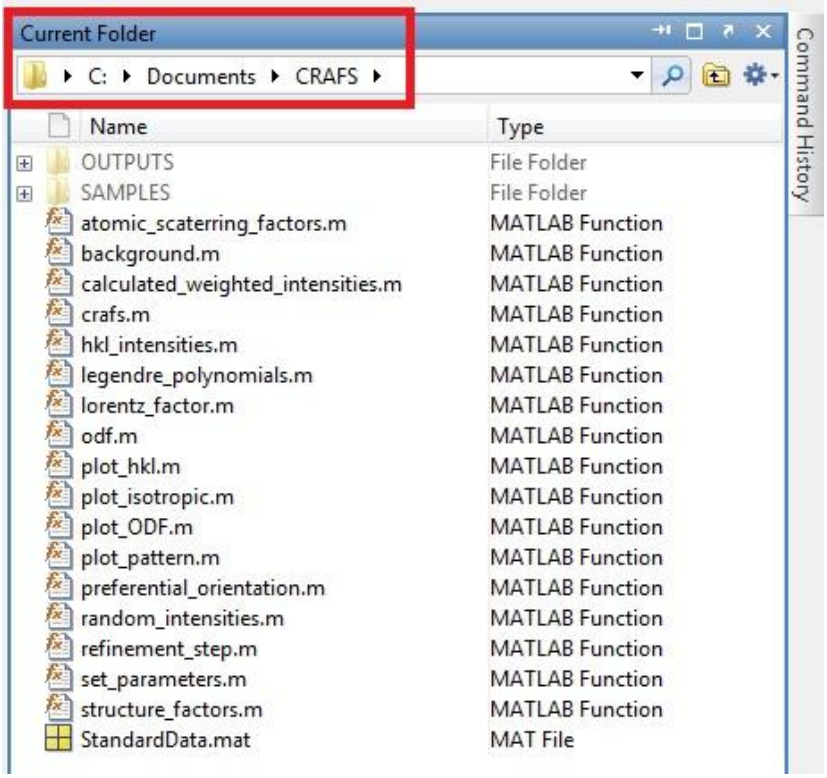
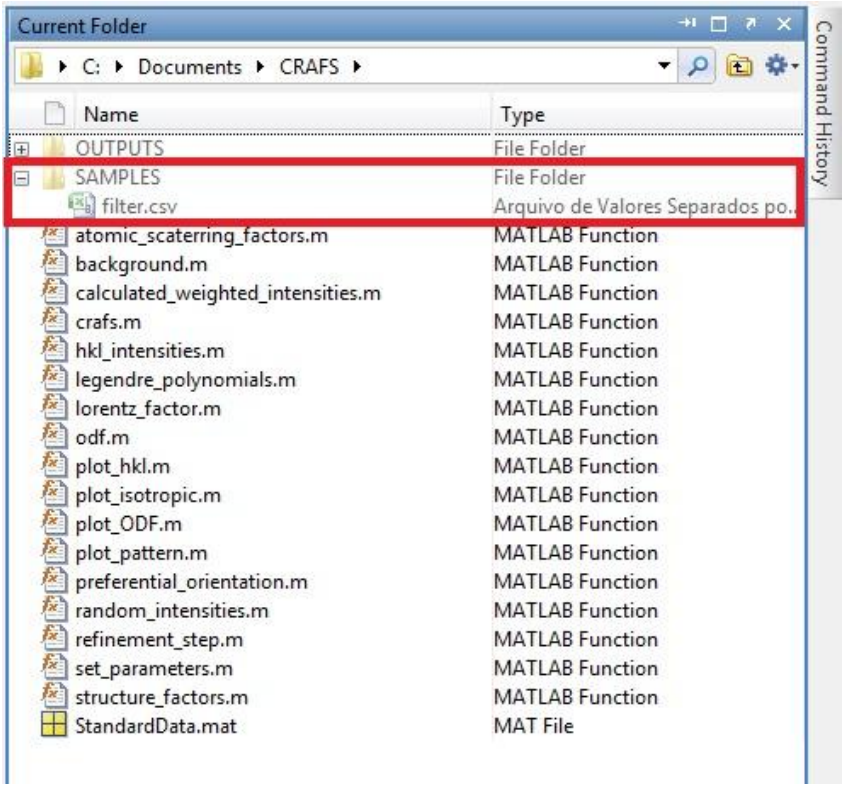
Extract the file CRAFS.zip to the folder Documents.



Open MATLAB and select the folder CRAFS as Current Folder



The file "*filename.csv*" to be analyzed must be in the folder SAMPLES



The command to analyze the pattern in "*filename.csv*" is

```
>>crafs('filename',Xinput)
```

Xinput is the input list of 33 model parameters separated by commas. If a parameter x in Xinput is x = 99, the algorithm understands that x is a free fitting coefficient that is going to be refined. If x ≠ 99, the algorithm understands that x is fixed and is going to be kept equal to the input number. The parameters must be given in the following order:

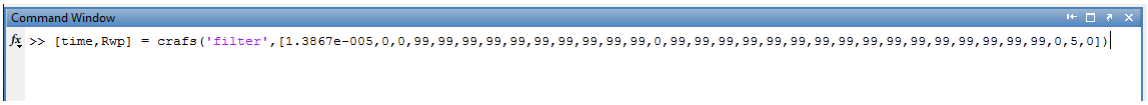
```
[cagl0,cagl1,cagl2,a,b,c,gamma,L200,LDiag,LDelta,L004,p200,pDiag,pDelta,p004,K,A0
,A1,A2,A3,A4,A5,A6,A7,A8,A9,C02,C04,C06,C08,muf,Gammaf,Af]
```

The coefficients $cagl_0$, $cagl_1$, $cagl_2$ are calibrations (not refinable) that describe instrumental broadening. The parameter $cagl_0$ must be positive.

