NOTE: CARBONXS IS A SUPERIOR PROGRAM, USE IT

J. DAHN

CARBONXS IS BETTER!

Structure Refinement Programs for Disordered Carbons - USERS MANUAL

By Hang Shi, J.N. Reimers and J.R. Dahn

This documentation describes two carbon structure refinement programs, HANGPROG.FOR and CARBONXS.FOR which can be used to determine the structural parameters of a disordered carbon according to the models described in references 1 and 2, which are included with this software.

1 DIFFRACTOMETER REQUIREMENTS

The programs are setup to accept data from powder diffractometers configured in the Bragg-Brentano pseudofocussing geometry. Samples must be flat plates. The incident beam slits must be of fixed angular divergence, chosen so that the beam does not extend beyond the edges of the sample at any angle (this is important at low angle). We have found that $1/2^o$ incident slits are a good choice for $CuK\alpha$ radiation for the angular range between 10^o and 130^o in scattering angle. The program assumes that a diffracted beam monochromator is present on the diffractometer. If your machine is not equipped with one, simply make the appropriate change to the expression for the polarization factor in the the programs.

2 SAMPLE TYPES

Thick Samples up to about $2.5mm$ thickness can be used to obtain maximum count rates for both programs. Since carbon has a small absorption factor, the beam penetrates throughout the sample, so that the sample cannot be considered infinitely thick. The programs take the absorption into account provided that the sample holder depth (thickness of the carbon in the sample well), the sample width (parallel to the beam direction, the beam width and the goniometer radius are supplied. Figure 1 shows these quantities. The actual absorption factor for the carbon as packed into the holder should be used. This is obtained by taking the absorption factor for bulk carbon ($9cm^{-1}$ for $CuK\alpha$) and multiplying by the sample density (as packed into the holder) divided by the carbon density. It is typical for such samples to have densities near $1g/cc$, so an absorption factor of

$$9cm^{-1}x1g/cc/2.2g/cc \cong 4cm^{-1}$$

often is used. These geometrical factors and absorption factors are supplied to the program in an input file as described below.

Thin samples on zero background holders can also be used. These samples should be less than $200\mu m$ thick. Both programs can be used and an estimate of the sample thickness is still required by the programs. Thick samples give much larger count rates than thin ones.

3 PROGRAMS ON DISK

The Disk included contains 2 directories, HANGPROG and CARBONXS

3.1 HANGPROG

In the directory HANGPROG, you will find the following files.

1. HANGPROG.FOR - fortran 77 source code. This has been compiled successfully on a SUN IPC workstation (SUN FORTRAN) using the command '$f77$ HANGPROG.FOR' and on IBM PCs using Microsoft Fortran with the command
'$FL - Gt$ HANGPROG.FOR'. If the program will not compile for you, consult a fortran expert at your location. The program will also compile using the 32 bit Lahey Fortran compiler - use the following commands for Lahey
$os386$ - installs Lahey Kernal
$F77L3$ Hangprog.for - Compiles and makes object file
UP $L32$ Hangprog; - Links
UP HANGPROG - Runs the Code.

2. SCAN.DAT - A sample data set measured on a soft carbon heated to 2850°C.

3. OUTPUT.DAT - The output file after refinement which contains 4 columns, 1 - scattering angle, 2 - measured counts, 3-calculated counts and 4-difference between measured and calculated counts.

4. CONTR.INI - the control file to control the refinement.

5. PARS.OUT - a file generated at the end of the refinement which shows the final refined parameter values and their statistical errors. The statistical errors assume that in the absence of counting noise that the theory would exactly agree with the data. It does not, so the error estimates are generally too small. Nevertheless, they are a useful guide.

6. HS.INC - A file which must be present in the directory where compilation is done.

3.2 CARBONXS

In the directory CARBONXS, you will find the following files

1. CARBONXS.FOR - fortran 77 source which compiles successfully as does HANGPROG.FOR using the SUN and Lahey compilers with the same commands. The program is too big for the simple Microsoft compiler.

2. SCAN.DAT - Same data file as SCAN.DAT used for HANGPROG

3. CARBON.INP - an input file which serves the same purpose as does contr.ini for HANGPROG

4. CARBON.OUT - the output file of parameters after refinement, including error estimates as above. The correlation matrix is also included.

5. CARBON.CMN - A common block setup segment which must be present during compilation.

6. CARBON.DAT - A four column output file which contains the same 4 columns as does OUTPUT.DAT for HANGPROG

4 DESCRIPTION OF THE THEORETICAL MODEL AND MEANING OF THE PARAMETERS

See references 1 and 2. The input and output files contain brief descriptions of the parameters.

5 SAMPLE FITS

Figures 2,3 and 4 show respectively data and calculations for a soft carbon heated to $2850°C$, using HANGPROG on a thick sample, HANGPROG on a thin sample and CARBONXS on a thin sample. The refined parameter values for the three refinements are tabulated in table 1 below. Each refinement used only a constant background.

As an aid in interpreting these refined parameters, we offer the following comments. $d(002)$ and a are the average layer spacing and the in-plane lattice constant, respectively. L_a is the basal plane coherence length in angstroms. M is the number of 2 layer stacks stacked to form the crystal (L_c = 2xMxd(002)). Both programs are using the two layer model (see references) for this calculation, so we are stacking AB registered two layer units. P is the probability for finding a random rotation or translation between adjacent 2-layer units, so $P/2$ is the probability for finding such a translation per layer. P_t is the probability of finding $a3R$ stacked sequence per 2-layer unit, so $P_t/2$ is the probability of finding $a3R$ stacked sequence per layer. $(< \delta^2 >)^{1/2}$ is the average value of the interlayer spacing fluctuation between adjacent 2-layer units, so that $(< \delta^2 >)^{1/2}/2$ is the average layer spacing fluctuation per layer. B is the Debye Waller factor, assumed isotropic. PO

is the preferred orientation parameter, which is unitless. NOTE THAT IN THE 2 LAYER MODEL CARBONXS RETURNS $P/2, P_t/2$ and $(< \delta^2 >)^{1/2}/2$ which are the relevant quantities PER LAYER. HANGPROG RETURNS P, P_t and $(< \delta^2 >)^{1/2}$ which must be divided by 2 to get the relevant quantities PER LAYER.

