Application Report – Origin

Methods of data managing towards surface characterization and quality control of surface-preconditioning

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Wear-prevention and one of its its prerequisites, namely surface exploring and surface conditioning of every gliding surface-pairing is a very important discipline to ensure the proper performance of countless mechanical equipment and thereby to avoid costs which otherwise would arise not only for spare parts, but also for compensation of down-times.
In fact wear causes annual cost of several billions of Euros and hence has remarkable impact on well-developed national economies. Hence, it may be well understood, that tremendous efforts are taken towards trouble-and wear-free, long lasting operations of ball-bearings and slide-bearings and every gliding pairing what so ever.

One of the less-prominent applications of this most general interest is found in printing industry, where the printing ink has to fulfills not only those requirements, which aim at rendering pictures and readable texts by color, contrast, hue and chroma. Additionally and by no means for secondary rank, the ink serves also as the lubricant for mechanically loaded printing forms.
Intimate knowledge of the surface properties involved are indispensable to ensure the proper function of inks and their interaction with the surfaces of the printing forms and other parts of the machinery.

Another application of surface characterization is relied to the printing industry as well. This means, that the microscopic surface-topologies of the various printing substrates like plastic films, aluminum-foils and of a broad variety of paper-webs is a focus of interest as well. Paper webs, per example, even super-calendared-ones, are relatively rough and imbibe a certain volume of fluid inks, which thus will fail to stay stick on the outermost surface and hence cannot contribute to gloss and surface-grade-up and the donation of a noble aspect. On the other hand, a well-balanced surface-roughness is certainly needed for successfully anchoring the inks on the printing substrate to ensure mechanical strength an durability.

With these general remarks we would like to provoke some interest to use ORIGIN as a software-tool, which makes available powerful methods of data managing towards surface characterization and quality-control of surface-preconditioning.

The power of ORIGIN is very well suited to be combined with well established commercially available surface-probing devices, which deliver an AD-converted signal which is generated by a micro-sapphire-sensor tip tracking across the surface profile. These profile-reading devices may trigger some remembrances to the signal-processing of record players, but they are far more sensitive with their profiling power and in fact allow accurate insight into the surface profile close to 10 nm. If reliable data-generation down to that level is backed by ORIGIN´s sophistication of data-managing and data-interpretation, some non-commercial and outstanding information about surface-profiles and figures of merit derived thereof may be the outcome.

So, starting towards this goal, Origin comes into the play with the import of an ASCII-file. This file has been generated by converting the analog, surface-replicating signal into a series of digital values, which represent the profile of the surface as long as signal aliasing has truly been avoided by choosing a sufficiently frequent sampling rate. For instance, if the tracking speed of the sensor tip is 500 µm /s and the surface-profile shall be sampled at every 1µm -increment of a total

tracking-length of 1 cm, the data vector, which is generated that way has a dimension of 10.000 and each component of this vector represents one "vertical" profile-value. The tracking-length may be extended to several centimeters and the tracking speed may be slowed down and the sampling rate may be enhanced, if the "horizontal" resolution is to be increased. Thus, vector dimensions far larger than 10.000 will be generated and fed into the worksheets of ORIGIN. Thus, ORIGIN deals with a demanding mass-data-handling and -conversion task.

1. Data-Import

Lets start with the import of a data-vector by selecting "import single ASCII " in the File-menu. Of course, if several data-reading-files are to be imported, this may be done by using "multiple ASCII" instead of. In every case it is good practice for the beginning to have the dialog-option activated. The dialog-window pops up and you should take care amongst other choices, that "start new columns" is selected as the valid "import mode". After having completed the import of a single file left-click on the B-column, than right-click and choose "properties" in the menu, which is coming up. Now You may feed in a descriptor into the comment-field. After "o.k.", right click again and select "set sampling interval" . Feeding in the sampling interval of the original data-generation and the physical unit of the sampling step is advisable to be prepared for an eventual Fourier-transformation you may want to perform.

After all that, which is completed within a few seconds, the screen should look like this:
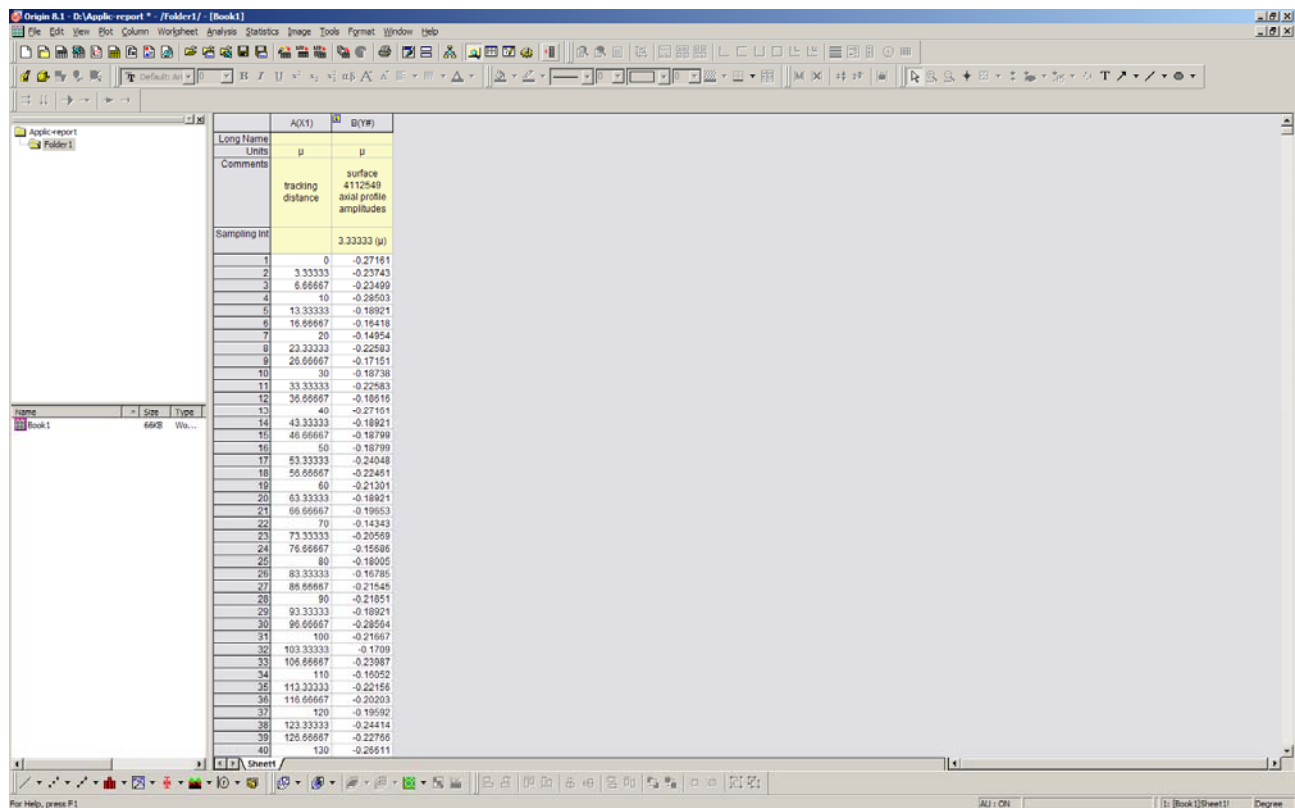
2. Plotting of the original data

Probably you are curious, what the surface profile is looking like. To get insight into these basics a plot of the data in worksheet 1 of book 1 is produced. Towards this, mark both columns of the sheet by left-clicking. Then, cross over to the plot-menu and select "line". A window with a crude plot is appearing, which after-wards may be refined by some editorial work.

Open the format-menu and select the sub-menu "layer" . Feed in the size of the plot as referred to

