

# TUTORIAL

## CRAFS

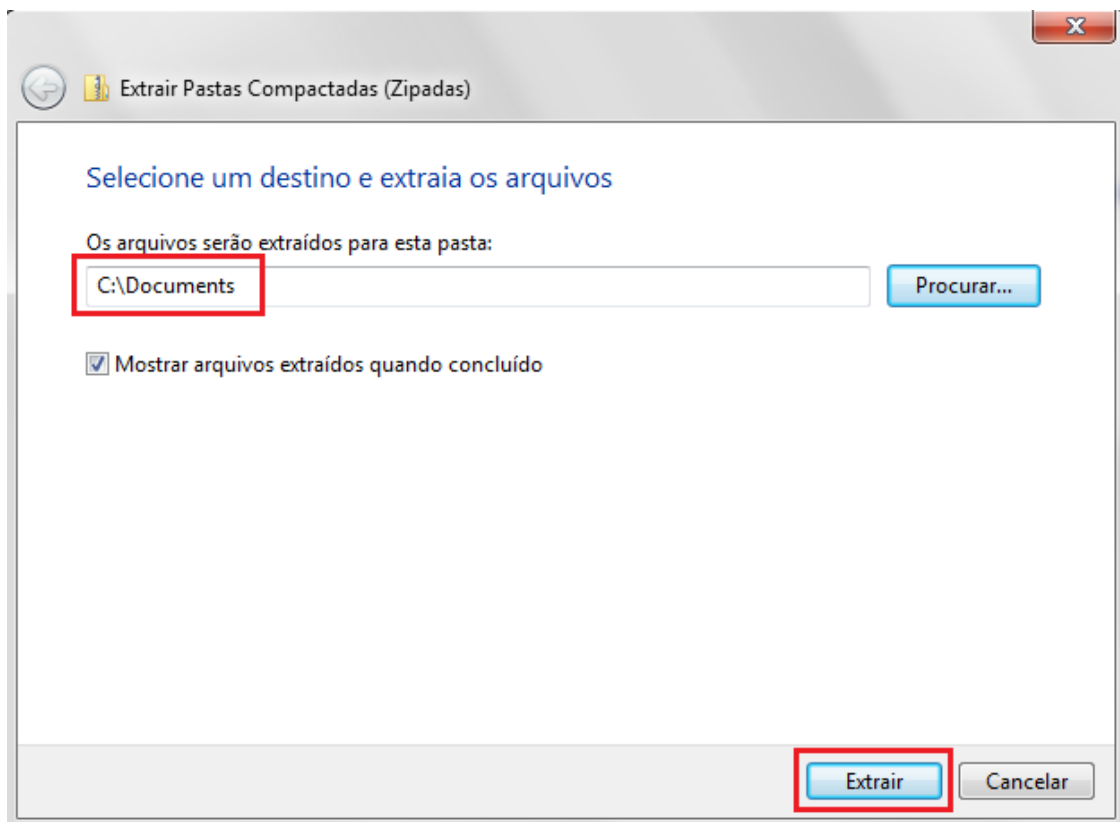
O CTBE integra o Centro Nacional de Pesquisa em Energia e Materiais (CNPEM) mantido pelo MCT