Low temperature carbons ($T < 2100°C$) are best refined using the so-called one layer model, which can be selected in each program. When refining such carbons, it is important that the background be chosen as a constant, so that meaningful fits can be obtained. A Polynomial background function is available in CARBONXS.

6 GENERAL COMMENTS ABOUT THE LIMITATIONS OF THE PROGRAMS

The diffractometer resolution function has not been included in the program. Thus if crystalline carbons, where $K\alpha_1$ and $K\alpha_2$ peaks are well resolved are encountered, the program will have difficulty. However, our experience of over 70 industrially available and home-made carbons shows no such occurrence. The program therefore uses the average $K\alpha$ wavelength.

If the carbon is very crystalline, the estimates for L_a and L_c will be unreliable, because the diffractometer resolution function will contribute to a large fraction of the peak width.

The programs are most impressive in their operation on carbons heated above 2100°C. The refined values of P and P_t are very good and extremely useful. We know of no other direct method to reliably extract these parameters, which measure the probability for stacking disorder of two types.

Examples of fits on low temperature carbons which can guide the user are given in reference 2.

7 DETAILED DESCRIPTION OF THE OPERATION OF HANGPROG

7.1 Introduction

This structure refinement program was developed at Simon Fraser Universityfor refining the X-raypowder diffraction patterns collected on disordered hard and soft carbons. The program minimizes the difference between the observed and calculated diffraction profiles in a least-squares sense by optimizing model parameters analogously to the popular Rietveld refinement method. Unlike the Rietveld method, which is designed for crystalline materials, our program allows the quantification of the finite size and disorder present in disordered layered materials like carbon fibers and cokes. For the details of the method

and the theory the reader should refer to the Ph. D thesis of Hang Shi at Simon Fraser University or to Hang Shi, J.N. Reimers and J.R. Dahn, *J. Appl. Cryst.* in press, a copy of which is included with the disks. Requests for the program, which is available on disk, should be directed to Jeff Dahn at Department of Physics, Simon Fraser University.

7.2 Getting Started

To use this program to fit a X-ray powder diffraction pattern collected on a carbon material, first compile this program on your own machine to get a executable file (we have developed the code on a SUN SPARC station using SUN FORTRAN 1.3.1). The program also compiles successfully and runs on PCs using microsoft fortran or Lahey Fortran. You will need the following two input files.

1. an X-ray data file named *scan.dat*
2. a control file with a name *contr.ini*

The raw data file *scan.dat* must be in following format

```
10.15004     1030.00
10.34995     1008.00
10.54999     1020.00
10.7500     1073.00
10.9500     990.000
11.1500     1015.00
11.3500     971.000
11.5500     927.000
11.7500     997.000
11.9500     949.000
12.1500     907.000
12.3500     902.000
12.5500     883.000
12.7500     921.000
12.9500     912.000
13.1500     874.000
13.3500     883.000
13.5500     930.000
13.7500     931.000
13.9500     881.000
14.1500     924.000
14.3500     865.000
```

The first column is the Scattering angle. The second column is the measured intensity. The control file *contr.ini* must have the following format,

```
CONTROL FILE OF PARAMETERS
1       A switch, 1 for fitting, 0 for calculating.
2       1 for the one layer model,2 for the two layer model
3       Number of Iterations desired
EXPERIMENTAL CONDITIONS
1.541800          the wave length  of X-ray in Angstrom
0.25          the depth of sample holder in cm
1.60          the width of sample holder in cm
17.30          the gonimeter radius in cm
0.15          the width of the X-ray beam in cm
PARAMETERS       STEPS   On/off     Description
28.546311       0.50000    1    Overall scale factor
846.231874       5.00000     1    Background constant
0.348573       0.01000    1    Isotropic thermal parameter
0.000000       0.00010    0    In-plane strain
0.115399       0.00500    1    g(1-layer) or 3R stacking Pt(2-layer)
3.388945       0.00200    1    d002, layer spacing (Angstrom)
2.463764       0.00200    1    a, a-axis (Angstrom)
0.553011       0.05000    1    P,random stacking probability
182.559811       1.00000     1    La, layer extent (Angstrom)
0.093969       0.00200    1    delta, layer fluctuation (Angstrom)
0.147609       0.01000    1    Preferred Orientation factor
4.000000       0.00100    0    Absorption factor (1/cm)
35.936856       0.50000    1    Average layer number
```

A sample *contr.ini* file is included with the programs on the distribution disk. The comments in the file *contr.ini* are not critical, only for clarity. The first three numbers of *contr.ini*allow you to choose which model (the one layer or the two layer) to be used foryour carbon.

One can also simply calculate the intensity based on a particular model by setting the switch in the first line at *contr.ini*. To avoid nonlinear divergences while fitting the carbon data, one needs reasonable values for the initial parameters. This is done by calculating the intensity for *guessed* paramters to see if it closely matches the data. Once the agreement is close, the parameters can be optimized automatically. For graphitic carbons, the two layer model has to be used, and for disordered carbons, the one layer model is needed.

