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CCP14

Tutorials and Examples

Powder Cell for Windows, Structure Visualisation/Manipulation, Powder Pattern Calculation and Profile Fitting by Werner Kraus and Gert Nolze

Performing Le Bail structureless whole pattern fitting using Powder Cell

The CCP14 Homepage is at ***http://www.ccp14.ac.uk***

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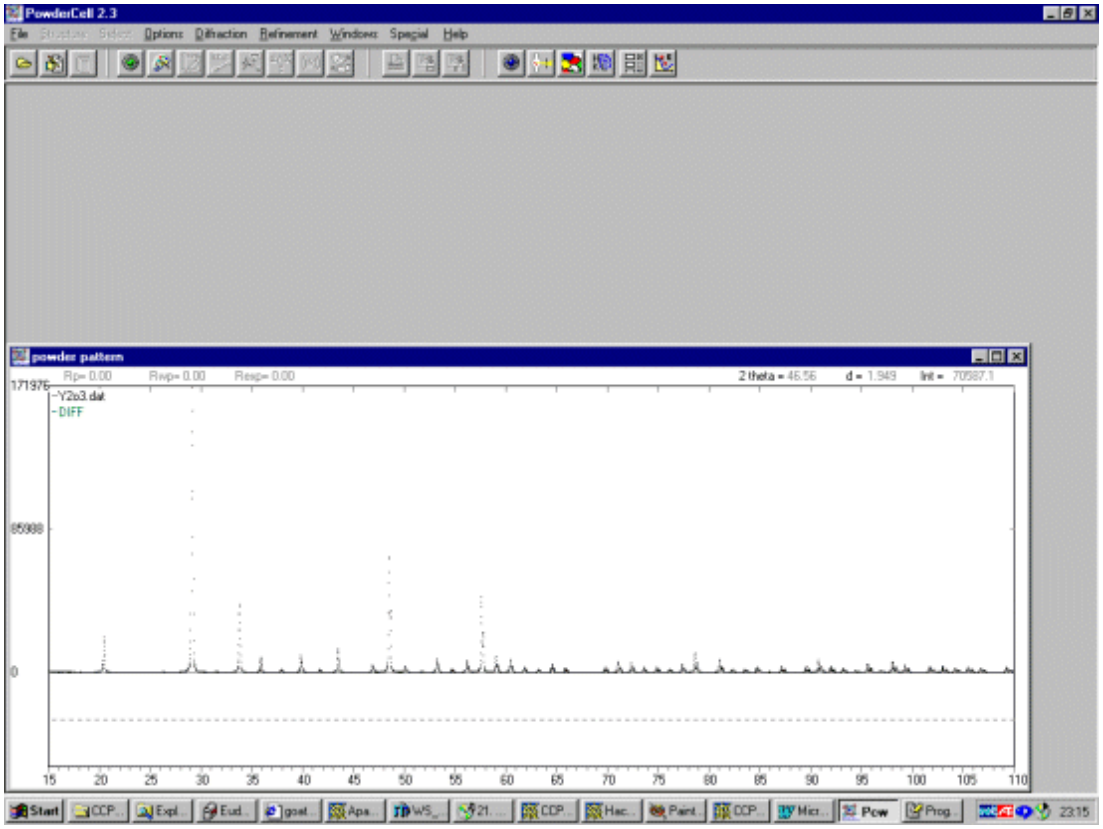
The following run-through is for Powder Cell 2.3 You may find for more complicated data involving nasty backgrounds and peak anisotropy, other programs such as LHPM-Rietica, Fullprof, GSAS, etc should be used to handle this. Powder Cell provides a very easy interface to perform simple Le Bail fitting.