the page or absolute dimensions and then click on format again and select the "axes"-sub-menu. Set the style of the axes and the scales according to your will. You may find it useful to re-edit all the elements like axis titles and also the legend of the graph by clicking on the titles and selecting "properties". An auxiliary window pops up and offers all the choices to alter the texts and their format and so on. If You want to take influence on the style of the graph´s line-trace, click on "Format" again, proceed to "plot" and select trace-width and color.
The screen could now look like that:
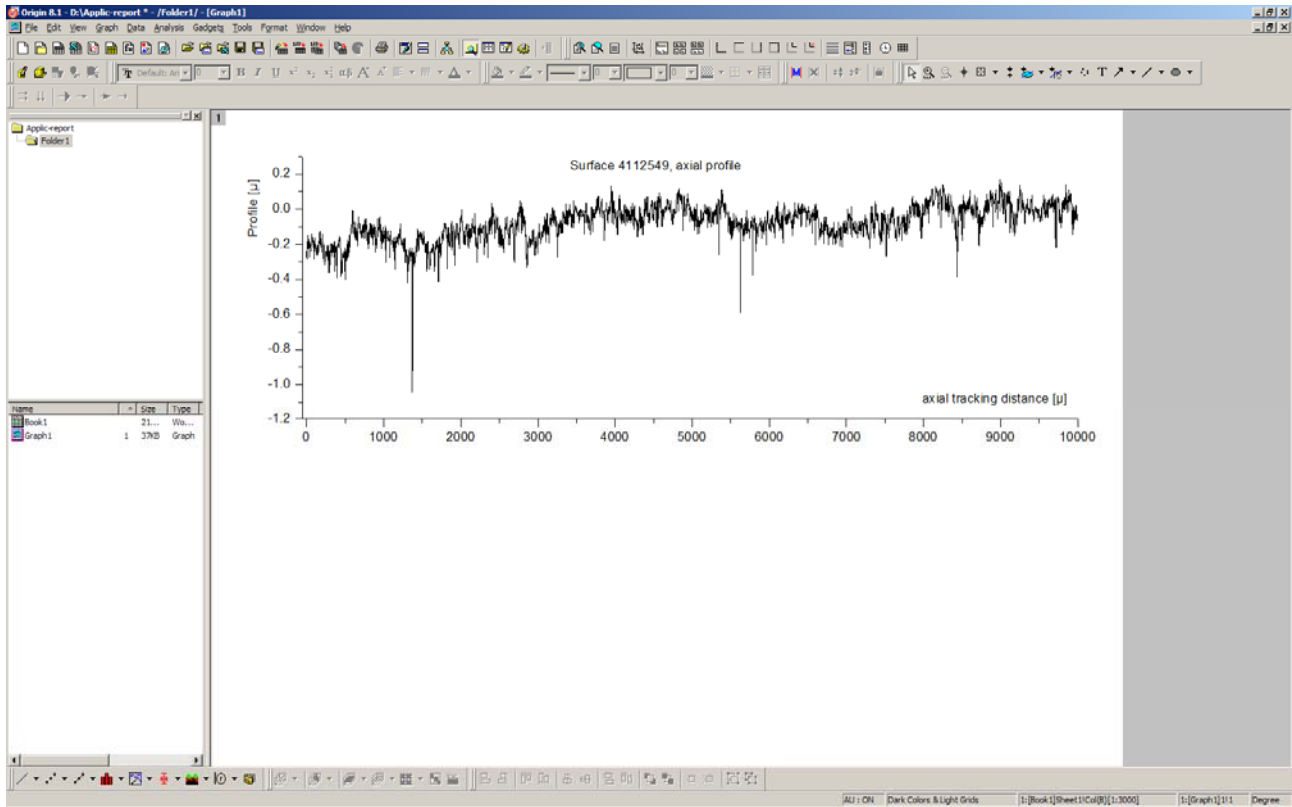
3. Data-Processing

In the first plot of the surface profile, which resulted from a probing of the surface specimen in an axial sense, you will probably discern some waviness of the surface as well as the roughness-component. With the aim of a closer specification of these both components of the total surface topology, it is certainly beneficial to separate both components from each other. This is best done by some sophistication of signal "processing", which is offered by ORIGIN in the menu "analysis" .

The data-series in the Y-column of the sheet is a vector in the so-called position space and may be linearly combined by a complete set of orthogonal functions in the canonically conjugate space of spatial frequencies. Such a complete and orthogonal set , per example, is the manifold of sine- and cosine- functions of all the spatial frequencies and hence, the data-vector may be transformed by Fourier-transformation in the spatial frequency-space and back again like it is done in the time- and frequency-domain by usual FFT. As a consequence, FFT-filtering, that means transformation into the frequency-domain, frequency clipping and back-transformation of the truncated vector into the position-space may be used to separate the HP-signal and the LP-signal in position-space.

While the new graph is the active window, look into the "analysis"-menu and change over to "signal processing" / "FFT-filters". Open dialog and check "auto-preview". Auto-preview is a very powerful

and encouraging tool for best control of what is going on in FFT-filtering after having set the various parameters of the transformation. The tool is enabled by having set the sampling interval in paragraph 1.

Select the filter-type, in this case High Pass, disable "keep DC Offset" and set the "Cutoff Frequency" to 2E-3. After a click somewhere into the window, you get a forecast of what you have effected. Then, having pressed o.k., the HP-Signal will be found in book 1 as additional columns and also in the graph as an additional trace. Now it may happen, that you are not really satisfied by the esthetics of the double-traced graph and you may wish to change that.

To do so, with the graph being still the active window, go to the menu "Format" and select "plot".

Two traces are listed as the content of layer 1. The filtered signal can be removed from the graph by deselecting it and clicking on the "apply"-button and after-wards on o.k. Right-click now into the graph and select "copy format" and "all". Having done so, go to the menu "Graph" and proceed with the sequence "new Layer" and "Bottom-X Left-Y. Now make active the new layer in the window by clicking on the layer 2 in the upper-left corner of the window. Right click somewhere in the layer 2 and choose "paste format".

After this little editorial work, You find a void layer in the window, which is to be filled with the filtered signal-graph. Towards this purpose, layer 2 should be still the active one. Activate the menu "Graph" and the command "add plot to layer" / "Line". A new dialog-window pops up and you should click on "col" to see, what data-columns You have available so far to be selected for plotting in layer 2. Choose "filtered X" as X-Axis (Abscissa) and "filtered Y" as ordinate. Then press "Add", "Apply" and "O.K.". Finally, re-editing the Y-axis-title (right-click and "properties") and the axis-scaling (menu "Format") , leads You to a new aspect of your graph:
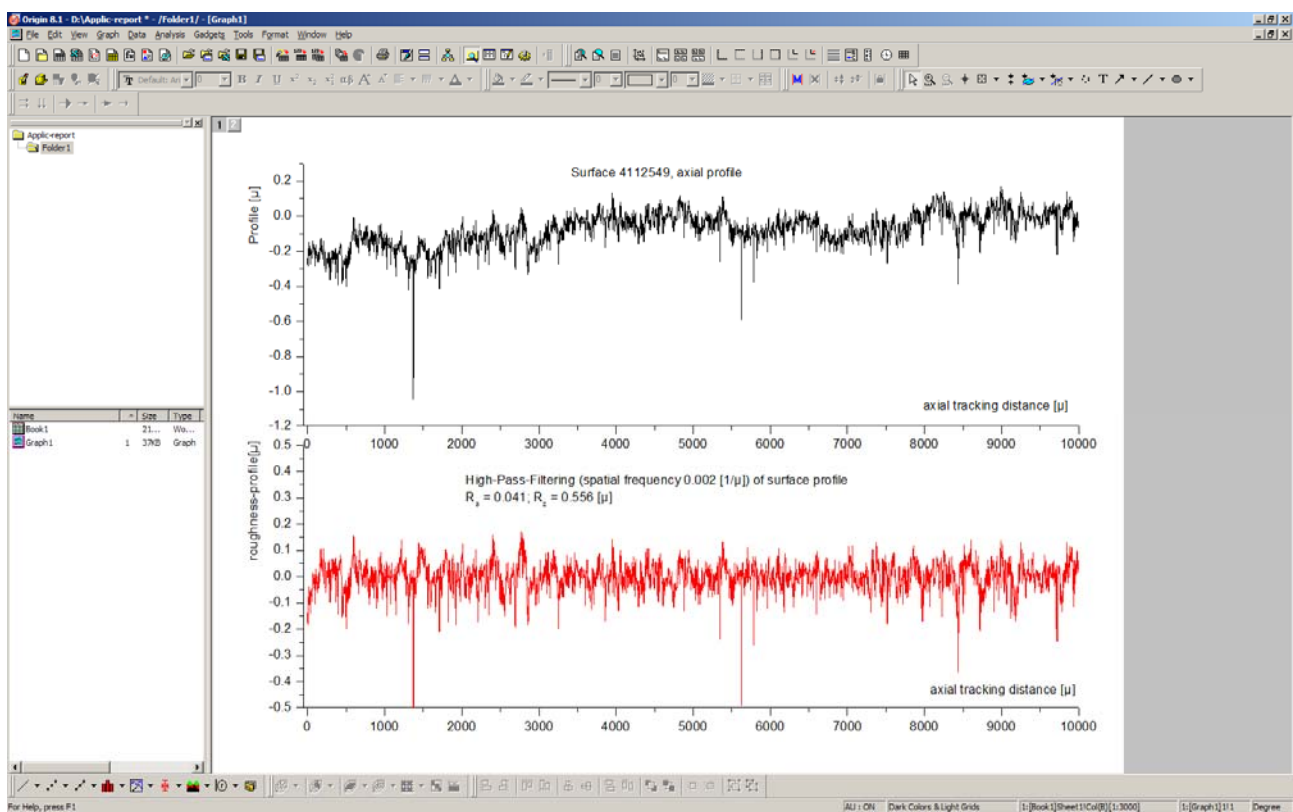
4. Additional Data-Processing

The roughness-profile (this is the profile, deprived of waviness) should now be processed further to get more insight into the surface-quality. For that purpose, two figures are normally distilled from

the roughness-profile. This will be done first, but by further steps we will go considerably beyond by the assistance of ORIGIN.