The maximum number of iterations can be set to prevent endless iteration with little further reduction in the goodness of fit. The next three columns are parameters and the steps. The steps are used to calculate the derivatives of $\partial\chi^2/\partial a_i$, where a_i is the

ith parameter. The steps should be about 1 percent of the parameter values, except for the lattice constants where the steps should be about 0.002 angstroms. The first column contains the parameters. You should estimate 13 parameters for the carbon you want to fit. Random guessing is not effective. One can get a good estimate based on the measured patterns. The third column is a switch whichallows you to decide which parameter you want to adjust. Sometimes, we only want to adjust some of these parameters. The On/Off switch in the *contr.ini* file is designed for this purpose.

7.3 Ready to Run

The usual procedure to fit a new carbon is

1. estimate a list of parameters,
2. decide which model to use (by looking the X-ray pattern)
3. set the switch to calculate the trial pattern
4. run the program
5. compare the calculated and measured intensities. The program will create an output file called output.dat which contains four columns. These are scattering angle, measured intensity, calculated

   intensity and the difference between them.
6. Readjust the parameters to get better agreement until you consider it is ready to use iteration procedure to automatically fit the data.

The running time depends on how many data were collected and which model is used. For a graphitic carbon with 2000 data points, it takes about one half hour on a SUN IPC and for a disordered carbon, the running time is shorter. A 486 machine is the minimum recommended computing power. When the program stops,
the following files will appear in the same directory.

contr.new the new contr.ini file with updated parameter values after iteration

chi.i a file listing the chi square value during the iteration.

status a run time file to watch the parameter changes.

status.m a similar run time file like status for watching how the program is doing.

output.dat the output file, which contains the fitted data and raw data as explained above.

pars.out an output file containing structural parameter information,

the correlation matrix, errors etc..

If you want to change some parameter, say No. of iteration, and the run the program again, you can copy *contr.new* to *contr.ini* as a new starting control file and do it again.

7.4 Program

The program was written in FORTRAN 77 at Department of Physics, Simon Fraser University and developed on a sun workstation. A brief description of the various subroutines is as follows,

MAIN main program, which calls in succession the subroutines ARRAY, FAC, MRQMIN, OUTINFO, FXP.

ARRAY Calculates a data array for integral usage.

FAC Calculates polarization factor and atomic scattering factor by using the expressions in the international tables for crystallography. The polarization factor incorporates those terms for a diffracted beam monochromator. If your diffractometer does not have such a monochromator, change the polarization factor in this program accordingly.

OUTINFO Write output files.

FXP Convolutes the model function to include the sample thickness etc..

MRQMIN a main subroutine for iteration, which calls MRQCOF, GAUSSJ,COVSRT.

GAUSSJ Gauss linear equation solver.

COVSRT a program which comes with GAUSSJ.

MRQCOF a subroutine to calculate the chi square, which calls DFDX.

DFDX derivative calculator, which calls FXP for evaluating the model values, which calls FUNC1 and FUNC2.

FUNC1 calculates the intensity for the one layer model.

FUNC2 calculates the intensity for the two layer model. Both FUNC1 and FUNC2 call the GOOL,SIC.

GOOL a subroutine for calculating the 00l intensity.

SIC a subroutine for calculating the hk0 intensity, which calls QGAUS1,QGAUS2.

QGAUS1,QGAUS2 two integral subroutines using GAUSS method to do fast integral calculations, which calls SFFI.

SFFI evaluate the model intensity for integral, which calls GF,ST.

GF a subroutine to calculates the interference function G.

ST a subroutine to calculate the density distribution in a rod.

Users should report to Hang Shi when they find errors in these codes.

8 DETAILED DESCRIPTION OF CARBONXS

This program was written by Jan Reimers and the code is much easier to follow than HANGPROG. The strategy for using the program is similar to that of HANGPROG. The program is MUCH FASTER and is more user friendly.

Key differences to Hangprog include:

1.*A* background function of the form similar to that typically used in the Rietveld method

2.*A* possibility to change the number of points in the tangent cylinder integral (# points in phi integral). Best set to 10 or more. Hangprog uses 50 points in the TC integral, so using 10 in CARBONXS gives a factor of 5 in speed.

3.*A* possibility to include intensity to 3 or more halfwidths of the intensity on the Bragg rods (assumed peak width). Best set to 3.

4. The possibility of refining the width of the M distribution (see reference 1).

5. This program runs about ten times as fast as HANGPROG, mainly because all needed derivatives are calculated analytically. In HANGPROG, the derivatives are evaluated numerically and the parameter steps for derivative taking must be given. This is not necessary when using CARBONXS.

6.*A* Sample input file (CARBON.INP) is included on the disk. The input file has the following structure.

Line 1 – Data file name (file contains scattering angle and counts in 2 columns)

line 2 – Start angle for refinement, End angle for refinement, wavelength, use every n^{th} data point only for the calculation (this speeds the program when you are just trying things out).

Line 3 – number of parameters included, number of points to include in the TC integral, number of halfwidths of the Bragg rods to include (use 3 or more), switch to select the one layer model (1) or the two layer model (2).

Line 4 – The fraction of bulk density that the sample is (less than 1), the goniometer radius in mm, the depth of the sample in mm, the width of the sample in mm, the width of the beam perpendicular to its direction (see Fig. 1).