We will be using Cubic Y2O3 as the example to be profiled using the following starting information

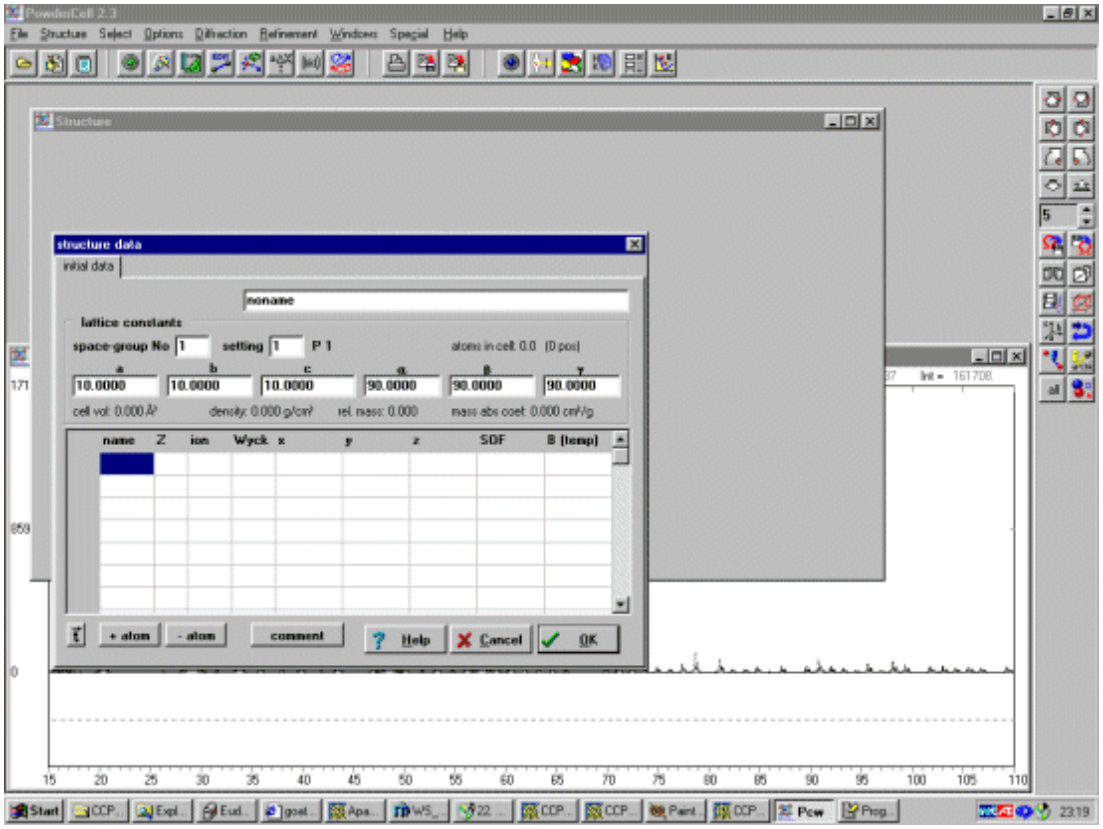
```
Spacegroup = I A 3 - (206)
CELL is 10.5981 10.5981 10.5981 90 90 90
```

For strutureless Le Bail fitting, Powder Cell 2.3 may complain there are no atoms but just ignore this (or you can give it a "dummy" atom to stop it complaining). You can also load any struture and just change the cell and spacegroup. For Le Bail, Powder Cell will ignore the atomic information.

Open up your powder diffraction data using **Diffraction, Load Powder Pattern**.