4.1. The two standard-figures are the so called R_a-value and the R_z-value. The former one is the arithmetic mean of the absolute signal-values, the R_z-value is figured out according to it´s definition

$$R_z = 1/5 \ (h_1 + h_2 + \cdots\cdots h_5);$$

by evaluating five heights h_i , that is the ordinate-distance between the deepest minimum and the highest maximum in the i-th subdivision of 5 equally-spaced subdivisions of the overall tracking length, summing them up and dividing the sum by 5. Thus, you end up with the mean of the five maximal amplitudes of each equidistant sub-partition of the total probing-distance of the roughness-profile. Both figures, R_a as well as R_z are matters of international standards.

Of course, R_a may be readily calculated by use of several tools of the menu "column". First go back to the workbook and it´s sheet (book1,sheet1). Select "Add New Columns" of the menu "Column" and add one new column. Highlight this new column E in the sheet and click on "Set Column Values " in the menu "Column". The dialog window which appears offers a very large mathematical manifold of entering formulas for calculations of the column-values. The simple formula, which does the job of calculating R_a is simply Mean(abs(col(D))). The text in the window reads now: col(E) = Mean(abs(col(D))). After clicking "Apply" and O.K. the R_a-value appears in every row of the new column E.

The R_z-value may be determined in the following way:
Make active the graph and therein layer 2. Then use the topic "statistics" / "open dialog of the menu "gadgets" . A dialog-offer is opened, which should be configured like this:
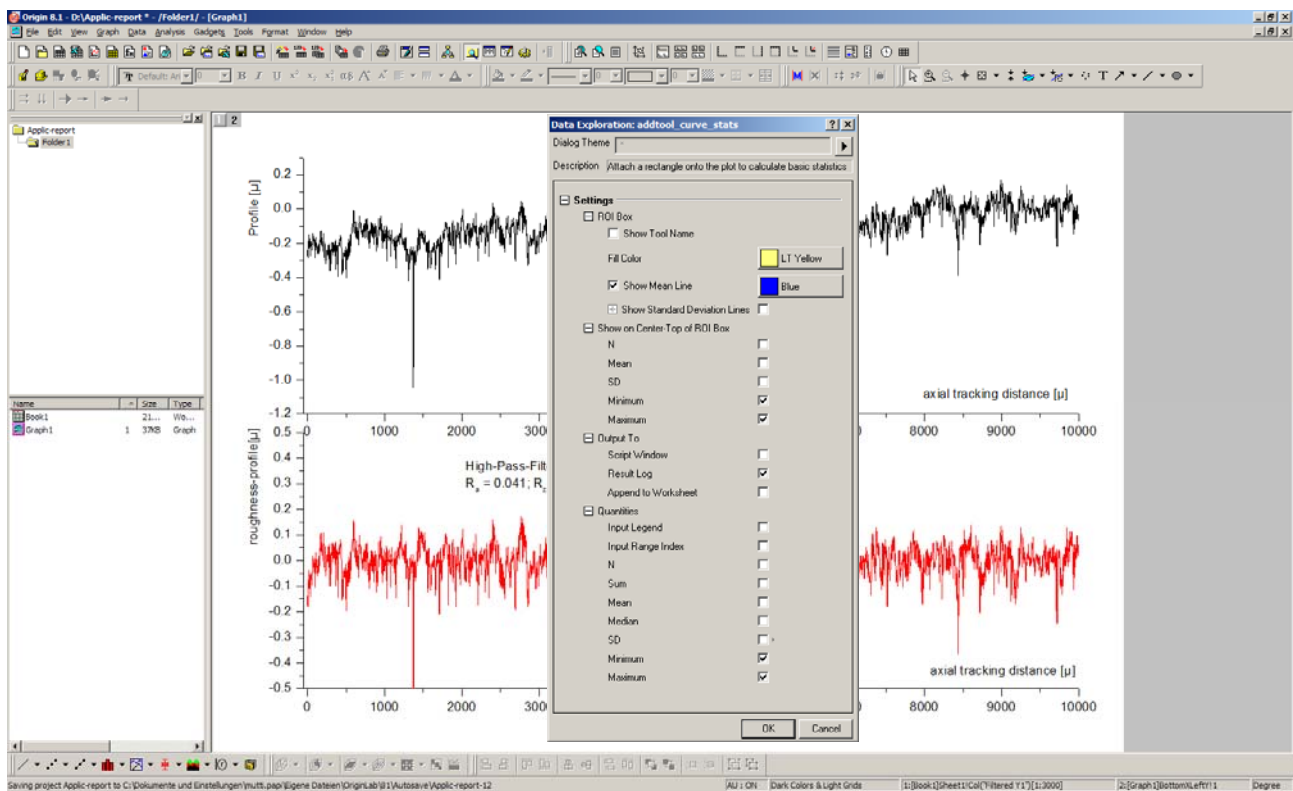
After pressing o.k. the window shows up a region of interest (ROI) and You may read off the x-interval of that ROI. Set the x-interval to the tracking length / 5. In the present case this is dx = 10.000/5 = 2000. What you see now is:
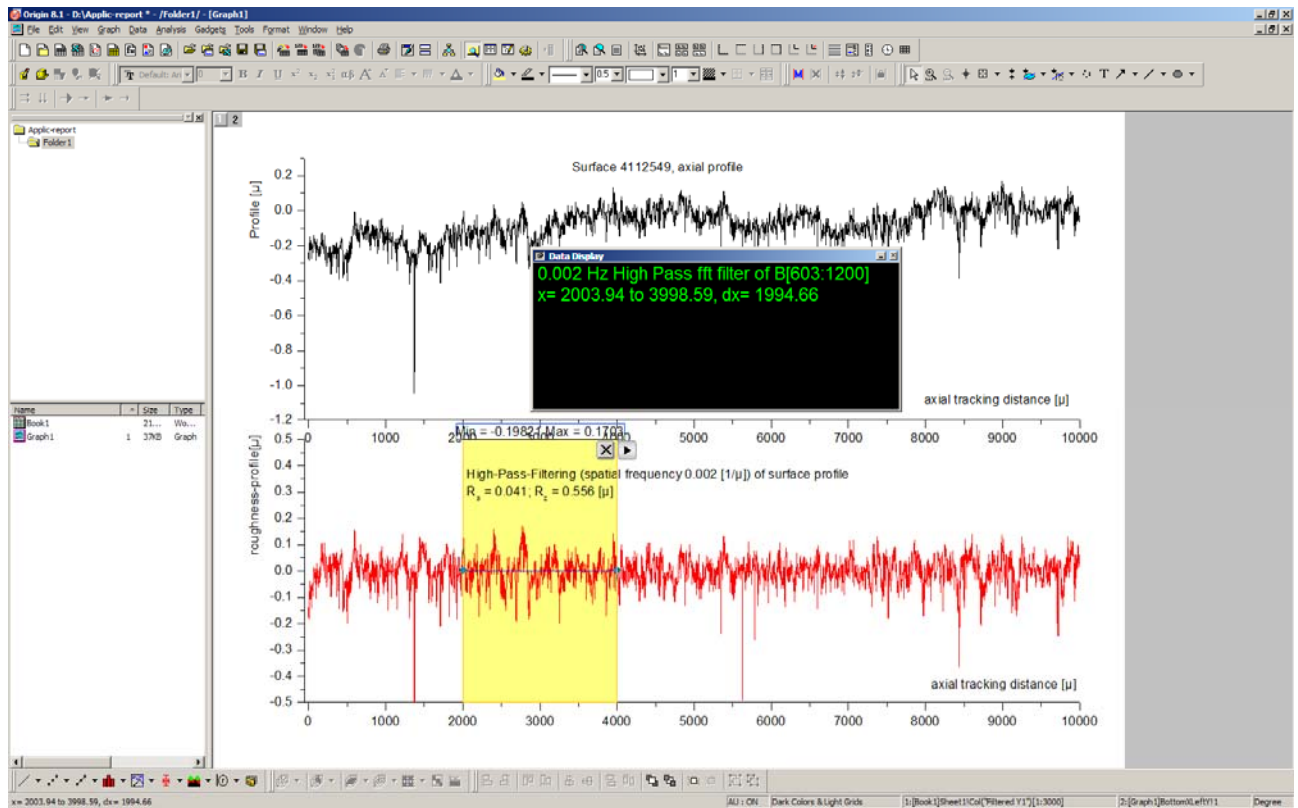
Shift the ROI-mask to the starting value of 0 and click on the triangle near the upper-right corner of the mask. Then select "new output". In the results-log you get the min.- and max-value of this ROI. Next, shift the ROI-mask to the right, such that the shifted left corner coincides with the former right corner and repeat pressing new output. Repeat that process five times totally and the results-log contains 5 pairs of values, min and max, for all the five equidistant ROI´s, which you shifted across the entire tracking-length. Now you should sum up the absolutes of these 10 values and divide the sum by 5. This is R_z.

Finally, the ROI-mask is removed by clicking on its cross and the freshly found R_a and the R_z-values may be written into layer 2 of the graph for the sake of characterizing the roughness-profile.