**Campus:** Rua Giuseppe Máximo Scolfaro, 10.000 - Pólo II de Alta Tecnologia - Campinas - SP

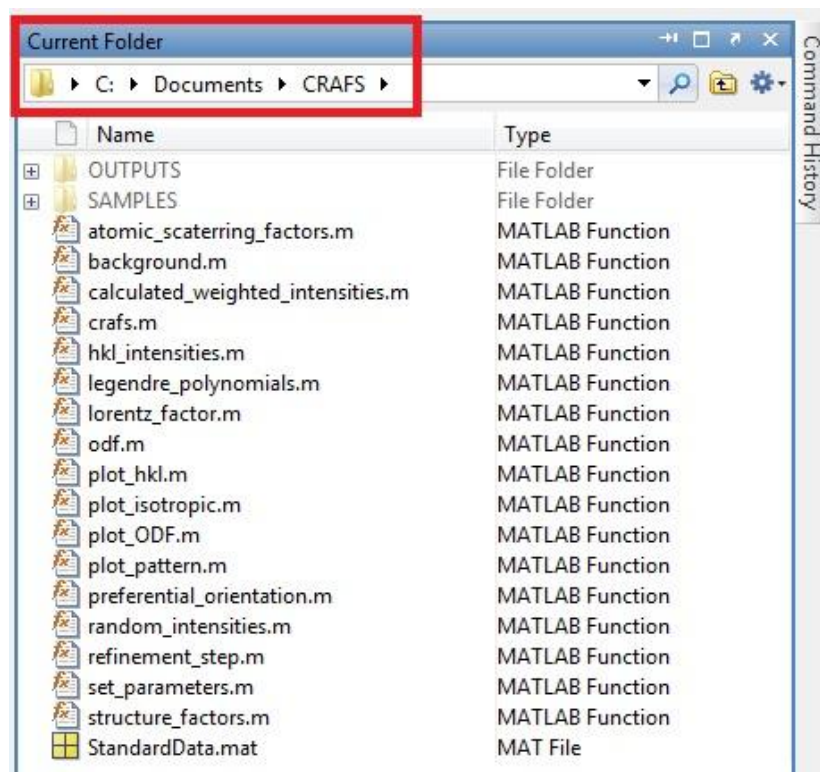
**Correspondência:** Caixa Postal 6170 - CEP: 13083-970 - Campinas - SP

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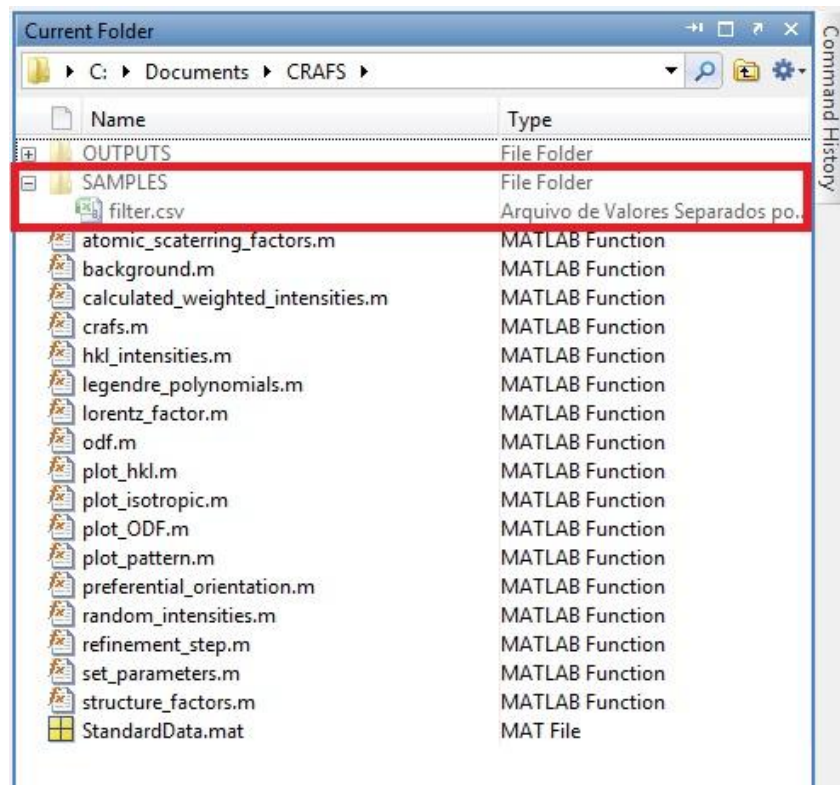
Extract the file CRAFS.zip to the folder Documents.



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  $x \neq 99$ , 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:

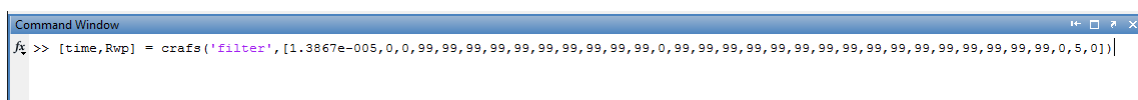
```
[cagl0,cagl1,cagl2,a,b,c,gamma,L200,LDiag,LDelta,L004,p200,pDiag,pDelta,p004,K,A0,A1,A2,A3,A4,A5,A6,A7,A8,A9,C02,C04,C06,C08,muf,Gammaf,Af]
```

