## MePS2dpl prepares spectra for fitting by PLRF version 19.

MePS2dpl code does the following

- extracts energies from names of MePS files and create separate directory for each energy (in the current folder)

- from each MePS file it cuts part of spectra which should be fitted and copies it to the corresponding directory. Names of these spectra are created automatically as number-of-file\_name-of-

sample\_energy.dpl, e.g. 13\_GaN\_16.dpl , i.e. 13<sup>th</sup> file in the series, sample GaN, energy 16 keV. The region which should be cut from MePS files is specified in the first line of the file

MePS2dat.ini as follows: first channel, last channel

-It creates file splist\_sorted.txt containing list of spectra to be fitted sorted from the lowest energy to the highest. This file is used by PLRF to get names of spectra to be fitted.

-It creates file matrix.txt which contains all spectra (each in separate column) shifted vertically with respect to each other. Vertical shifting is by multiplication by factor given in the third line of the file MePS2dat.ini. This file can be used to plot all spectra as the following figure for GaN crystal. Sometimes it might be useful.



-It creates also file mesh.txt containing 2D histogram positron energy versus lifetime. Bin width for the lifetime axis is specified in the second line of the file MePS2dat.ini.It allows to make the following 2D plot (it is again for GaN crystal)



## Content of the Initial file for MePS2dpl code MePS2dpl.ini:

32000,52000 !first and last channel of the part of spectra to be fitted 10 bin width (in channels) for horizontal axis of 2D histogram in file mesh.txt 5.0 !multiplication factor used for vertical shift of spectra in file matrix.txt

PLRF code (version 19) is then started in the standard way using the initial file PLRF19.ini only in the section <code>#spectrum</code> one should write <code>splist\_sorted.txt!</code> (i.e. the name of sorted list created by MePS2dpl followed by !). It tells PLRF to fit sequence of spectra located in folders where they were sorted out by MePS2dpl.

Results of fitting will be automatically copied to appropriate folders and will have names number-of-file\_name-of-sample\_energy-fnumber-of-fit.suffix

Output files have standard suffixes used by PLRF

\*.ini – input file

\*.res-output file with results of fitting

\*.p1-file containing experimental spectrum and model function for plotting

\*.cnt-the same format as the input file but with parameter values obtained from fitting. It enables e.g. to release some parameter and start next fitting run with parameters close to the optimum values.

In addition it creates file name-of-sample-fnumber-of-fit.lst (e.g. GaN-fl.lst) which contains table with all fitted parameters + their errors for all spectra.

Number-of-fit is added to each file. It allows to start PLRF repeatedly with different model functions, e.g. one and two component fitting, and results of previous fitting will not be overwritten. User will be asked to enter fit number after start of PLRF.

An examples of PLRF input file PLRF19.ini for fitting of sequence of spectra measured on MEPS. In this example the spectra are fitted by two components + Ps contribution (consisting of p-Ps and o-Ps part)

#spectrum 1,3 splist\_sorted.txt! 9999 1,9999 #calibration(ns) 0.003 #parameters #bcg 1 bcg 10.0 0.001 0.00 1000.0 0 0.00 10000.00 2 TO -1.0 0.1 #RF 1 3 DT 0.014 0.001 -1.20 1.20 0 4 RFwa 0.344 0.001 0.00 1.20 0 5 RFwb 0.206 0.001 0.00 1.20 0 #inverse spectrum 6 linv 0.000 0.000 0.00 0.10 0 #source 0,0 #sample 0 2.1 7 tau1 0.100 0.001 0.01 0.30 1 8 int1 0.01 0.0 100.0 1 45.0 9 tau2 0.380 0.001 0.01 10.0 1 10 int2 50.0 0.01 0.0 100.0 1 11 tau3p 0.125 0.001 0.01 10.0 1 12 tau3o 1.5 0.001 0.01 100.0 1 13 intr 75.0 0.01 0.0 100.0 1 #commands FIX,11,13 SEEK,100 SIMPLEX MINIMIZE RETURN

Output file (GaN sample, E = 1 keV)

spectra:

1\_GaN\_1.dpl total area: 7.508e+06 counts

number of parameters: 12 number of free parameters : 10 number of fixed parameters: 2

Background and TO

1 bcg(1) 15.46317 +/- 0.00096 2 T0(1) 1284.7128 +/- 0.00003

RF model 1 mirrored double-Gaussian

3 DT(1)	0.06662 +/- 0.00000
4 wa(1)	0.34396 +/- 0.00002
5 wa(1)	0.56481 +/- 0.00000

inverse spectrum

6 I\_inv(1) 0.00000 +/- 0.00000

source model: 0 component(s), 0 complex component(s)

sample model: independent 2 exponential component(s) 1 complex component(s)

7 tau1	0.04590 +/- 0.0052
8   1	49.97713 +/- 0.00041
9 tau2	0.38710 +/- 0.00001
10  2	45.59789 +/- 0.00040
11 tau1c1	3.86084 +/- 0.00004
12 tau2c1	0.12500 +/- 0.00000
13 Irat1	75.00000 +/- 0.00000
lrc1	4.42498

spectrum 1 RF total FWHM: 0.406914 ns

spectrum 1 chi2 per degrees of freedom: 1.309463 +/- 0.014150