May be you don´t want to conserve col (E) of the worksheet. Delete it.

The whole process so far is very rapid, if you developed some skill. However, the job can be done even more rapidly and if it is not a single evaluation but a every-once re-occurring routine operation, it is advisable to write a LAB-TALK-script, which is run in the script window. Such a script is given in the appendix-file "Labtalk-Origin8_1-Rz-Ra.txt".

Open the menu "window" and select "script window". Load the fore-mentioned script into the script window (open....) and make active the worksheet with the roughness-profile. Enter the column-index of that column, which contains the interesting roughness-filtered as the z-value in the first command-line of the script and let it run. At a glimpse, you will find the results in the script window and in a new column of the worksheet, too.
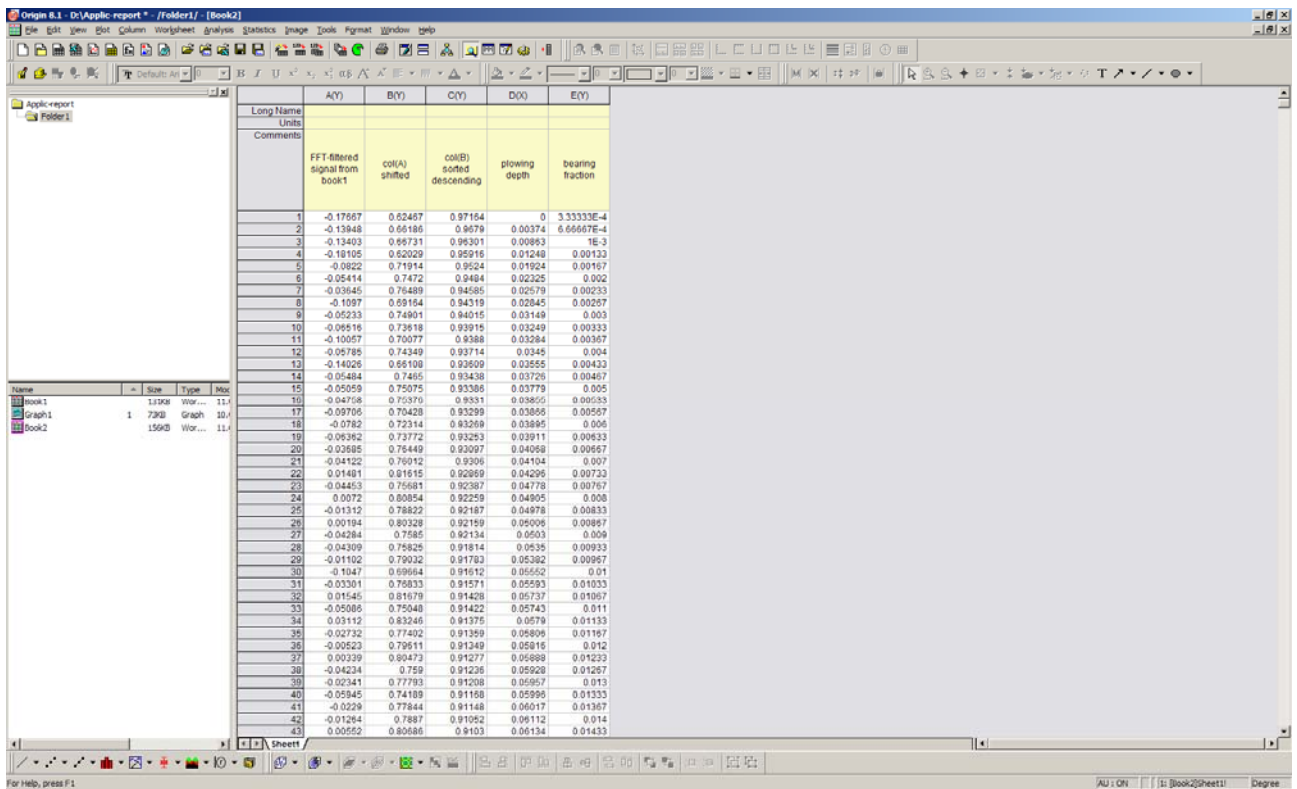
4.2 The bearing fraction of the surface
The term bearing-fraction describes that fractional part of the overall-surface-topology, which will

bear an ideally smooth , that means a completely flush (down to sub-nano-scales of roughness) gliding counterpart. Of course, if you look into the graph of the roughness-profile, you readily get aware of the fact, that the bearing fraction at the first kiss-point, that means at the outermost surface-contact, will be a minimum and about ten ahead minus something small. But in the course of initial wear which sets in until the gliding pairing comes to a stationary condition, the gliding partner is penetrating and plowing into the counter surface until a sufficient bearing fraction has been self-created which is able to carry the load of the gliding pairing. Thus, for those, who are skilled in the art and have to fight against wear and malfunction of lubrication, the functional inter-dependence between bearing fraction and plowing-depth is an interesting feature and a criterion to judge the quality of the surface topology.

The slope of the bearing fraction-curve may serve as a figure of merit for the wear-resistance of the surface: This curve being steep would mean, that the gliding partner is borne by more than sufficient material, but no lubricant is distributed within the roughness-voids of the surface-profile. Under those circumstances, it is to be expected, that hydrodynamic pressure in the gliding gap is paramount. At the other hand, if the slope is flat, the bearing fraction will not be able to support the normal load in the gliding gap. Thus, as a consequence, one is lead to the expectation, that the slope of the bearing-fraction-curve (also called Abbot-curve) is best if in between. Lubrication is very well controlled to be between the so called boundary condition (lubricant too scarcely distributed) and the full (elasto)hydrodynamic separation of the gliding partners. The latter gliding condition is not always welcome. Per example, it is prohibitive in printing business, because the printing form would run under severe and disastrous scumming and toning-condition. If cars are driven with slicks, that is tires without profile, aquaplaning is the consequence on wet roads. Reflect a little bit about the analogies.

Aiming at the bearing fraction, we start with book 1 and make a copy of just that column which contains the FFT-filtered Y-roughness-signal (col(D). Then we create a new book. Open the file-menu and press "New" and then "workbook". The new book is appearing under the name book 2 and two columns in it´s sheet 1. The copy of book 1, col(D) is pasted into column A of the new book 2. Next, col(B) is highlighted and its elements are calculated by use of the column-menu and the command "set column values " and the expression col(B)= col(A)+abs(min(col(A))). Still by use of the column-menu, add three new columns to the worksheet. Then, Col(C) is filled first with a copy of col(B) and then sorted by use of the (sort column / descending)-command of the worksheet-menu. Col(D) is calculated again by the command "set column values" within the menu "column" and the expression col(D) = max(col(B))-col(C). Finally, scroll to the last row of the sheet and memorize the index-number i_{max} of the last row. Now, highlight col(E) and calculate the values of this column by the expression col(E) = i / i_{max} , where instead of i_{max} you have to write-down just that number You memorized as the index of the last row. After little editorial work, the sheet 1 of book 2 should look like that:

|	A(Y)	B(Y)	C(Y)	D(X)	E(Y)
Long Name					
Units					
Comments	FFT-filtered signal from book1	col(A) shifted	col(B) sorted descending	plowing depth	bearing fraction
1	-0.17567	0.62467	0.97164	0	3.33333E-4
2	-0.13948	0.66186	0.9679	0.00374	6.66667E-4
3	-0.13403	0.66731	0.96301	0.00863	1E-3
4	-0.18105	0.62029	0.95916	0.01248	0.00133
5	-0.0822	0.71914	0.9524	0.01924	0.00167
6	-0.05414	0.7472	0.9484	0.02325	0.002
7	-0.03645	0.76489	0.94585	0.02579	0.00233
8	-0.1097	0.69164	0.94319	0.02845	0.00267
9	-0.05233	0.74901	0.94015	0.03149	0.003
10	-0.06516	0.73618	0.93915	0.03249	0.00333
11	-0.10057	0.70077	0.9388	0.03284	0.00367
12	-0.05785	0.74349	0.93714	0.0345	0.004
13	-0.14026	0.66108	0.93609	0.03555	0.00433
14	-0.05484	0.7465	0.93438	0.03726	0.00467
15	-0.05059	0.75075	0.93386	0.03779	0.005
16	-0.04758	0.75376	0.9331	0.03855	0.00533
17	-0.09706	0.70428	0.93299	0.03866	0.00567
18	-0.0782	0.72314	0.93269	0.03895	0.006
19	-0.06362	0.73772	0.93253	0.03911	0.00633
20	-0.03685	0.76449	0.93097	0.04068	0.00667
21	-0.04122	0.76012	0.9306	0.04104	0.007
22	0.01481	0.91615	0.92869	0.04296	0.00733
23	-0.04453	0.75681	0.92387	0.04778	0.00767
24	0.0072	0.80854	0.92259	0.04905	0.008
25	-0.01312	0.78822	0.92187	0.04978	0.00833
26	0.00194	0.80328	0.92159	0.05006	0.00867
27	-0.04284	0.7585	0.92134	0.0503	0.009
28	-0.04309	0.75825	0.91814	0.0535	0.00933
29	-0.01102	0.79032	0.91783	0.05382	0.00967
30	-0.1047	0.69664	0.91612	0.05552	0.01
31	-0.03301	0.76833	0.91571	0.05593	0.01033
32	0.01545	0.81679	0.91428	0.05737	0.01067
33	-0.05086	0.75048	0.91422	0.05743	0.011
34	0.03112	0.83246	0.91375	0.0579	0.01133
35	-0.02732	0.77402	0.91359	0.05806	0.01167
36	-0.00523	0.79611	0.91349	0.05816	0.012
37	0.00339	0.80473	0.91277	0.05888	0.01233
38	-0.04234	0.759	0.91236	0.05928	0.01267
39	-0.02341	0.77793	0.91208	0.05957	0.013
40	-0.05945	0.74189	0.91168	0.05996	0.01333
41	-0.0229	0.77844	0.91148	0.06017	0.01367
42	-0.01264	0.7887	0.91052	0.06112	0.014
43	0.00552	0.80686	0.9103	0.06134	0.01433

Please observe, that col(D) is made of type X.