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

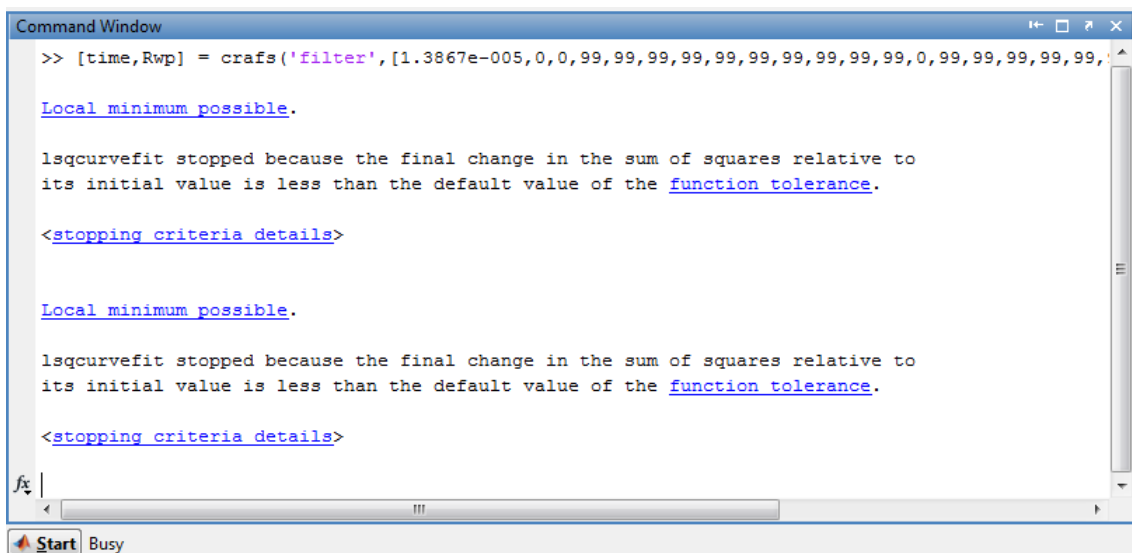
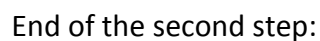
To analyze the filter paper from the example enter the following command in the 'Command Window':

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

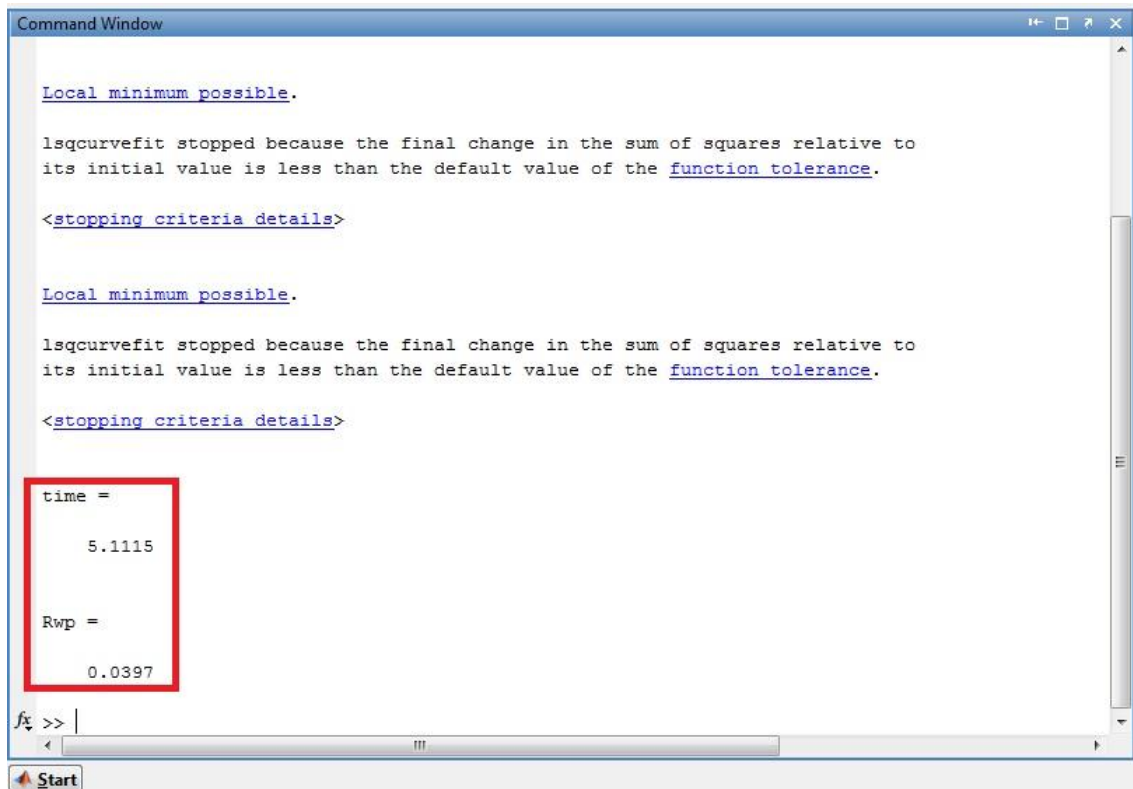
'time' and 'Rwp' in brackets returns the runtime of analysis and the residue.



