This aims to be a very short introduction to how to use the pyxrr x-ray reflectivity simulation tool.

1. Important Files and Folders

Base Directory:	
pyxrr/	Folder containing the subroutines and modules for reflectivity calculation, the database and lots more
pyxrr/core.py	Python wrapper for xrr.c routines
pyxrr/functions.py	Helper functions for pyxrr.py
pyxrr/wrap4leastsq.py	Wrapper for scipy's leastsq fitting routine
pyxrr/xrr.c	C sources of reflectivity calculation routine R(θ)
pyxrr/xrr_sc.c	Same as above but for single core processing
pyxrr/materials.sqlite	Database containing dispersion corrections f1+f2, atomic properties and densities
pyxrr/locale	Folder containing translations
contrib/	Folder containing scripts and examples that use pyxrr and make it usable (the GUI must be placed here)
contrib/fit_interactive.py	Outer example script for interactive least squares fitting
contrib/fit_auto.py	Example for automated least squares fitting
contrib/multilayer_gammaopt.py	Outer example script for searching the optimum gamma parameter
contrib/pyxrr_GUI_v0.6.pyw	Graphical User Interface (GUI) for the simplified use of pyxrr
contrib/samples/	Folder containing samples files defining the multilayer (see below)
contrib/samples/measurements/	Folder containing the measured data files
contrib/results/	Folder containing saved projects/results/simulations
contrib/tmp/	Temporary folder containing results of last iteration

`setup.py`	Installation script

2. Multilayer Sample Files

Every Multilayer consists of a Substrate, Groups of Layers and the Ambience. The Groups can be stacked to a given number of periods. An example for a samplefile is given below.
If a line ends with a comma (,) or a backslash (\) the next line is included in the processing.

EXAMPLE.param

```
Ambience: code=H20, name=Water, rho=1.0

Group: name=protection, sigma=5, periods=1, grad_d=0
Layer: code=B4C, d=100, name=B4C_protection, rho=2.5

Group: name=ML, sigma=3, periods=100, grad_d=0.01
Layer: code=Mo, d=6, name=Mo_absorber, rho=9.4, sigma=1.5
Layer: code=B4C, d=3, name=B4C_barrier1, rho=2.3, sigma=1.3
Layer: code=Si, d=15, name=Si_spacer, rho=2.3, sigma=1.6
Layer: code=B4C, d=5, name=B4C_barrier2, rho=2.3, sigma=1.4

Substrate: code=SiO2, name=Glass, rho=2.34, sigma=1.1

Measurement: file=measurements/mosi_hzg4.njc, x_axis=twotheta, energy=8.905, fit_range=0.2->inf,
resolution=0.01, background=-4., scale=1.0, offset=0, weigthing=statistical, pol=0.5
Measurement: file=measurements/mosi_hasylab.fio, x_axis=theta, energy=10.0, fit_range=0.2->10.,
resolution=0.001, background=-5., scale=1.0, offset=0, weigthing=z, pol=0
Measurement: energy=10.0
```

Explanation:
Italic grey attributes are **optional**. Their default values are listed below.
Red parameters are new in this version.

Keyword	Definition	Default value
code	Chemical formula of the material. Case sensitive. F.e.: La0.25Ca0.75MnO3	-
name	Name to distinguish later.	code
periods	Number of Periods. How many repeats of the current group?	1
grad_d	Linear gradient in period thickness in % growth per layer.	0
sigma	RMS roughness of the **upper** interface in Å.	0
rho	density of the layer in g/cm³.	from database
d	Layer thickness in Å.	-
file	Path to the file containing measured data. Can be .njc, .raw, .x00, .val, .asc, .fio or simple 2-columned data	-
x_axis	specify the independent (x-axis) quantity given in the measurement file. Possible values: *theta twotheta qz_A qz_nm*	
energy	Photon energy of the measurement in keV	8
twotheta	1 if x-values are 2θ, 0 if they are θ	0
fit_range	θ_min->θ_max , Interval that will be evaluated for fitting simulated data (same unit as x_axis)	0->inf
rebin	Rebinning is necessary if the measured data is unequally spaced in theta. Possible values: *average* (combine several data points to maximum step width) *interpolate* (interpolate data to minimum step width, resulting in more data points)	interpolate
resolution	FWHM of a gaussian shaped device resolution in θ/°.	0
background	Common logarithm of background Reflectivity (log10(R_noise))	-10

scale	Scaling parameter for shifting Reflectivity values. (For Primary beam intensity uncertainties) Should be adjusted by hand in the beginning.	1
offset	θ offset in measured data in °.	0
weighting	Weighting of the errorfunction. Possible values: **z** = Weights are given in 3rd column of measurement file **statistical** = 1/σ , where σ is standard deviation of the Intensities (or proportional to it)	no weighting
pol	Polarization state of incident x-rays. (0 = perpendicular, 1 = parallel, 0.5 = unpolarized) This has **negligible** influence for θ<10°	0

3.Theoretical Model (short)

pyxrr employs the Fresnel equations to calculate the reflection coefficients at each interface.
The interference of the reflected waves is calculated using the transfer matrix method (Abeles formalism).
Interface roughness is taken account for by implementing Nevot and Croce's formula for error-function shaped interfaces.

See for example:
http://en.wikipedia.org/wiki/Transfer-matrix_method_%28optics%29