Finally, by plotting col(E(Y)) versus col(D(X)), you produce a graph of the bearing-fraction. Of course, You may change the stile of the graph with all of the editorial possibilities, ORIGIN is offering.

At the end, we will extract a characterizing figure out of the graph. This is the slope of the linear ascent of the sigmoid. This slope, as already mentioned, may serve as an index for the wear- and lubrication-properties of the surface.

Use the "Gadget"-menu and "Quick Fit". Adjust the fitting mask just to cover the linearly ascending middle-part of the curve.
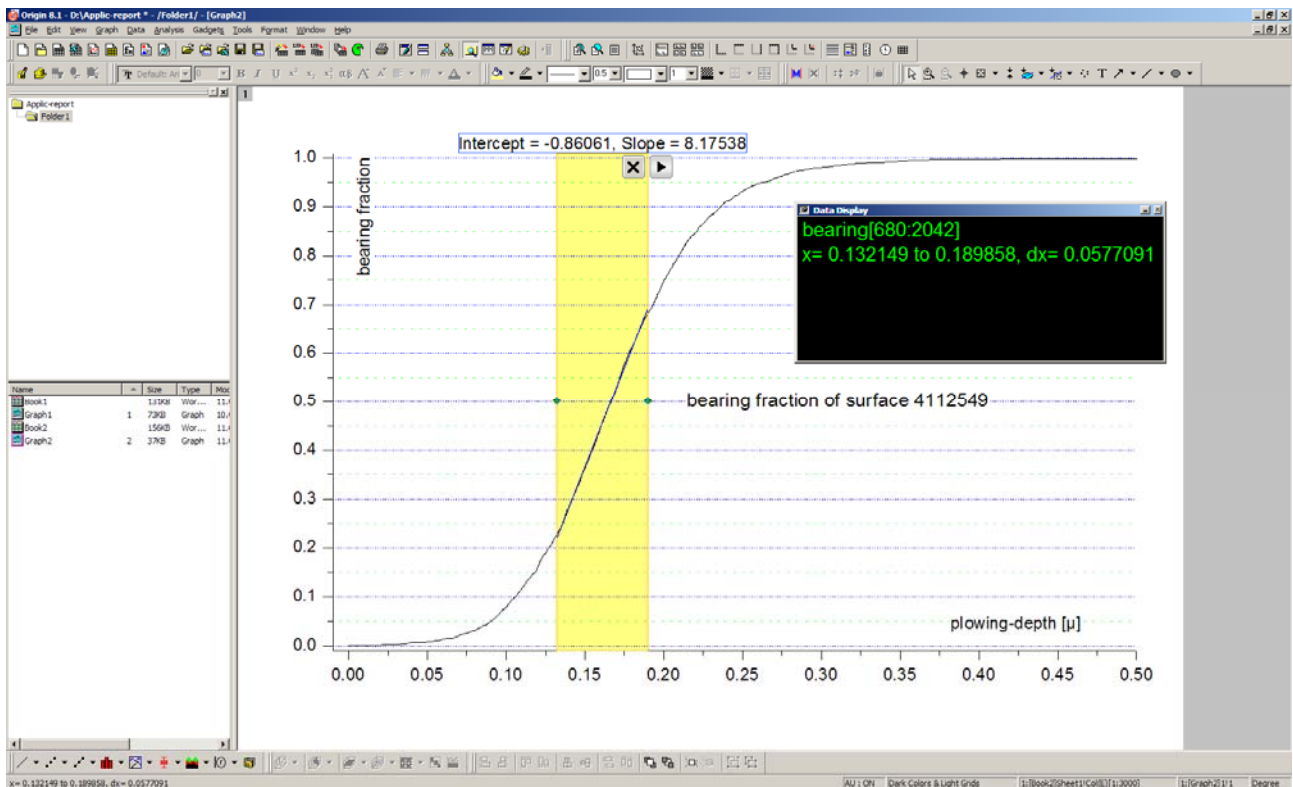
Next, click on the little arrow at the upper-right corner of the mask and press "new output". Then cancel all the windows and the mask, which are no longer needed and you have the graph again with the fitting line. Now make active the workbook 2 and you will find two new columns with the fitting data. Merely for the purpose of esthetics, you may wish to pronounce the fit-line by making visible some points with a different color. This is achieved in the following way:

Make active book2 and highlight the two columns with the fitting data. Cross over to the worksheet-menu and select "reduce rows" /"open dialog". Feed in, per example "delete 9, skip1, starting 2, output = input" . Press o.k. and the two columns will be reduced to one/tenth of their original length. Now go back to the graph and select the menu "Format / Plot" and select the layer content "Quick fit". In the dialog-field "Plot-Type" the selection "Line plus symbol" should be made and the symbol can be edited as well as the line itself by using all the offers in the right part of the window. After-wards, the graph may look like this one ,
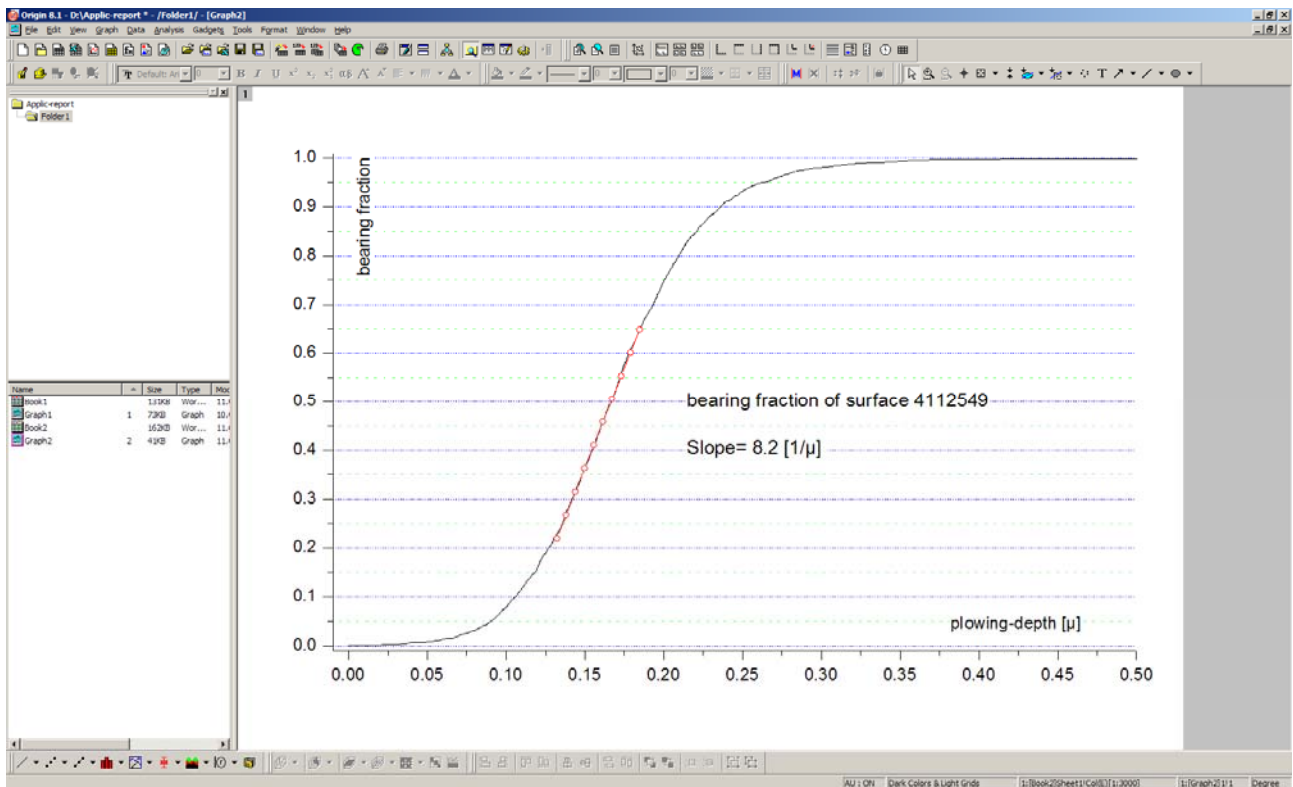
where-off, per example, you may read, that a bearing fraction of about 40%, where the gliding pairing eventually works in a stationary way, is reached in a profile-or plowing-depth of 0.15 µm.