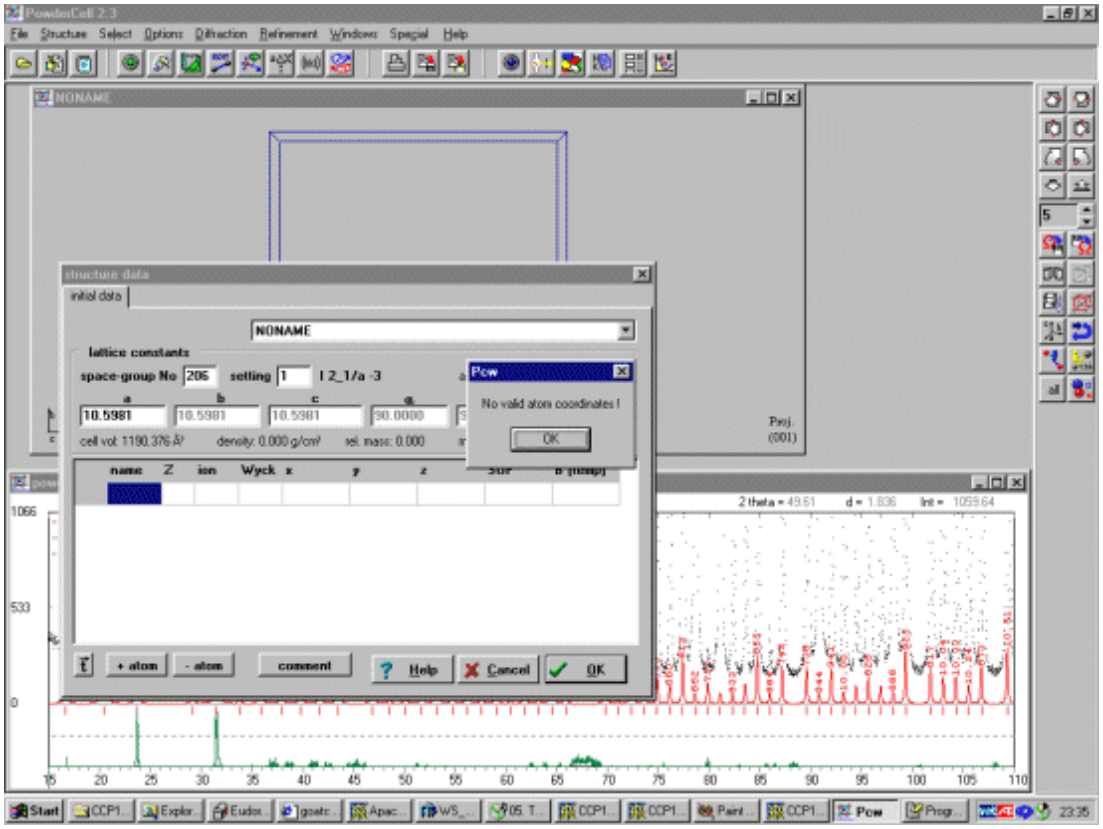


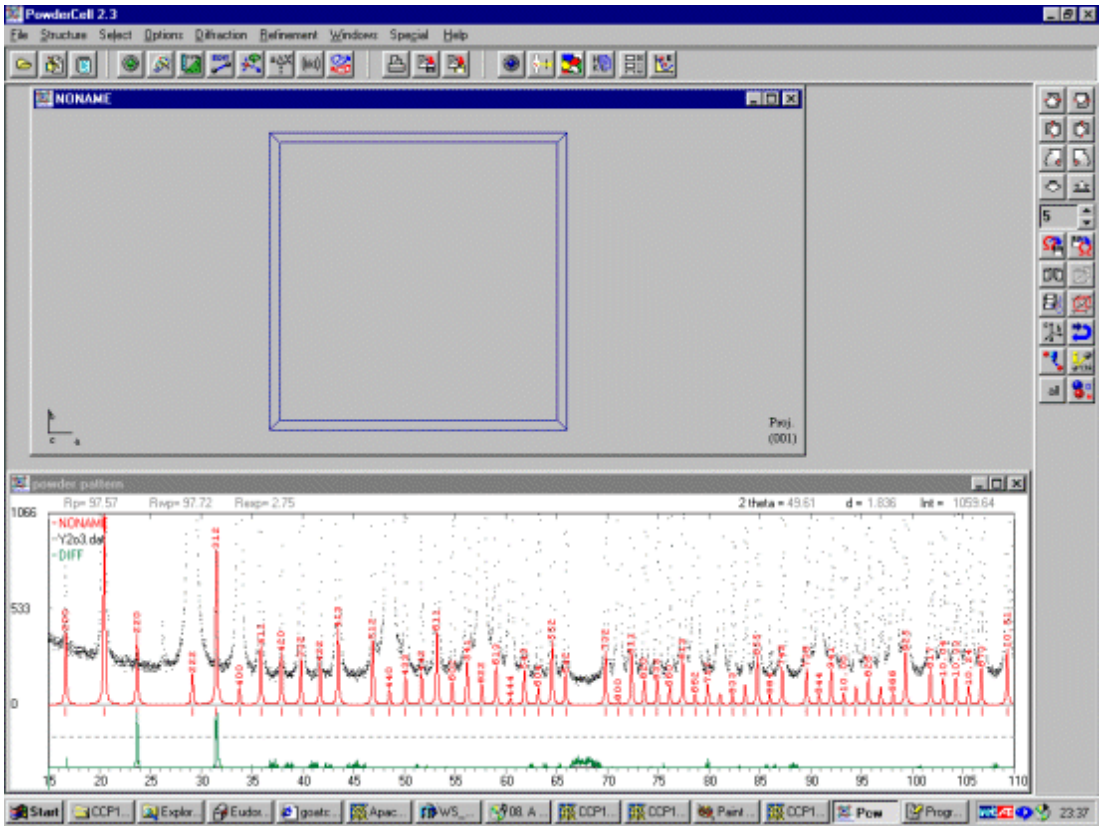
In this case, we will enter a new structure from scratch by selecting **File, New**.