To analyze the filter paper from the example enter the following command in the 'Command Window':

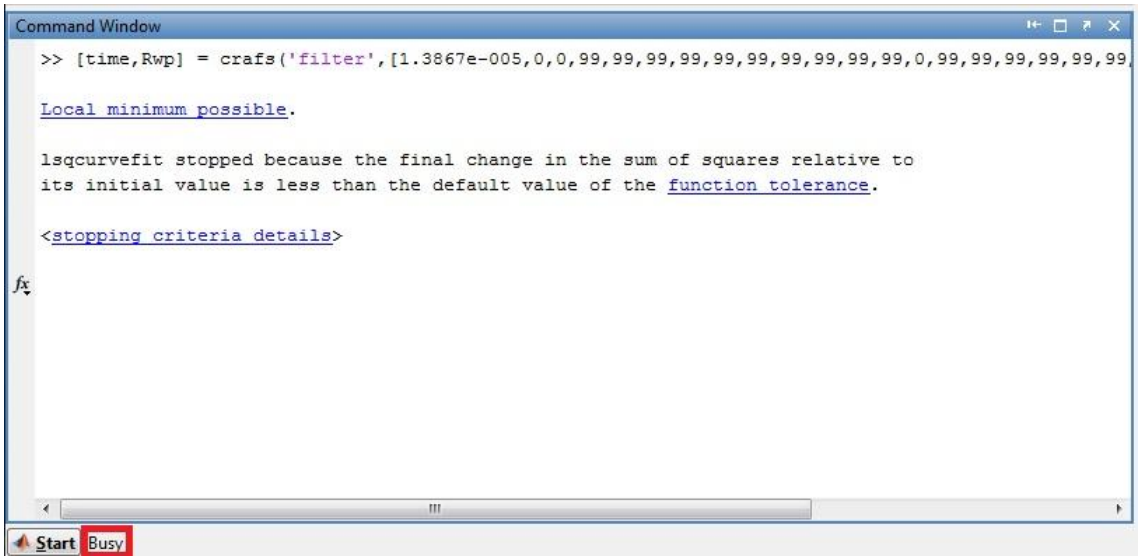
```
>>[time,Rwp] = crafs('filter',[1.3867e-005,0,0,99,99,99,99,99,99,
99,99,99,99,0,99,99,99,99,99,99,99,99,99,99,99,99,99,99,99,99,0,5,0])
```

'time' and 'Rwp' in brackets returns the runtime of analysis and the residue.

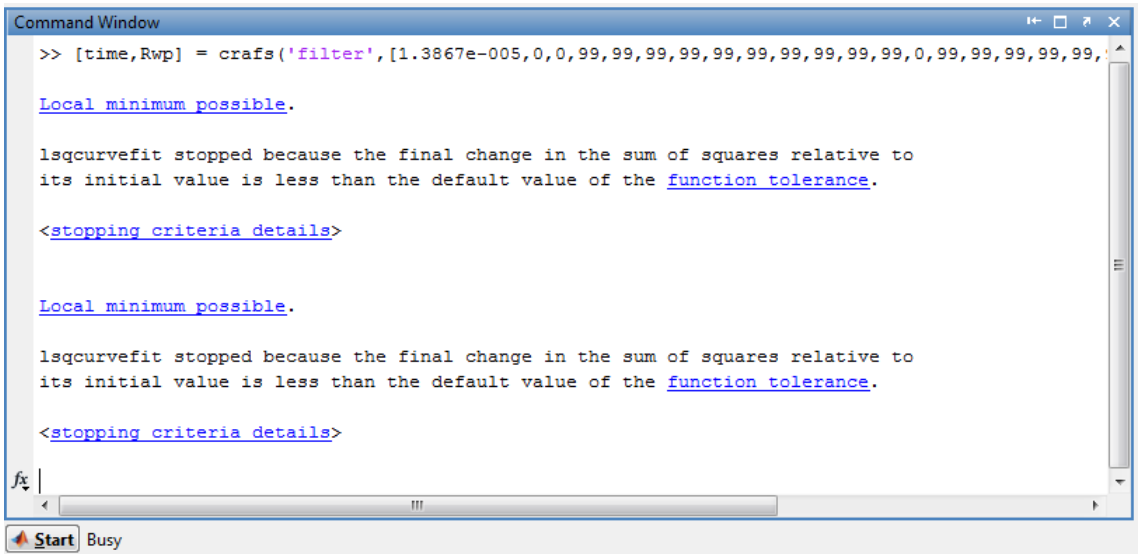


The analysis will be done in three steps. At the end of each step MATLAB shows on screen a message indicating the end of the refinement.