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



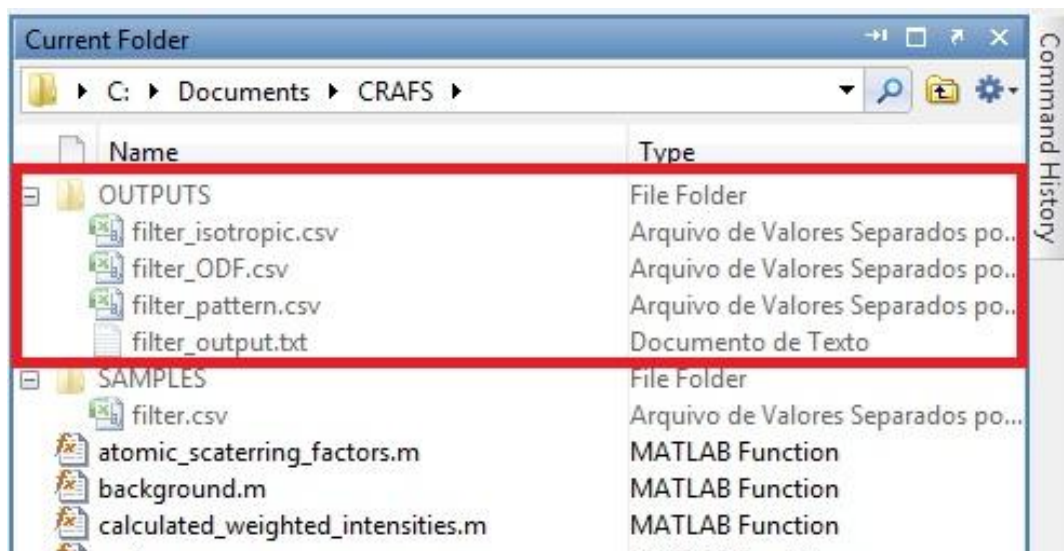
End of the third step. The program returns the values of time and Rwp:



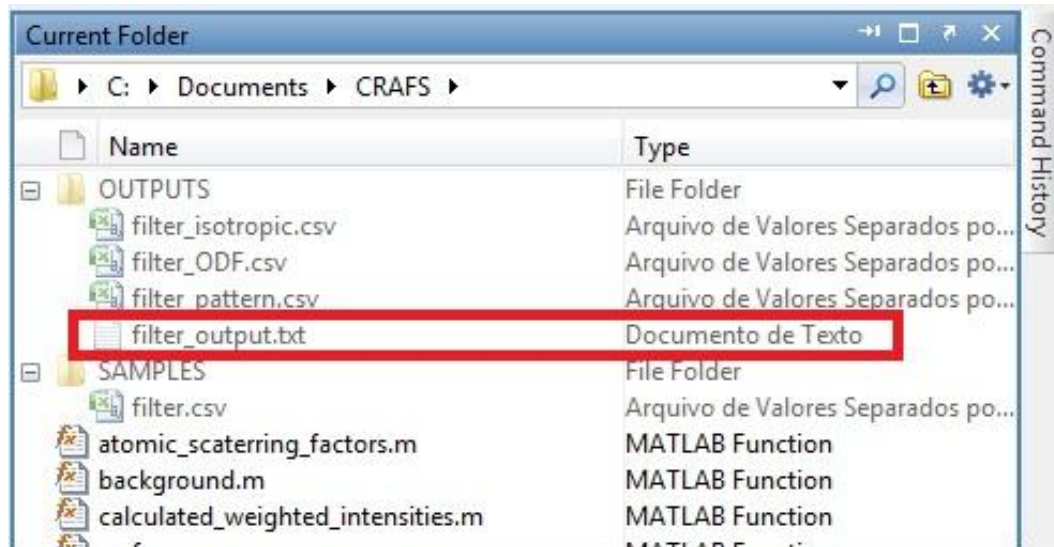
The screenshot shows the MATLAB Command Window. It displays two identical blocks of text, each preceded by the underlined phrase "Local minimum possible.". Each block states: "lsqcurvefit stopped because the final change in the sum of squares relative to its initial value is less than the default value of the function tolerance." followed by "<stopping criteria details>". Below this, the output variables are shown: "time =" followed by the value "5.1115", and "Rwp =" followed by the value "0.0397". These two lines are enclosed in a red rectangular box. At the bottom, the prompt "fx >>|" is visible.

```
Local minimum possible.  
  
lsqcurvefit stopped because the final change in the sum of squares relative to  
its initial value is less than the default value of the function tolerance.  
  
<stopping criteria details>  
  
Local minimum possible.  
  
lsqcurvefit stopped because the final change in the sum of squares relative to  
its initial value is less than the default value of the function tolerance.  
  
<stopping criteria details>  
  
time =  
  
    5.1115  
  
Rwp =  
  
    0.0397  
  
fx >>|
```

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.

The screenshot shows a text editor window titled 'Editor - C:\Documents\CRAFS\OUTPUTS\filter\_output.txt'. The file contains a list of parameters and their values, with some parameters marked with an asterisk to indicate they were fixed during refinement. The parameters are listed as follows:

```
1 *cagl0 = 1.386700e-005
2 *cagl1 = 0
3 *cagl2 = 0
4 a = 7.844780e+000
5 b = 8.218750e+000
6 c = 1.038985e+001
7 gamma = 9.560074e+001
8 L200 = 6.430757e+001
9 LDiag = 5.404461e+001
10 LDelta = -8.523090e+000
11 L004 = 2.554427e+002
12 p200 = 9.028607e-001
13 pDiag = 6.605469e-001
14 *pDelta = 0
15 p004 = 1.940432e-001
16 K = 1.600616e-005
17 A0 = 2.571224e+002
18 A1 = -6.843197e+000
19 A2 = -9.048942e+001
20 A3 = 6.575430e+001
21 A4 = 1.867338e+001
22 A5 = -3.575923e+001
23 A6 = 1.031319e+001
24 A7 = 1.776136e+001
25 A8 = -8.714801e+000
26 A9 = -3.472281e+000
27 C02 = 6.609810e-001
28 C04 = 2.655997e-001
29 C06 = 9.657666e-002
30 C08 = 8.112145e-003
31 *muf = 0
32 *Gammaf = 5
33 *Af = 0
34 Rwp = 3.970361e-002
35 Qcr = 8.517641e+000
36 Qexp = 1.911362e+001
37
```