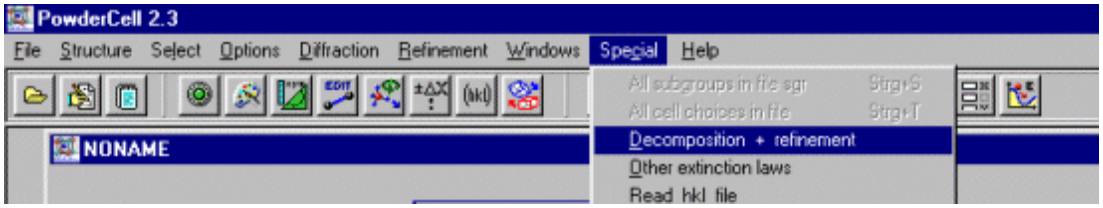
Enter the Spacegroup and Cell and Press OK. Powder Cell will complain there are no atoms but just ignore this.

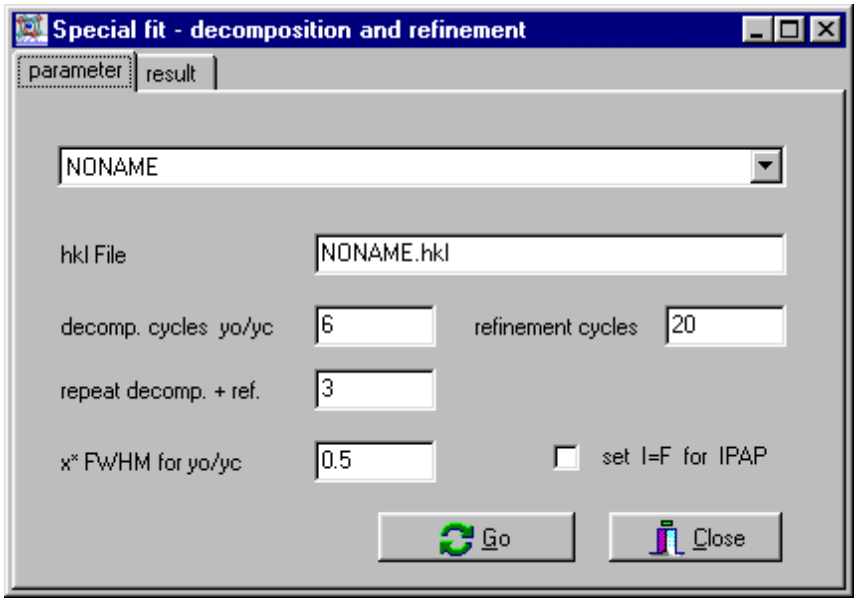
```
Spacegroup = I A 3 - (206)
CELL is 10.5981 10.5981 10.5981 90 90 90
```


PowderCell 2.3
File Structure Select Options Diffraction Refinement Windows Special Help
NONAME
structure data
initial data
NONAME
lattice constants
space-group No 206 setting 1 I 2_1/a -3
a b c α
10.5981 10.5981 10.5981 90.0000
cell vol: 1190.376 Å³ density: 0.000 g/cm³ rel. mass: 0.000
name Z ion Wyck x y z
+ atom - atom comment Help Cancel OK
Pcw
No valid atom coordinates !
OK
Proj. (001)
2 theta = 49.61 d = 1.836 Int = 1059.64
Start CCP1... Explor... Eudox... goetc... Apac... WS_... 05 T... CCP1... CCP1... Paint... CCP1... Pcw Prog... 23:35