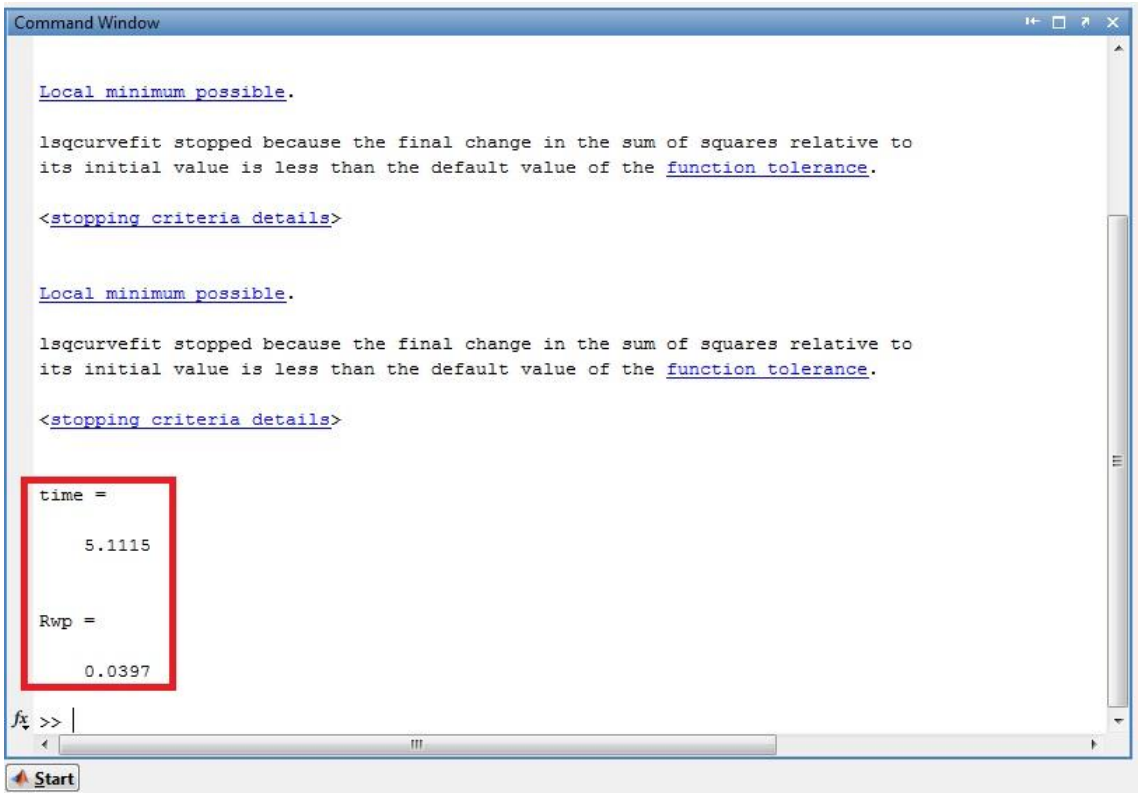
During the runtime of the program MATLAB will appear as 'Busy'.



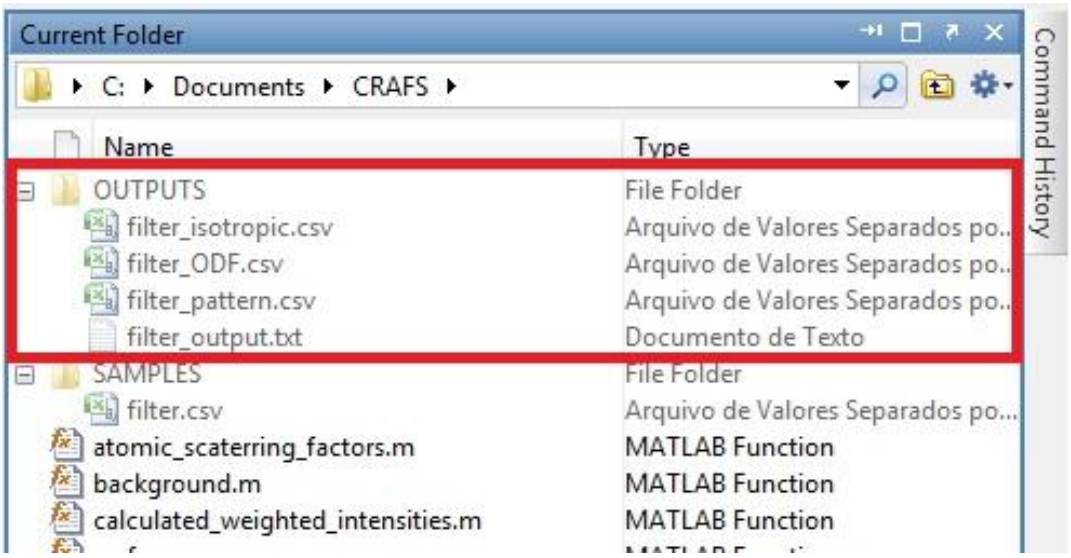
End of the second step:



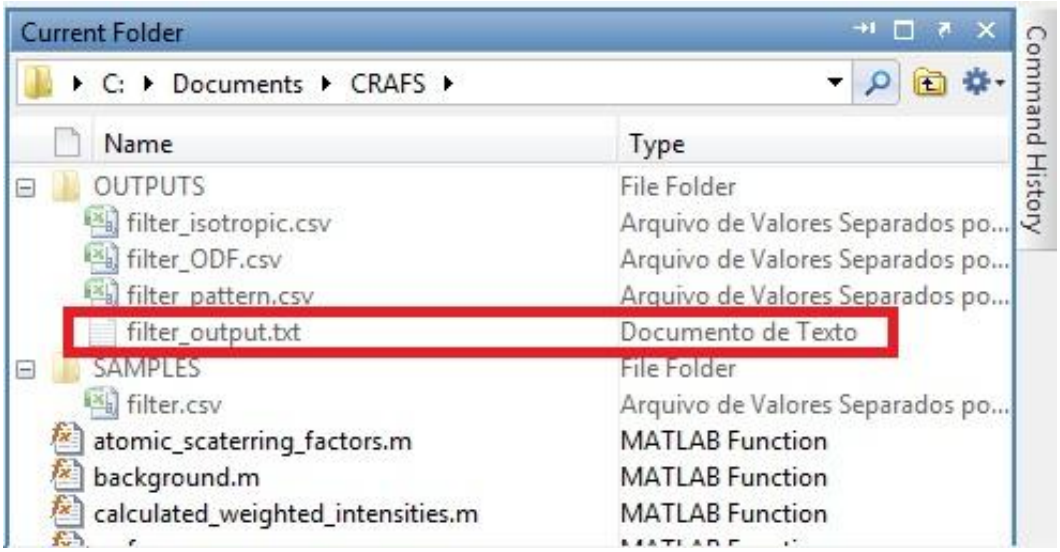
End of the third step. The program returns the values of time and Rwp:



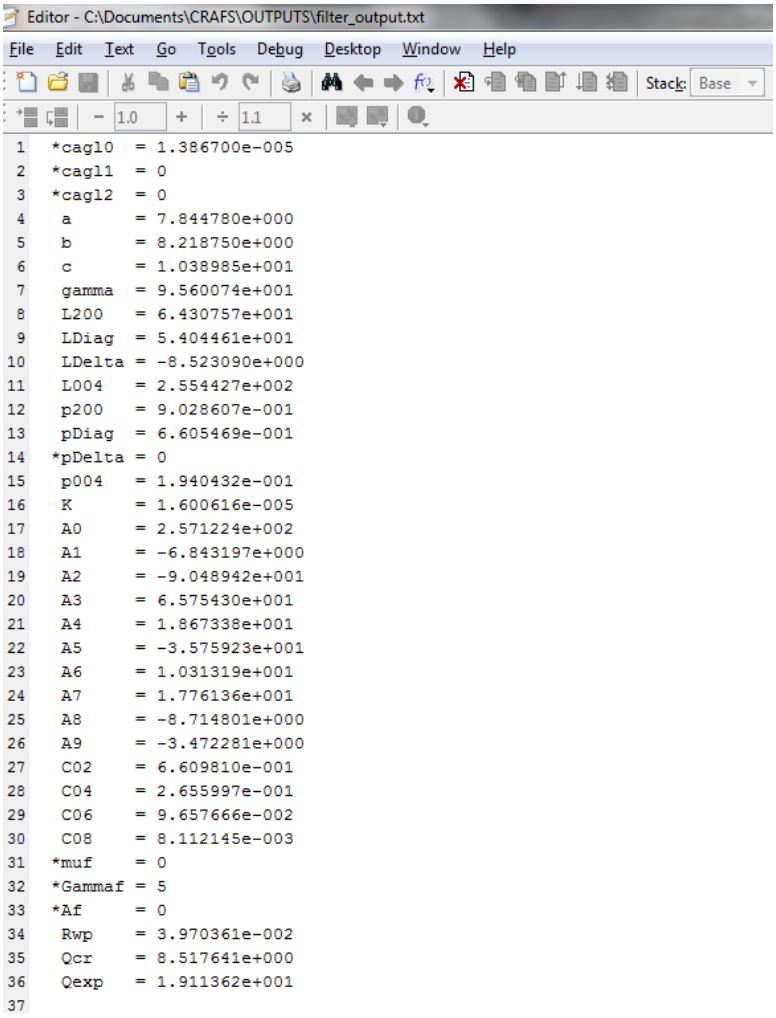
The output files will be saved in the folder OUTPUTS



The output coefficients are saved in the folder OUTPUTS with the name filename_output.txt.



The parameters preceded by "*" indicate that they were kept fixed during the refinement.



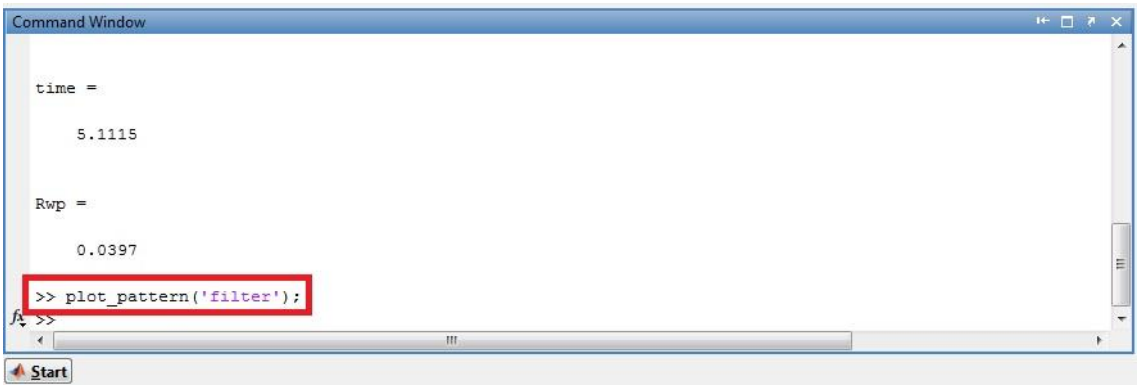
Plotting Graphs

The command to plot the two-dimensional diffraction patterns is:

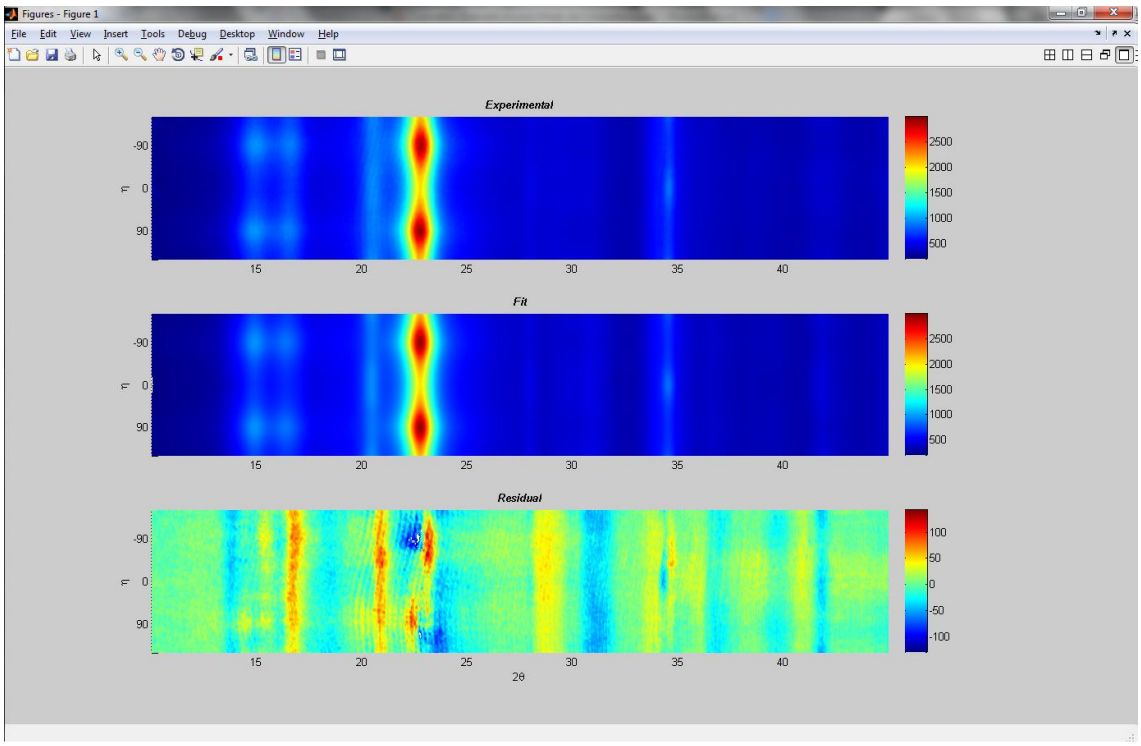
>>plot_pattern('filename');

To plot the the two-dimensional diffraction patterns for the file "filter.csv" enter the command in "Command Window":

>>plot_pattern('filter');



MATLAB creates a figure with the experimental pattern at the top, followed by the calculated pattern and residual.



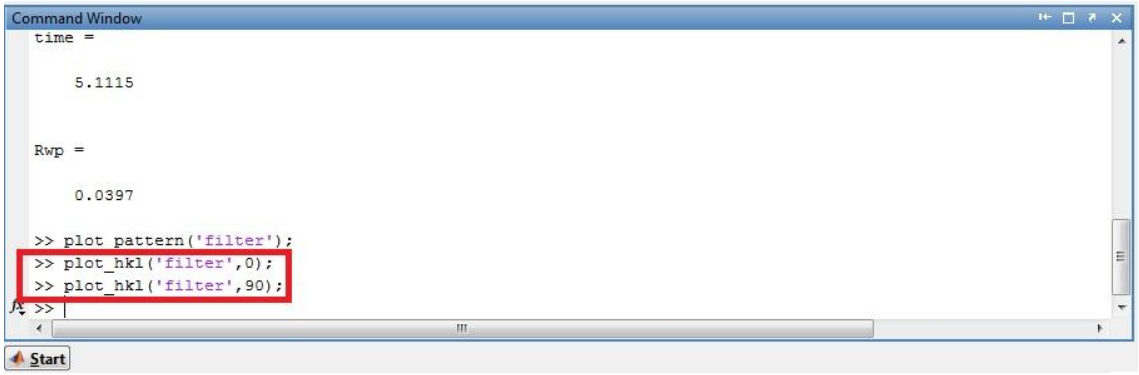
The command to plot the diffractogram for a specific angle eta is:

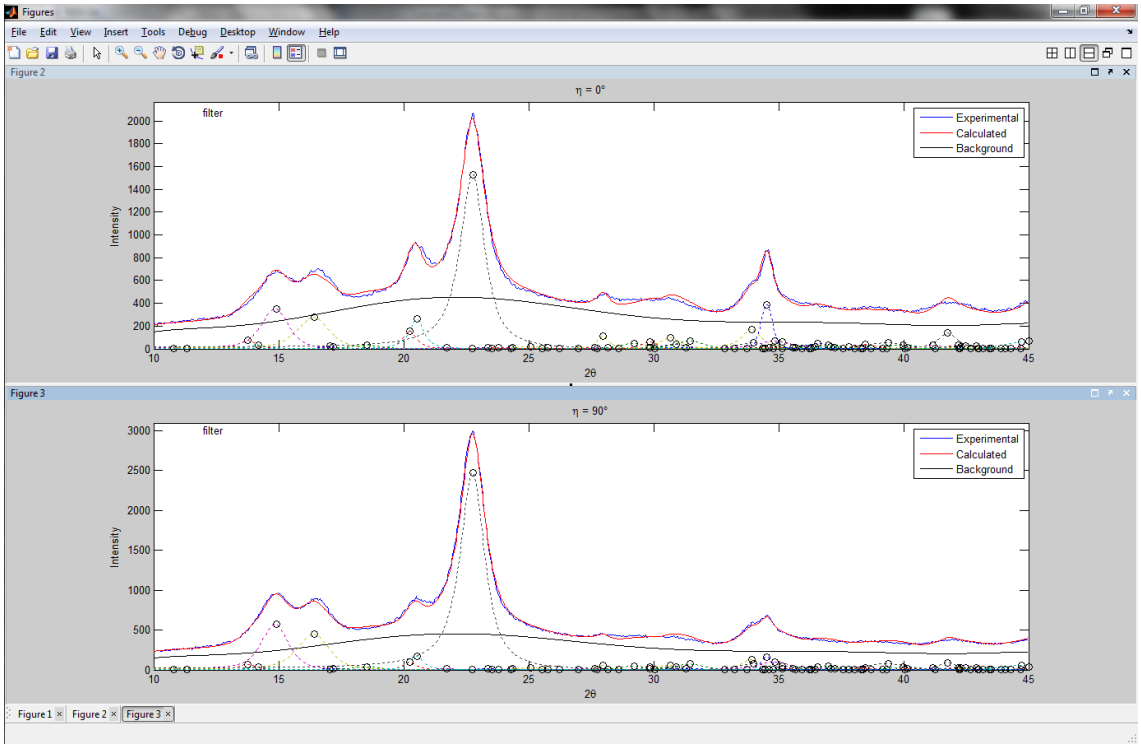
>>plot_hkl('filename',eta_angle);

In the example we plot the diffractograms for eta 0 and 90, respectively.

>>plot_hkl('filter',0);

>>plot_hkl('filter',90);