Line 5 – The maximum number of iterations, The smallest change in χ^2 that the program will accept,

Line 6 - Debugging tools, do not fiddle with these

Line 7 - Scale factor, switch (1=refine, 0=don't refine)
Line 8 - Constant Background, switch
Line 9 - Background S, switch
Line 10 - Background $S**2$, switch
Line 11 - Background $S**3$, switch
Line 12 - Background $S**4$, switch
Line 13 - Background $1/S$, switch
Line 14 – a lattice constant (angstroms), switch
Line 15 – d_{002}, switch
Line 16 – $L_a(angstroms)$, switch
Line 17 – M TOTAL number of layers, switch
Line 18 – SM width of M distribution, switch
Line 19 - In plane strain (be careful with this one), switch
Line 20 - Interplane strain per layer, switch
Line 21 - Probability of Random Stacking PER LAYER (for both models), switch
Line 22 – g(one layer model) or Probability of $3R$ stacking PER LAYER (2 layer model), switch
Line 23 - Debye Waller (Temperature Factor) (angstroms$**2$), switch
Line 24 - Preferred Orientation Factor, switch

9 FINAL REMARKS

All problems with the program should be reported to Jeff Dahn.
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email jeff@dahn.phys.sfu.ca

10 REFERENCES

1. Hang Shi, J.N. Reimers and J.R. Dahn, Accepted for publication in J.Applied Crystallography
2. Hang Shi, PhD. Thesis, Physics Dept., Simon Fraser University, Burnaby B.C., Canada $V5A1S6$

Table 1: Refined parameters for the carbon fits shown in figures 2,3 and 4

PARAMETER	HANGPROG THICK SAMPLE	HANGPROG THIN SAMPLE	CARBONXS THIN SAMPLE
d(002) (Å)	3.367	3.361	3.363
a (Å)	2.458	2.458	2.458
L_a (Å)	301(11)	211(2)	210(2)
2M	90	88	82
P/2	0.277	0.267	0.276
$P_t/2$	0.059	0.070	0.064
$(\langle d^2 \rangle)^{1/2}/2$ (Å)	0.042	0.057	0.055
B $(Å)^2$	1.24	1.01	0.69
PO	0.63	0.41	0.33

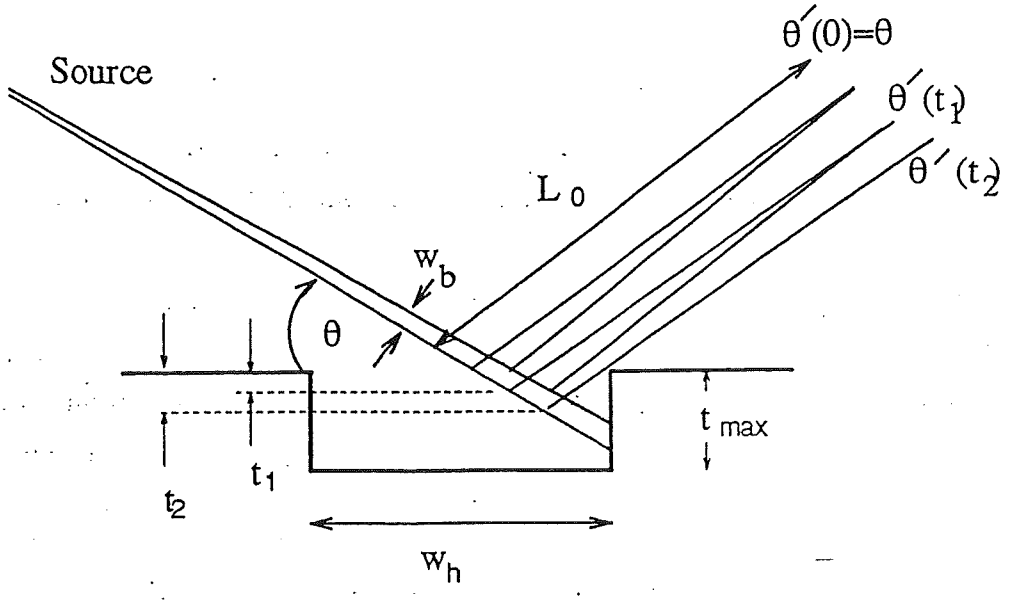


Figure 1. Sample holder geometry.