To facilitate the sequence of calculations towards the bearing-fraction, a LAB-TALK-script is given in the appendix under the file-name "Labtalk-Origin8_1-Traganteil.txt", which may be run as a worksheet-script in book 2, after having filled col(A) with the FFT-filtered roughness-profile of interest. It should be noticed, that the second part of this script prepares the prerequisites needed in what follows next.

4.3 The lubrication-imbibe-volume

wear-fighting by proper lubrication (be it boundary-lubrication or full lubrication in the (elasto)-hydrodynamic lubrication-regime may be considerably backed by knowledge of the volume of the lubrication film, which is contained in the roughness-profile of one square-meter of the surface.

Knowledge of what we call the imbibe-volume of the surface, may also be helpful in characterization of printing-substrates, whose surface-topology and capillarity must be filled and leveled with fluid ink.

Hence, let us proceed towards a calculation and a graph of this very interesting feature. For that purpose, we go back to book 2 and make a copy of the filtered signal (col(A), in this case) and paste it into col(A) of a newly made book 3. From now on, Book 3 is the active one. Go to the window-menu and tick on "script-window". The void window, appearing now should be filled with the script "Labtalk-Origin8_1-Traganteil.txt" by clicking on the file-menu of that window, than clicking on open... and following the pathway to that directory, where You have buried in the script.

Next, highlight all the text of the script and press <enter>. The calculation is going on as you may discern in the lower-left corner of the screen. After a few seconds, the screen is rearranged an you find a book named data 2 being active. The only worksheet of this book should have 11 rows filled and is an excerpt of the columns D and E of book 3. These latter columns are the bearing fraction again as calculated "manually" in paragraph 4.2 . The book "data2" is needed now for calculation of the Lub-film-volume.

We go back now to book 1 and make a copy of the "filtered X" and "filtered Y" These are the columns C(X) and D(Y) in our case. The copy of these two columns is pasted into a new book, which is book 4 in our actual case. Following the description already given above, we open the script- window for that book 4 and feed in the script "Labtalk-Origin8_1-Lubfilm.txt".

Highlighting the full text of the script and pressing <enter> will start the automated calculation of the lubfilm-volumn. The result is found in columns A27(X2) and A26(Y2) at the out-most right corner of the sheet, which in the course of the calculation was blown up a little bit. These two last columns are plotted now to yield the display of the lubfilm-volume versus the bearing fraction. After the usual stiling and by using spline-interpolation for the Line+Symbol-Plot, you may see this graph as the culmination of your work.
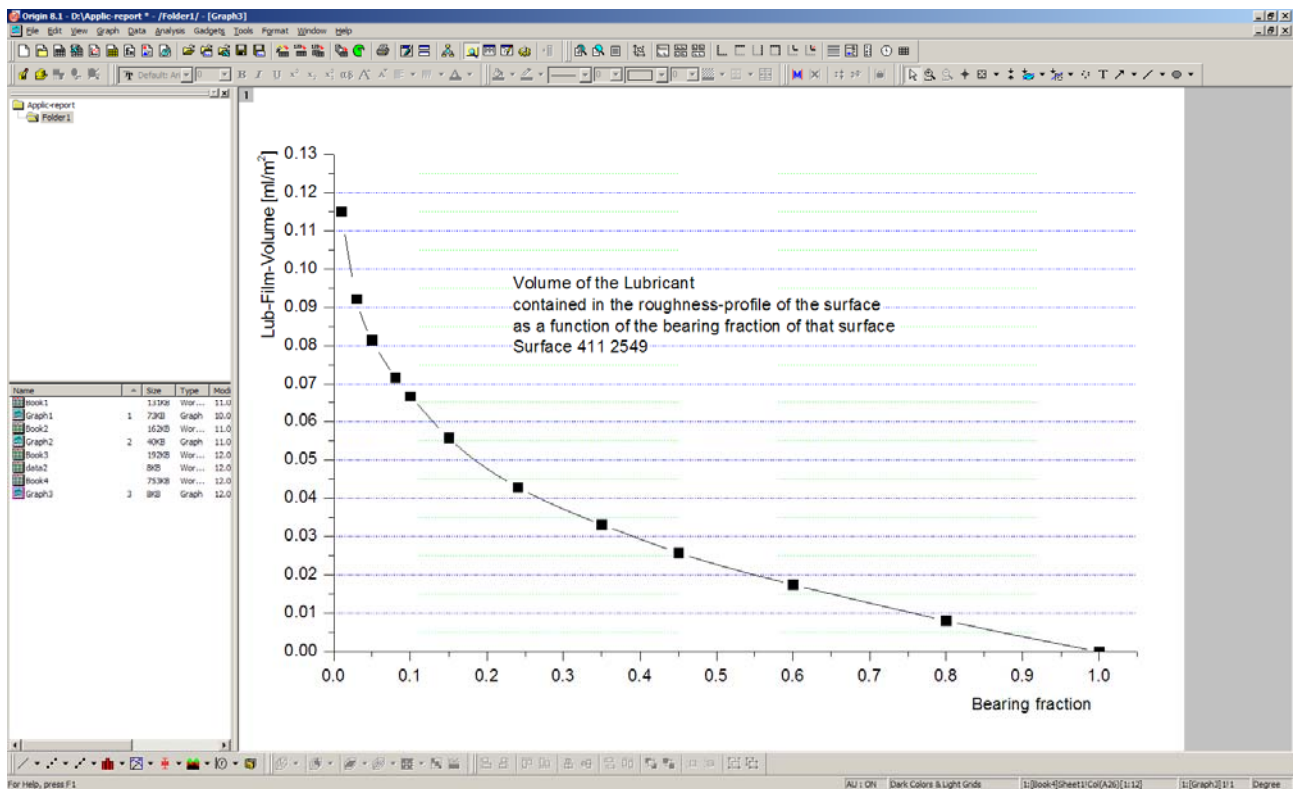
4.4 The fingerprint of the surface-finishing tools.

After having found a process, which produces the right surfaces for Your purposes, You may wish to document a fingerprint of the finishing tools, which are engaged e.g. in milling and grinding the surface in the case of hard-stuff or producing it in the case of paper-webs or alike.

Generally spoken, there are two kinds of fingerprints: Those, which have stochastic qualities and others with periodic as well as stochastic features.

4.4.1

The fingerprint of the former ones is readily inspected by making a histogram of the roughness-profile reading. Go back to book1, col(D). This is the column with the filtered roughness Y-data. Highlight it and select statistics/histogram in the plot-menu. A histogram with prefixed display-parameters is appearing. This may be altered by going to the format-menu and selecting "plot". Most important is the "Data"-sub-menu, where you should deactivate the automatic binning and change bin-size subsequently. Feed in 0.01 in our case. Then eventually choose a normal distribution to be compared with the histogram. Line and pattern may be chosen at will as well as the spacing between the hist-bars. Finally, You may have combined a graph as shown below.

The arrows may be inscribed by using the arrow-tool, which is activated by going to the menu "view" and there to "tool bars" The position of the arrows may be fixed by right-clicking on each arrow and using the choices of the "programming control".