## Plotting Graphs

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

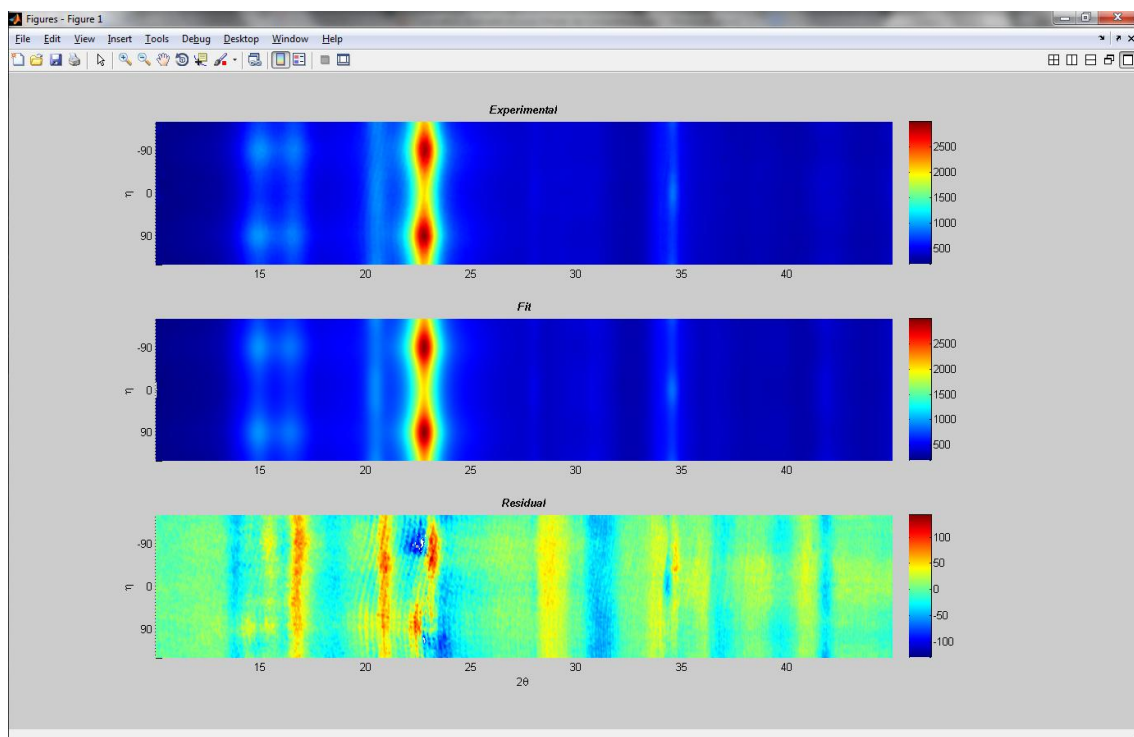
```
>>plot_pattern('filename');
```

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.



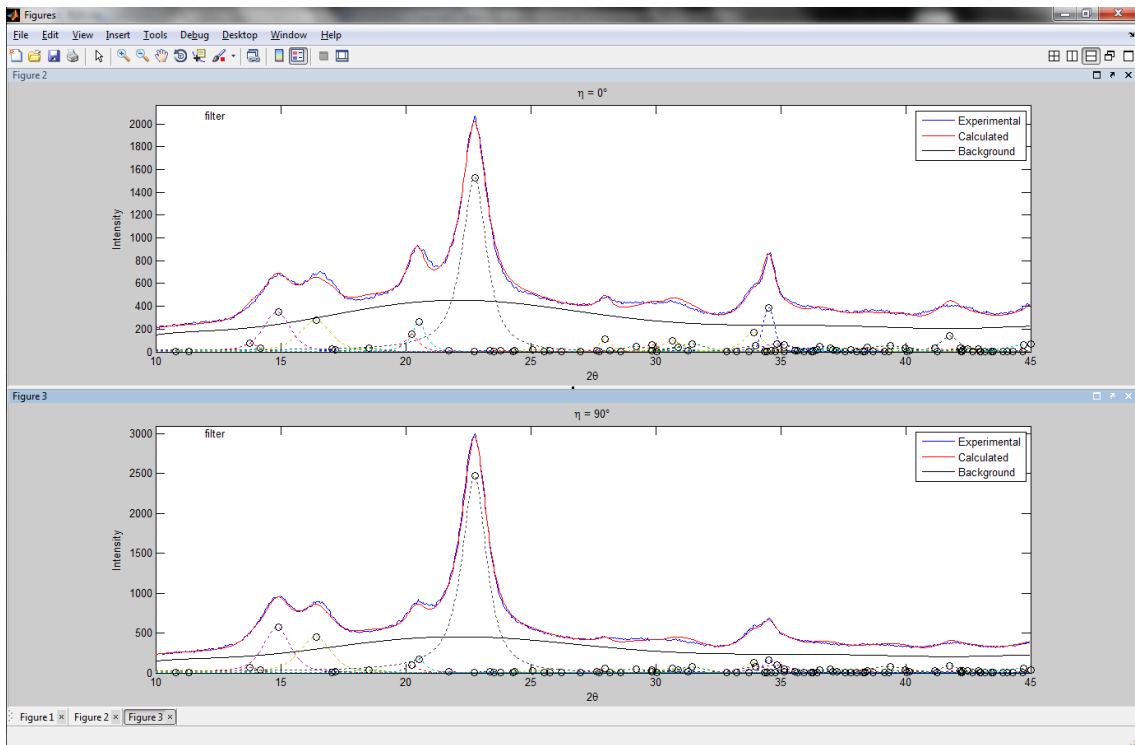
The command to plot the diffractogram for a specific angle eta is:

```
>>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( $\mu$ ) is:

```
>>plot_ODF('filename')
```

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

```
>>plot_ODF('filter')
```



```

Command Window

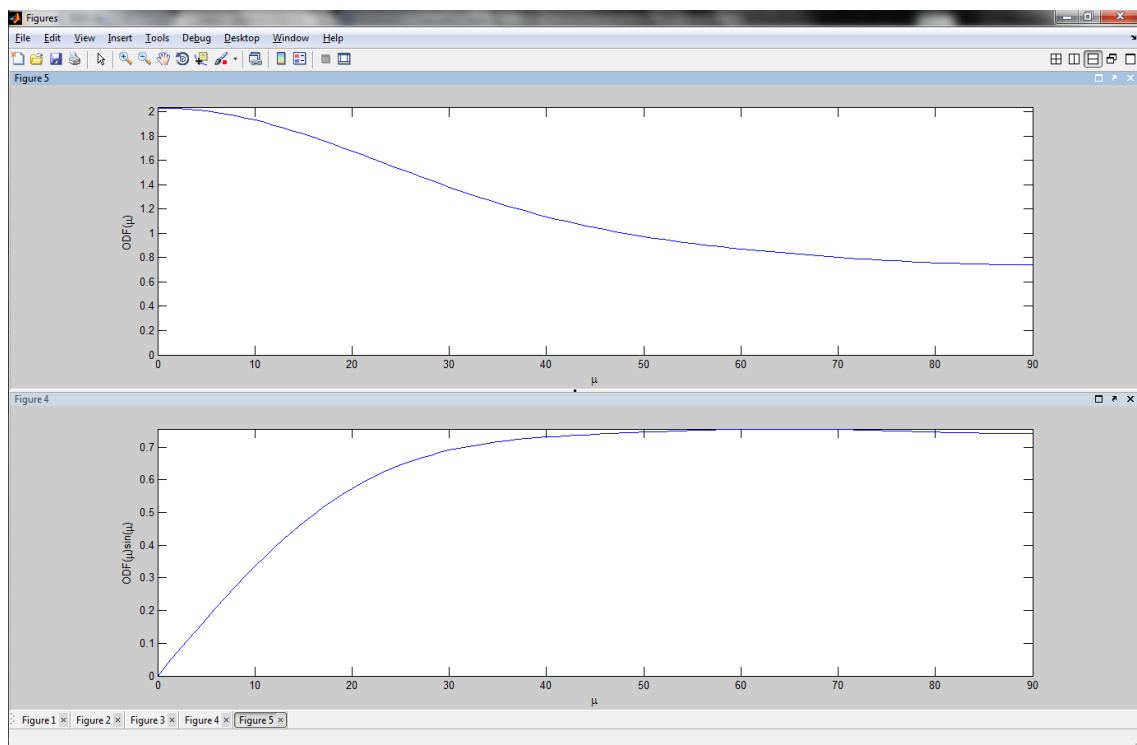
5.1115

Rwp =

0.0397

>> plot_pattern('filter');
>> plot_hkl('filter',0);
>> plot_hkl('filter',90);
>> 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.