t_{max} = sample holder depth

w_h = holder width

w_b = beam width

L_0 = goniometer radius

Figure 2

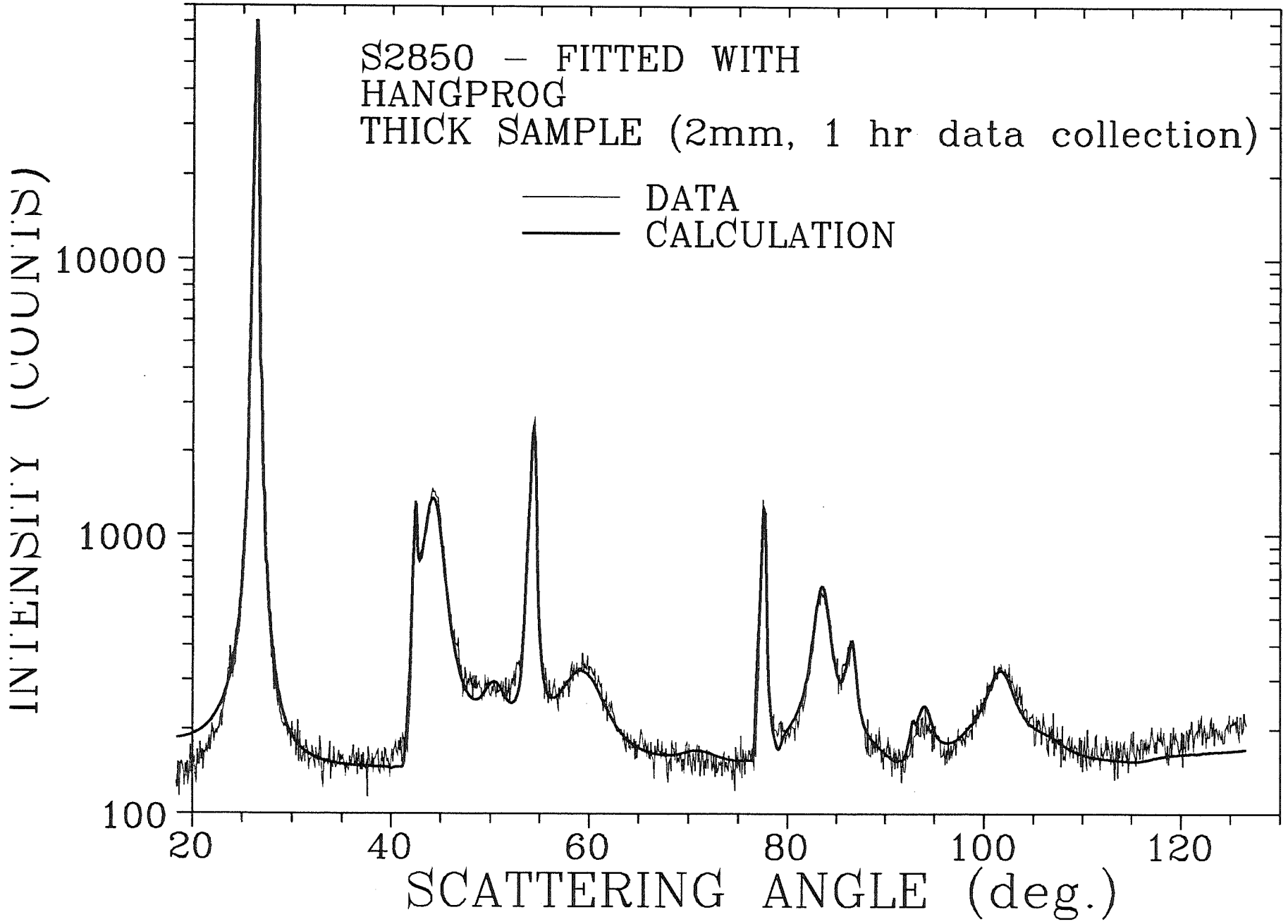

S2850 – FITTED WITH
HANGPROG
THICK SAMPLE (2mm, 1 hr data collection)
DATA
CALCULATION
INTENSITY (COUNTS)
10000
1000
100
20
40
60
80
100
120
SCATTERING ANGLE (deg.)