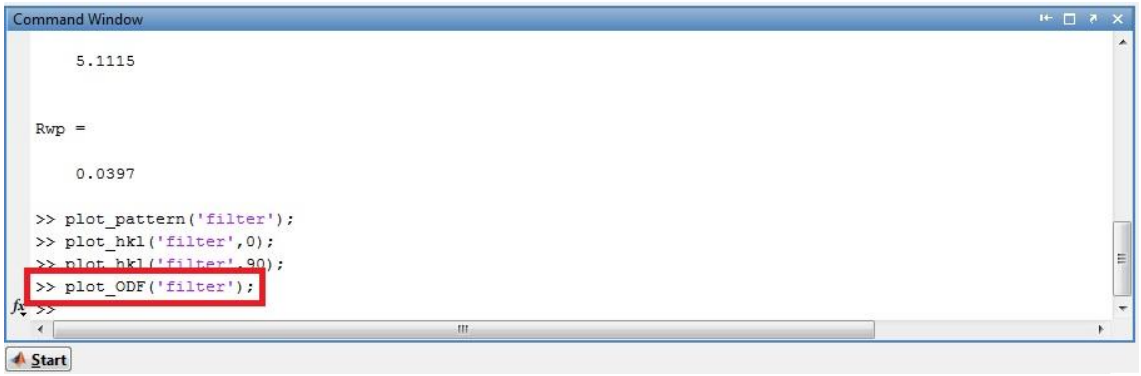


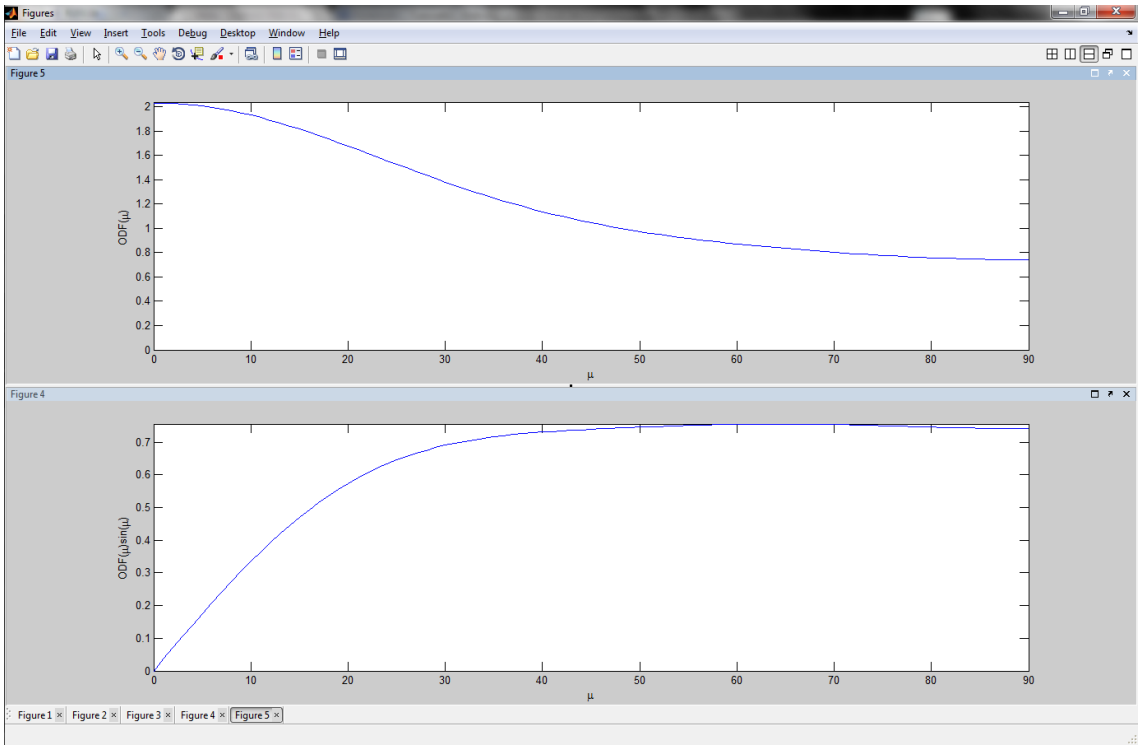
The command to plot the ODF and ODFsin(μ) is:

>>plot_ODF('filename')

To plot the ODF and ODFsin(μ) for the filter in the example, enter the command:

>>plot_ODF('filter')



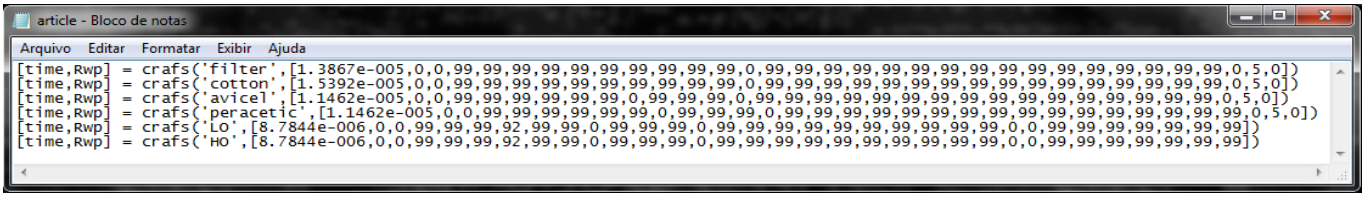


Multiple Refinements

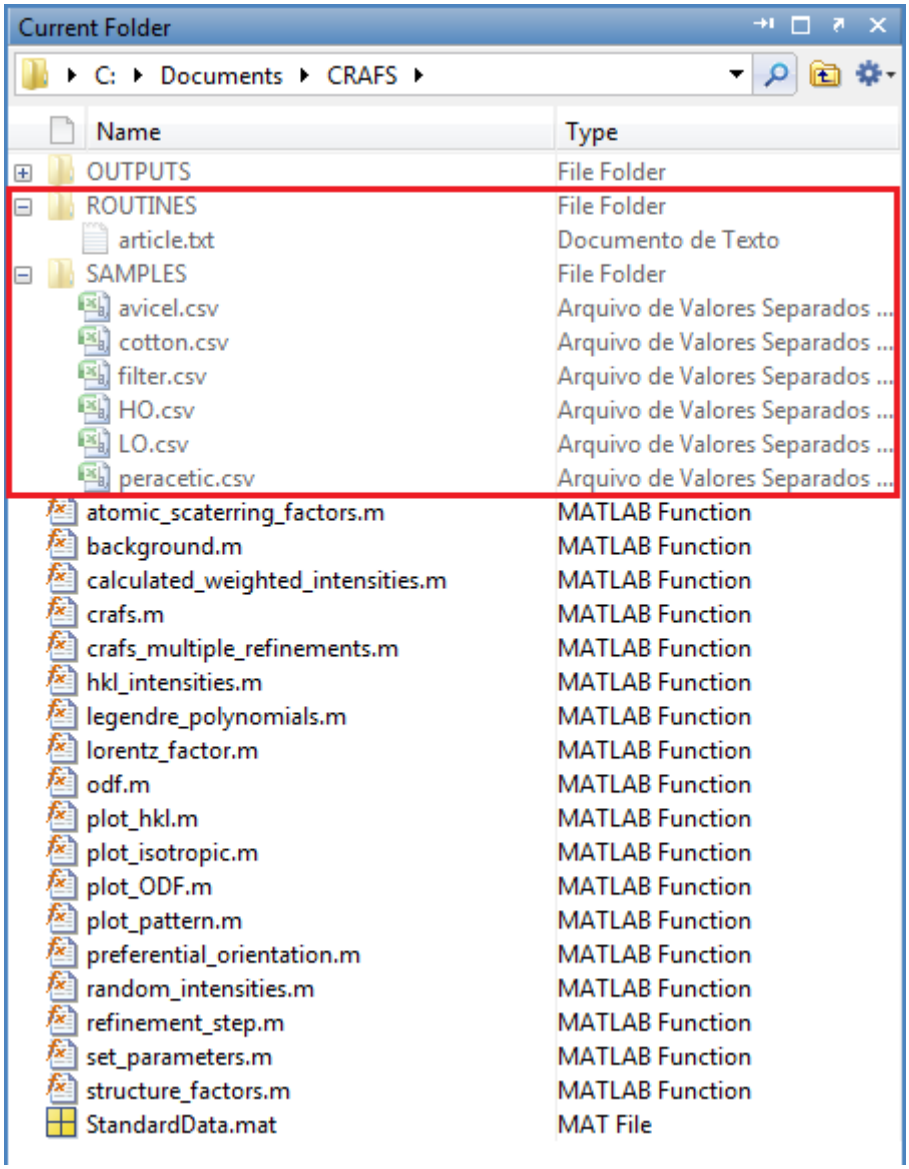
To make multiple refinements first open notepad and create a txt file.