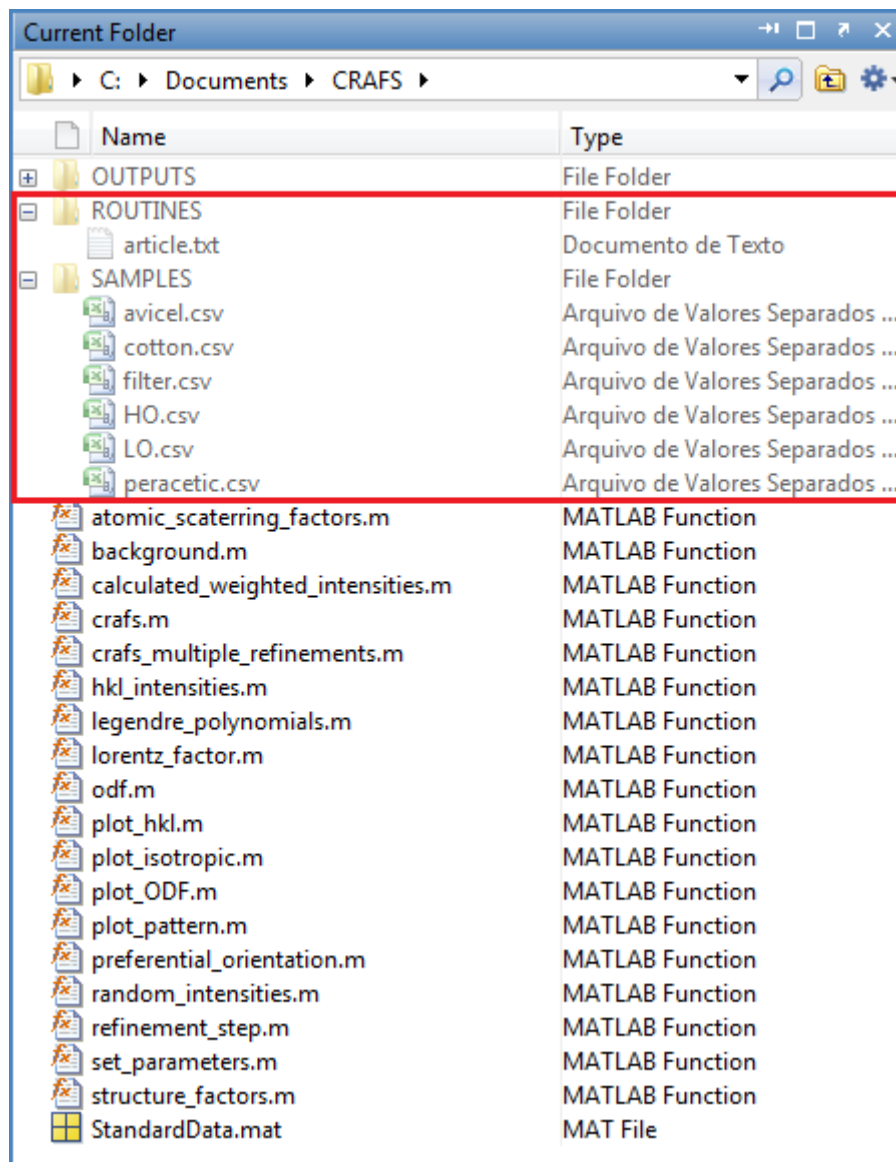
As an example, let's run the refinement of the six samples used in the article.

```

article - Bloco de notas
Arquivo Editar Formatar Exibir Ajuda
[time,Rwp] = crafs('filter',[1.3867e-005,0,0,99,99,99,99,99,99,99,99,0,99,99,99,99,99,99,99,99,99,99,0,5,0])
[time,Rwp] = crafs('cotton',[1.5392e-005,0,0,99,99,99,99,99,99,99,99,0,99,99,99,99,99,99,99,99,99,99,0,5,0])
[time,Rwp] = crafs('avicel',[1.1462e-005,0,0,99,99,99,99,99,99,99,99,0,99,99,99,99,99,99,99,99,99,99,0,5,0])
[time,Rwp] = crafs('peracetic',[1.1462e-005,0,0,99,99,99,99,99,99,99,99,0,99,99,99,99,99,99,99,99,99,99,0,5,0])
[time,Rwp] = crafs('LO',[8.7844e-006,0,0,99,99,99,92,99,99,0,99,99,99,0,99,99,99,99,99,99,99,99,0,0,99,99,99,99,99])
[time,Rwp] = crafs('HO',[8.7844e-006,0,0,99,99,99,92,99,99,0,99,99,99,0,99,99,99,99,99,99,99,99,0,0,99,99,99,99,99])

```

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.