Figure 3

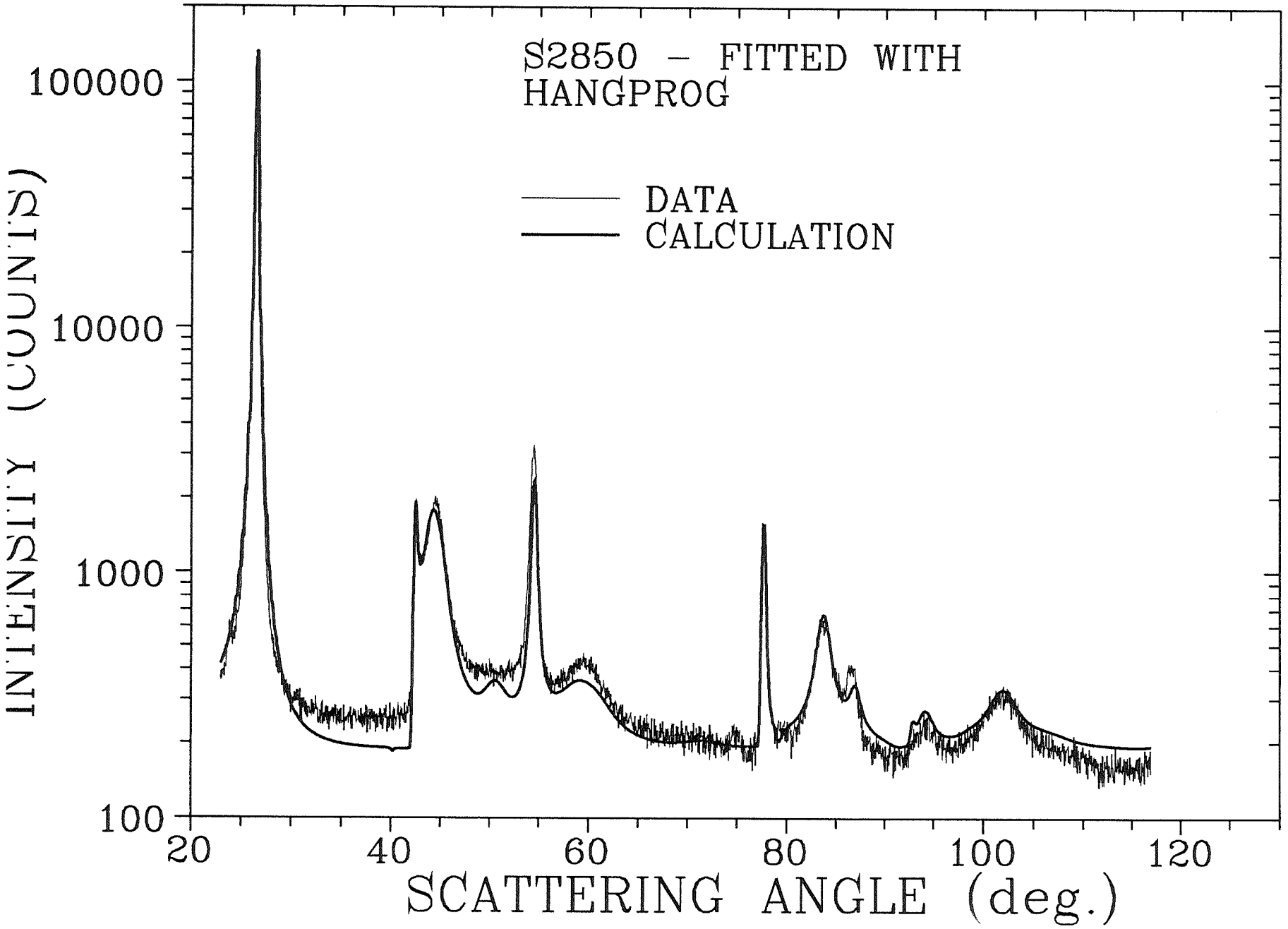
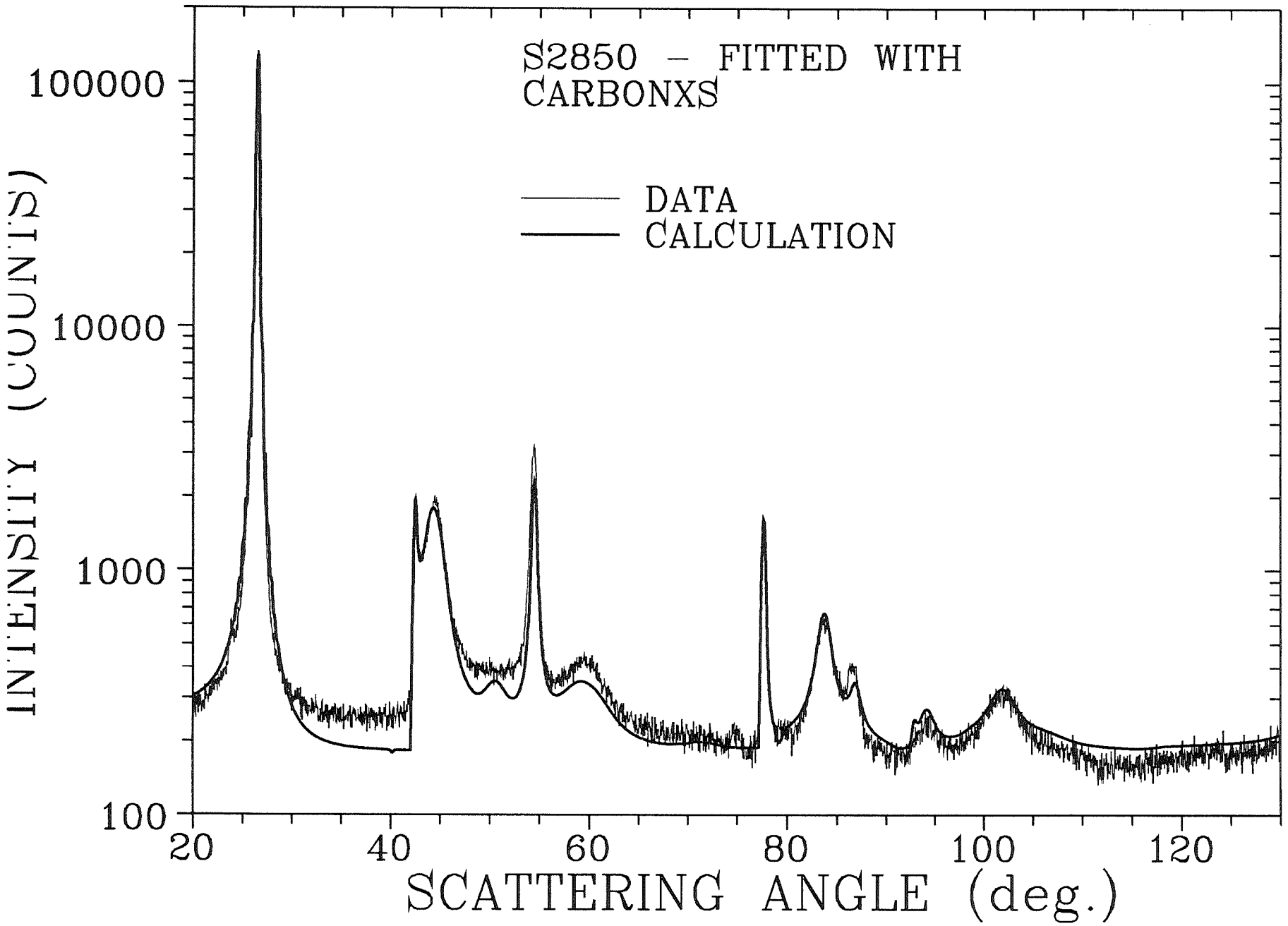

S2850 – FITTED WITH HANGPROG
DATA
CALCULATION
INTENSITY (COUNTS)
100000
10000
1000
100
20
40
60
80
100
120
SCATTERING ANGLE (deg.)

Figure 4.


S2850 – FITTED WITH CARBONXS
DATA
CALCULATION
INTENSITY (COUNTS)
100000
10000
1000
100
20
40
60
80
100
120
SCATTERING ANGLE (deg.)