Type the full command line of all the refinements you want to do, each line corresponds to a refinement.

As an example, let's run the refinement of the six samples used in the article.



The txt file with the commands of refinement must be saved in the folder ROUTINES. In the example let's use the name 'article.txt'. It is important to remember that the csv files with the experimental data must be in the folder SAMPLES.



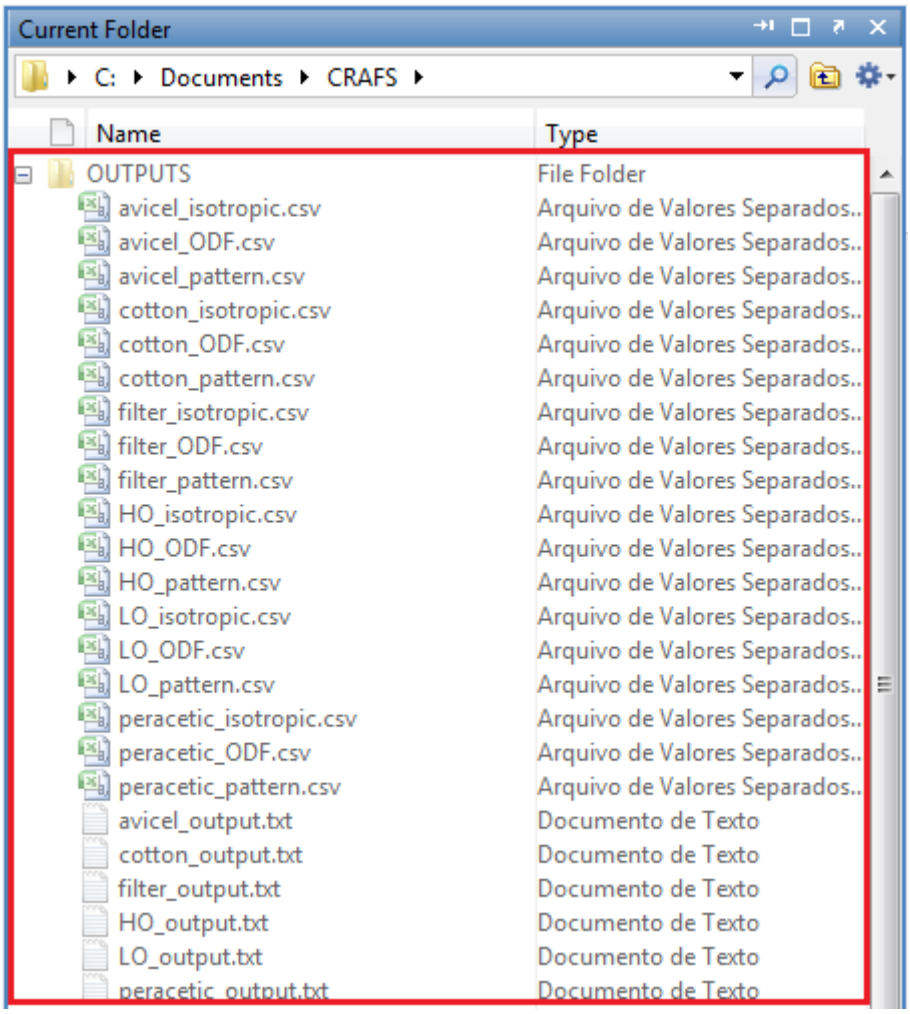
The command to perform the multiple refinements is:

>> crafs_multiple_refinements('routine_name')

To perform the multiple refinements of the example, enter the command:

>> crafs_multiple_refinements('article')

MATLAB will perform the refinements in the order that they were written in txt file. The output files will be saved in the folder OUTPUTS.


Current Folder
C: ▸ Documents ▸ CRAFS ▸
Name
Type
OUTPUTS
File Folder
avicel_isotropic.csv
avicel_ODF.csv
avicel_pattern.csv
cotton_isotropic.csv
cotton_ODF.csv
cotton_pattern.csv
filter_isotropic.csv
filter_ODF.csv
filter_pattern.csv
HO_isotropic.csv
HO_ODF.csv
HO_pattern.csv
LO_isotropic.csv
LO_ODF.csv
LO_pattern.csv
peracetic_isotropic.csv
peracetic_ODF.csv
peracetic_pattern.csv
Arquivo de Valores Separados..
avicel_output.txt
cotton_output.txt
filter_output.txt
HO_output.txt
LO_output.txt
peracetic_output.txt
Documento de Texto