Determination of crystallite sizes by the Scherrer formula and a fitting procedure.

Pd.org is an origin file which contains the *Wide Angle X-ray Scattering* patterns of two black Pd powders prepared in different way. The contribution due to the instrumental broadening has been already taken into account. The broadening of the peaks can suggest you which sample has smaller particles.

Pd1.dat and **Pd2.dat** contains only the data related to the first two peaks of the patterns reported in **Pd.org.**. These two files have to be used as input files of the program *fitts.exe*.

Please, now, run

To the question

1) hit **Enter**

2) write the file name (Pd1.dat or Pd2.dat)

3) 1.54 (is the wavelength used CuKα)

4) N

5) N

6) N

7) 2

At this point by a graphical way it is possible to find the best initial parameters to start the minimization.

Remember that each profile is described by a pseudo-Voigt. For each pseudo-Voigt 4 parameters are requested:

A1=peak Intensity

A2= peak location

A3=parameter related to the full with at half maximum.

A4=parameter varying between 0 and 1 expressing the Gauss and/or Cauchy content of the peak

In order to describe also the background it is necessary use a polynomial function. In the present case a straight line is enough (2 parameters).

At the end of the fit with the *F2 Key* it is possible to know the value of the minimized parameters and by the Scherer equation the crystallite sizes can be determine.