KS 285° THICK

# of raw data pts	1151	Raw theta limits	15.00 to 130.00
# of data pts used	1151	Theta limits used	15.00 to 130.00
Max # of it's	8	Min delta Chi^2	0.00100
# of pts in TCI	10	TCI range	+/- 3 Sigma
Relative Density	0.500	Stacking Model	2 layer
Goniometer Radius	185.000(mm)	X-ray Beam Width	1.500(mm)
Sample Well Depth	2.000(mm)	Sample Well Width	25.000(mm)

CARBON XS
2 layer model
KS 285° THICK

Iter #	Chi^2	Alambda
1	5.53439	0.10E-01
2	5.53308	0.10E-02

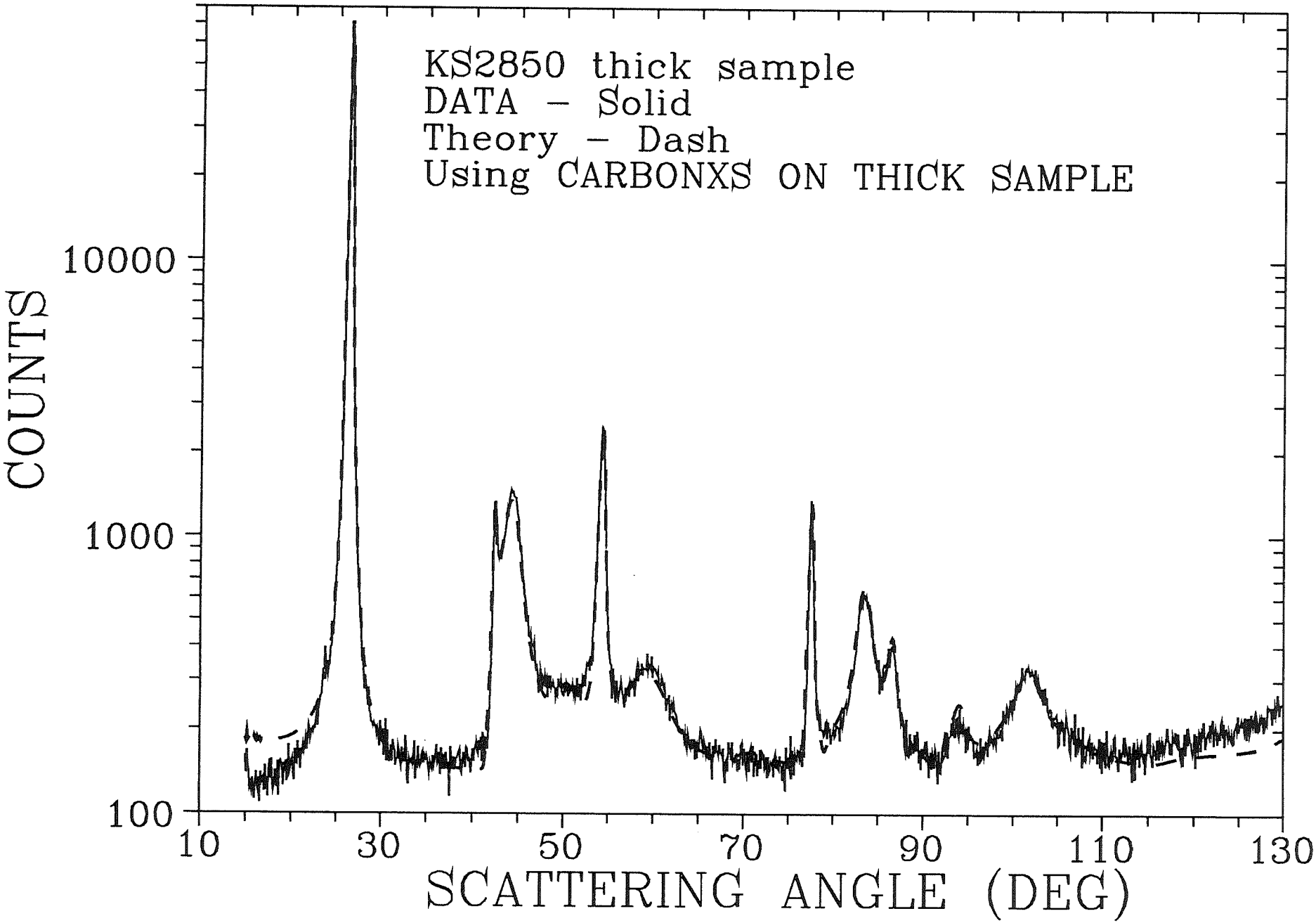
Correlation Matrix

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	100	6	0	0	0	0	0	0	-4	99	12	0	0	7	10	-4	6	4
2	6	100	0	0	0	0	0	-8	0	6	-4	0	0	-19	-26	20	49	-5
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	-8	0	0	0	0	0	100	0	0	0	0	0	2	17	-11	-8	5
9	-4	0	0	0	0	0	0	0	100	-3	-10	0	0	-2	0	1	0	0
10	99	6	0	0	0	0	0	0	-3	100	0	0	0	0	11	-4	4	4
11	12	-4	0	0	0	0	0	0	-10	0	100	0	0	68	0	0	-6	6
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	7	-19	0	0	0	0	0	2	-2	0	68	0	0	100	3	-2	-16	11
15	10	-26	0	0	0	0	0	17	0	11	0	0	0	3	100	-81	-17	-3
16	-4	20	0	0	0	0	0	-11	1	-4	0	0	0	-2	-81	100	14	2
17	6	49	0	0	0	0	0	-8	0	4	-6	0	0	-16	-17	14	100	-59
18	4	-5	0	0	0	0	0	5	0	4	6	0	0	11	-3	2	-59	100

Final Parameters

Old Value	New Value(esd)	Description
17100.	17170.(754)	Scale Factor
140.	140.(1)	Background Constant
0.000	0.00000	Background S
0.000	0.00000	Background S**2
0.000	0.00000	Background S**3
0.000	0.00000	Background S**4
0.000	0.00043	Background 1/S
2.457	2.4572(1)	A, In plane Cell constant (Angstroms)
3.364	3.36429(9)	002, Interlayer Spacing (Angstroms)
309.	308.(17)	La, Coherence Length in the AB Plane
96.	96.(1)	M, Total Number of Layers
2.000	2.00000	SM, Width of M Distribution
0.000	0.00001	DAB, In plane strain
0.043	0.0433(8)	del, Inter Plane Strain
0.289	0.289(8)	Pr, Probability of Random Stacking
0.060	0.054(7)	Pt, Probability of 3R stacking
1.04	1.04(7)	Debye Waller (Temperature) Factor (Angstroms**2)
0.63	0.63(1)	PO, Preferred Orientation Factor