The width of the distribution (FWHM) and the descriptive statistical properties, which may be configured by all the offers of "Analysis/statistics/open dialog" may be helpful as characterizing figures. These figures, which can be output to a new book or to the results-log or to a worksheet, may be transferred to the graph by means of copy and paste and can be edited there by right-clicking and adjusting the "properties....".
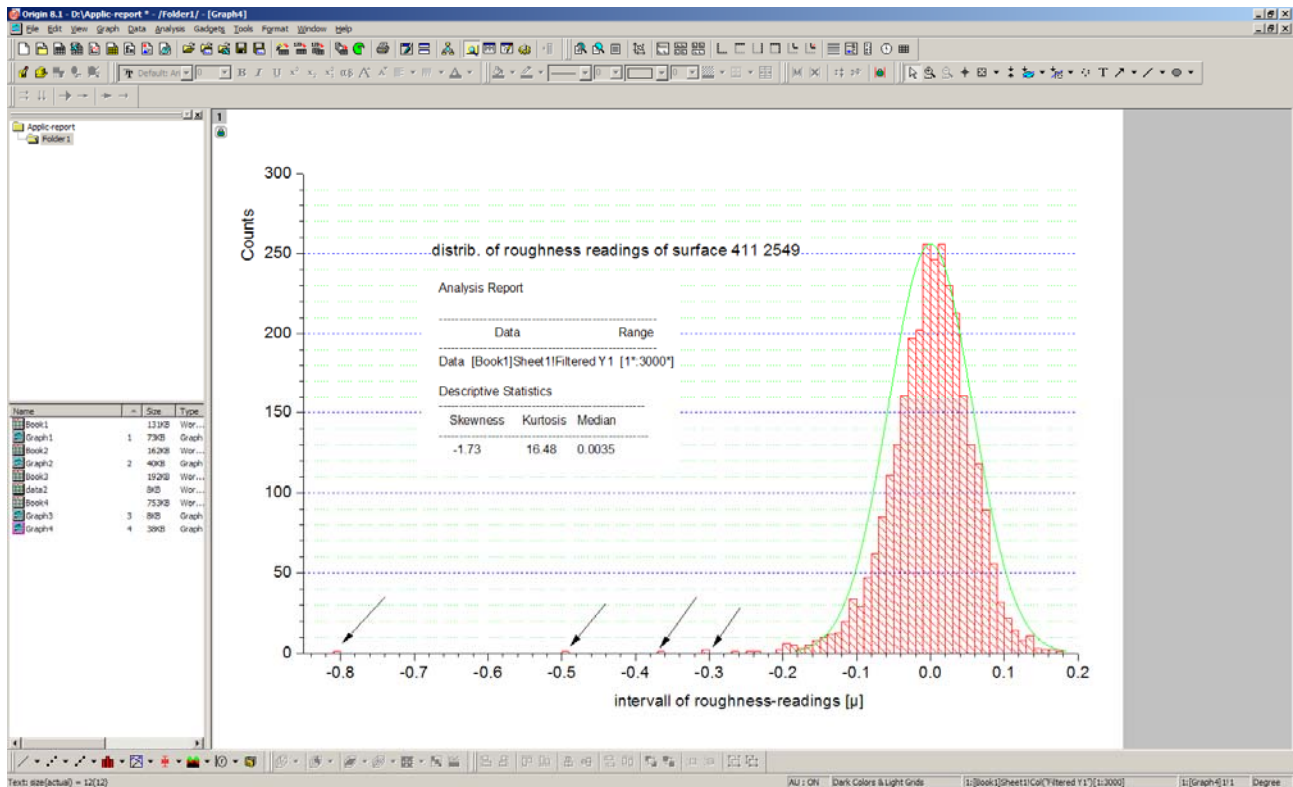

4.4.2

The fingerprint of the spatially periodic type is documented by using FFT again. To demonstrate, how it may work, we import a new profile into book 5 and make a plot of the new data. This is graph 5. After inspection, you probably are convinced, that the baseline of this graph is an artifact due to the fact, that this profile is the result of a circumferential tracking of a cylindrical body like a roller-bearing or a piston. We would not like to go into the details here, but instead of, we would like to demonstrate the power of ORIGIN as applied to baseline-correction.

Let the graph 5 be the active window. Now go to the menu "Analysis" and proceed to "peak-analyser" in the sub-menu "peaks and baseline" . Open the dialog and choose the goal " subtract baseline". Press "Next" and run through and act on the following sequence:

Baseline mode: User defined; Enable Auto-find; Number of points 12; Find; Disable Auto-find; Modify; Add; Done; Next; Interpolation Method: B-Spline; Subtracted data: <new>,<new>;

Baseline: none ; As a result you are now in front of a screen like that:
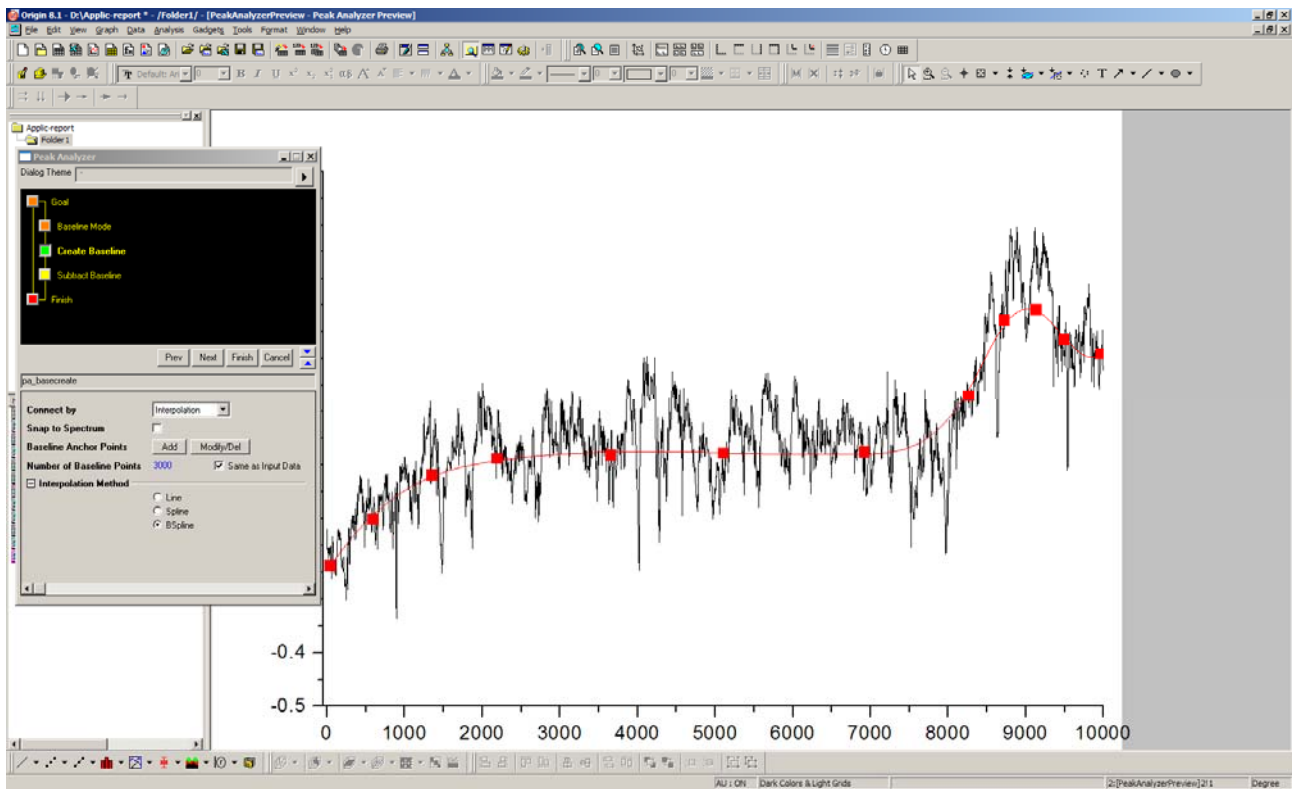
Finally, press "Finish". Go to book 5 now and you will find there two new columns with the baseline-subtracted data. Highlight the corrected Y-column and right-click to set the sampling interval. Now you are well prepared to start the fingerprint-finding by using FFT.