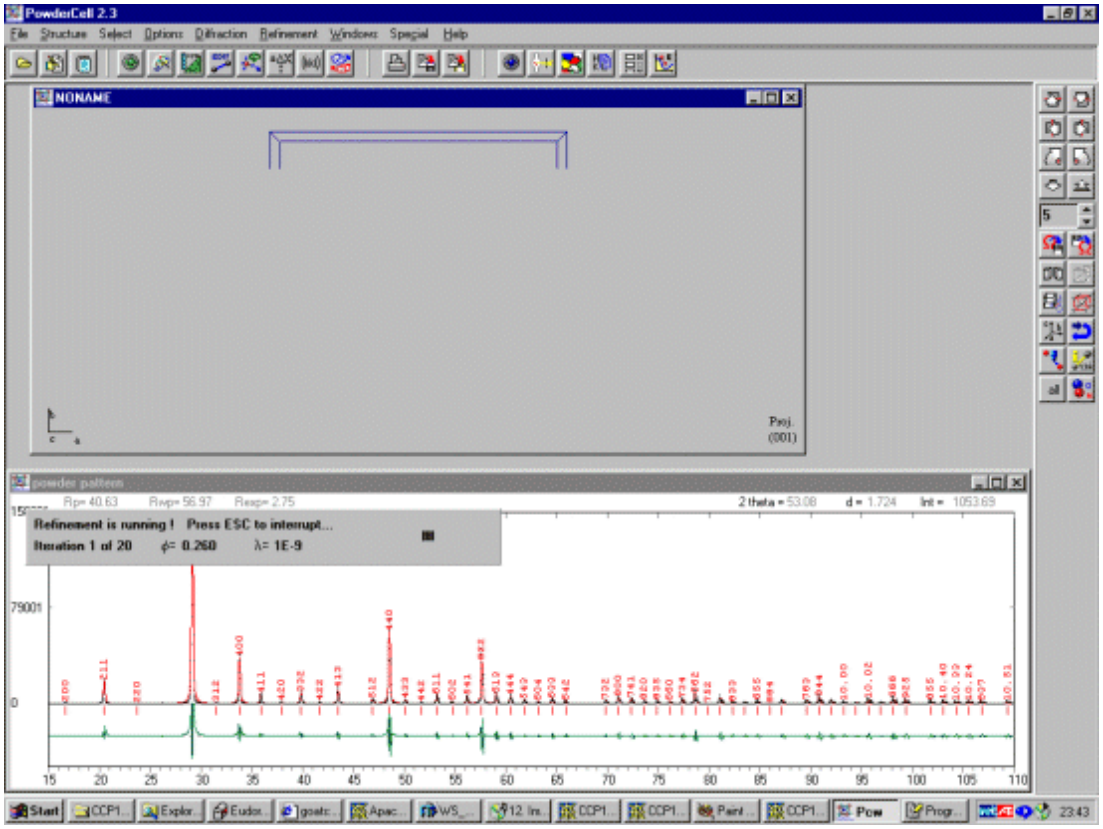

PowderCell 2.3
File Structure Select Options Diffraction Refinement Windows Special Help
NONAME
Proj. (001)
powder pattern
Rp= 97.57 Rwp= 97.72 Rexp= 2.75
2 theta = 49.61 d = 1.836 Int = 1059.64
NONAME
Y2o3.dat
DIFF
Start CCP1... Explor... Eudox... goetc... Apac... WS_... 08 A... CCP1... CCP1... Paint... CCP1... Pcw Prog... 23:37