First add a second layer to graph 5 and plot the baseline-corrected profile into that layer. The difference between the original profile, which contains the artifact and the corrected profile is now in front of your eyes.
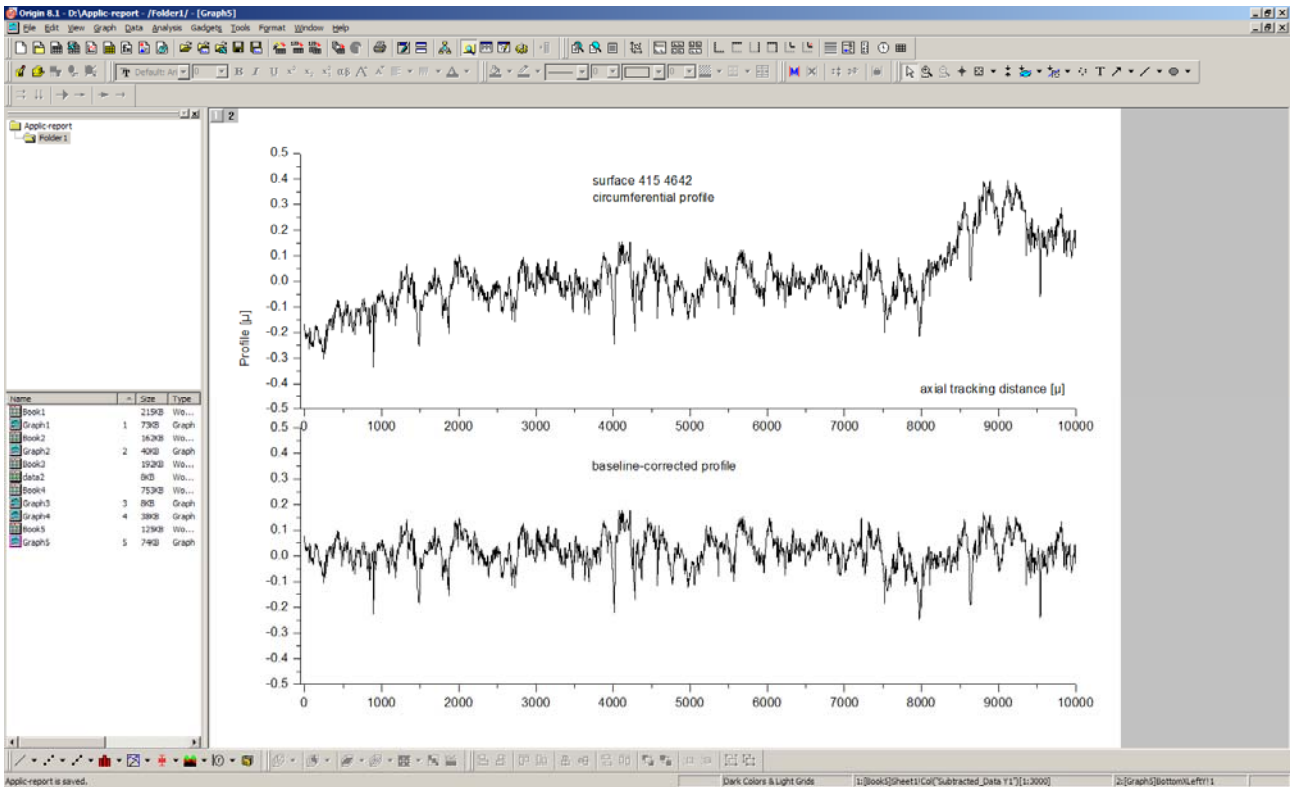
Make active layer 2 and cross over to "Analysis" again, "signal processing" and "FFT". Open the dialog and make the settings as displayed here:
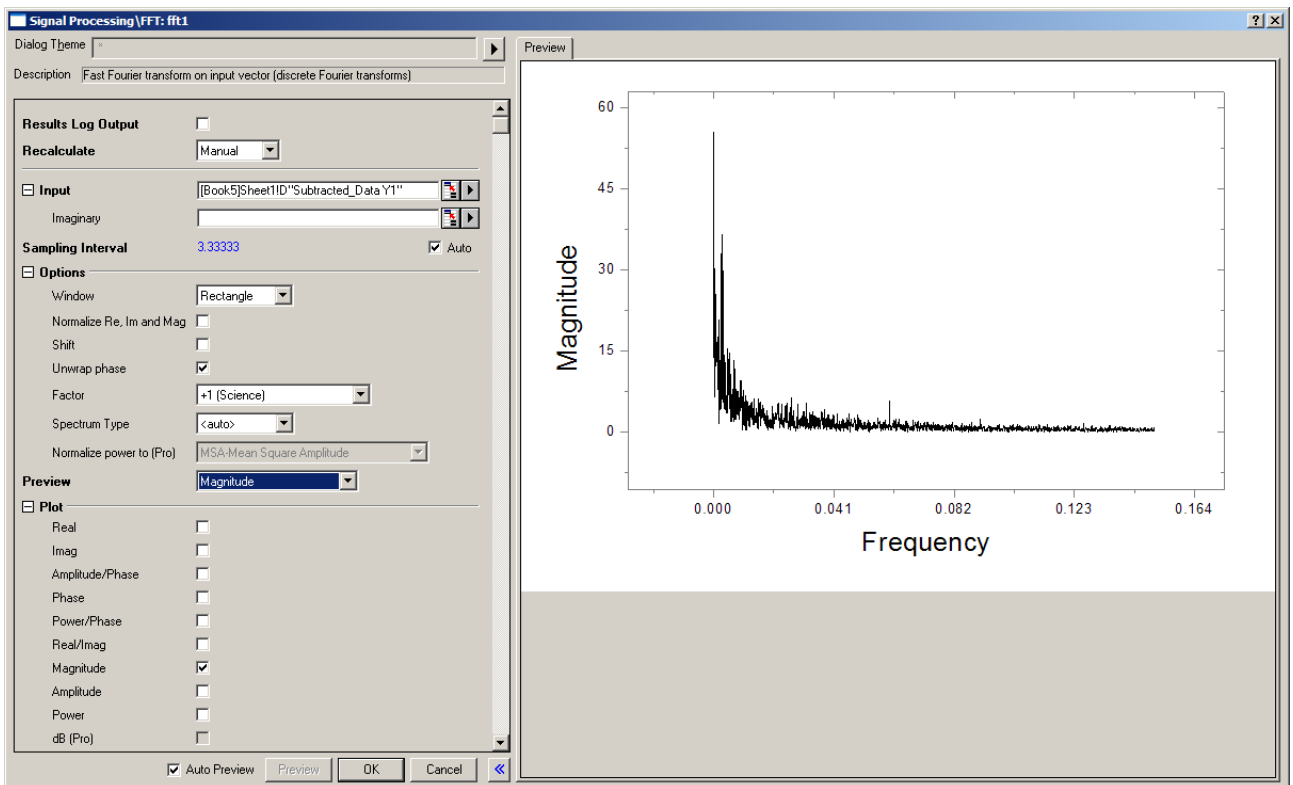
At the bottom of the dialog window, the "Result Data sheet" is chosen to be "[<input>]<new>". The "Result Graph-sheet" should be disabled. Next, press o.K. and go back to book 5. An additional sheet, named "FFT Result Data" is appended to this book and you can plot now these data. Expand the plot for the relevant range and make the necessary editorial work to end up with a graph as follows:
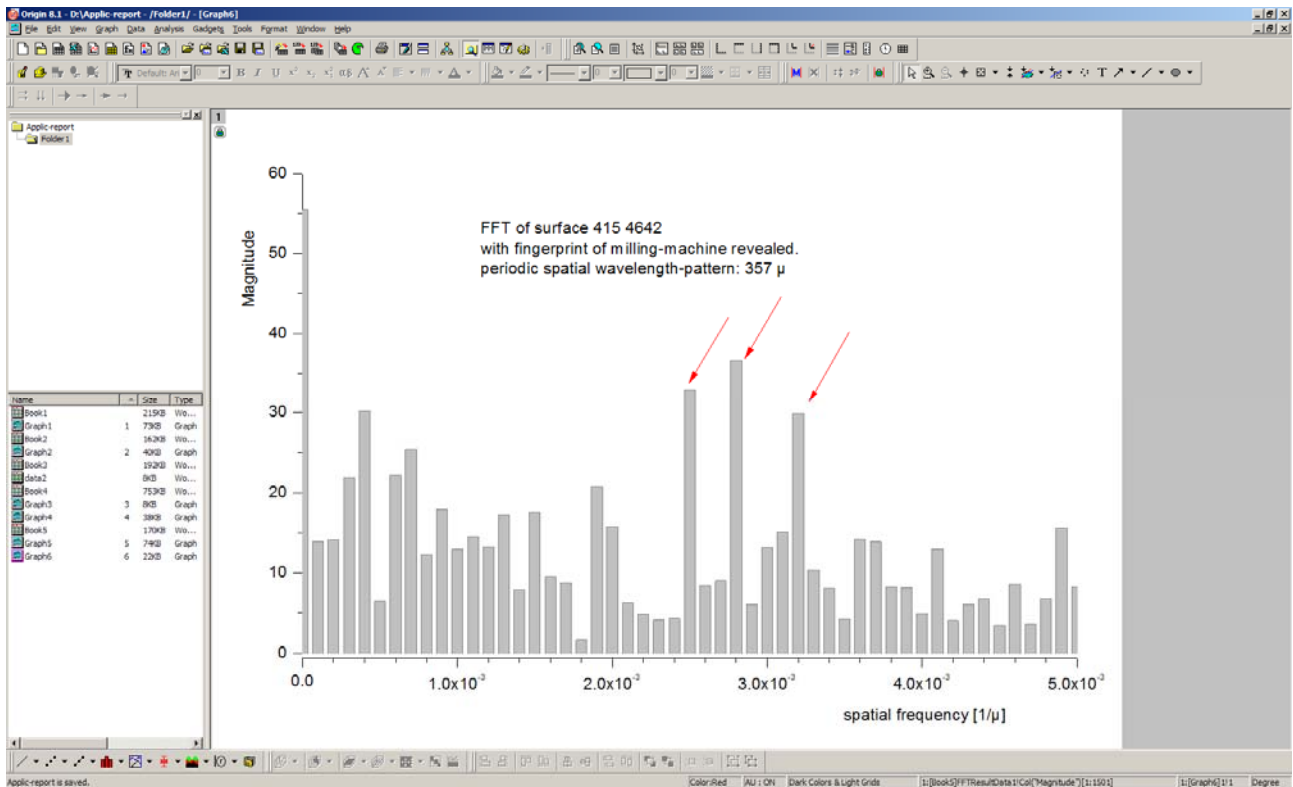
This graph clearly reveals, that improvement in surface-finishing should be effected, because there is a clear periodical pattern in the surface-profile with a group of spatial frequencies around 2.8(-3) [1/µ] . This corresponds to a spatial wavelength of 357 µ . Such a periodic pattern in one of the surfaces of a gliding pairing may trigger a continuously forced normal as well as translational vibration (resonance or else) of the contact and provoke severe wear as a consequence.