To start the Le Bailing Fitting, enter **Special, Decomposition and Refinement**

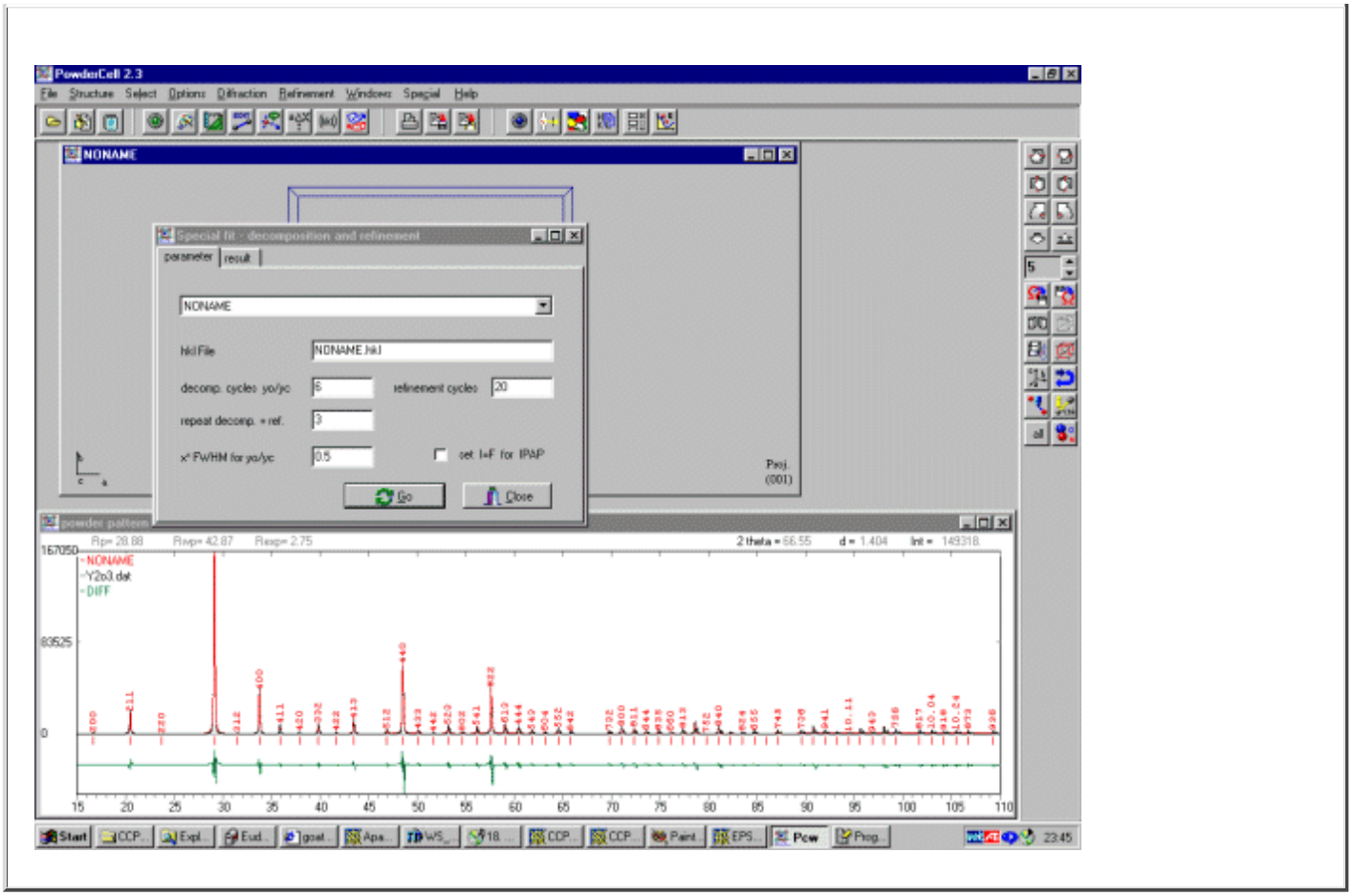




Now select **GO** and the Le Bail fitting should start and converge. If it does not, enter **Refinement, Parameters** and deselect some relevant parameters which may be dependent on the type of pattern you are trying to fit.



Done. With the Green different plot below the powder pattern. Display options can be enabled and disabled by selecting the right mouse button and the required option. An HKL file will be present in the same directory as the powder data and there is also the option of reading in Shelx files to optimise them to the powder data.



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