Lc = 323.6(1.7)


KS2850 thick sample
DATA - Solid
Theory - Dash
Using CARBONXS ON THICK SAMPLE
COUNTS
10000
1000
100
10
30
50
70
90
110
130
SCATTERING ANGLE (DEG)

KS900

# of raw data pts :	576	Raw theta limits :	5.00 to 120.00
# of data pts used :	526	Theta limits used :	15.00 to 120.00
Max # of it's :	8	Min delta Chi^2 :	0.00100
# of pts in TCI :	10	TCI range :	+/- 3 Sigma
Relative Density :	0.500	Stacking Model :	1 layer
Goniometer Radius :	173.000(mm)	X-ray Beam Width :	1.500(mm)
Sample Well Depth :	2.500(mm)	Sample Well Width :	16.000(mm)

Cabon X5

1 layer model

KS900

Iter #	Chi^2	Alambda
1	43.81709	0.10E+01
2	43.81414	0.10E+00

Correlation Matrix

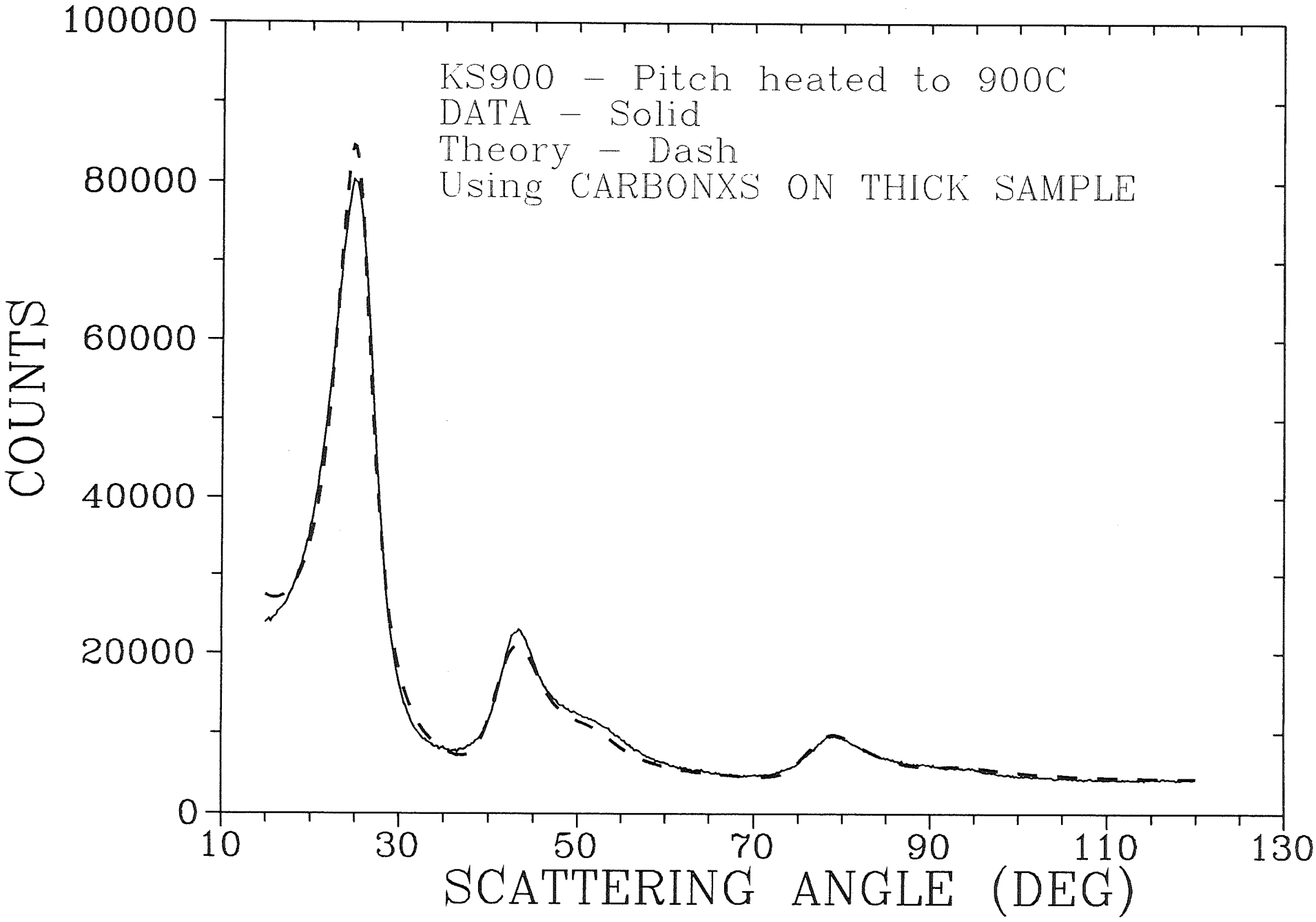
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	100	39	0	0	0	0	-24	31	-26	89	0	0	0	-7	0	-10	51	0	
2	39	100	0	0	0	0	-89	10	-36	1	0	0	0	4	0	-16	77	0	
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
7	-24	-89	0	0	0	0	100	-4	43	17	0	0	0	2	0	29	-50	0	
8	31	10	0	0	0	0	-4	100	-3	33	0	0	0	20	0	20	15	0	
9	-26	-36	0	0	0	0	43	-3	100	-2	0	0	0	-4	0	10	-25	0	
10	89	1	0	0	0	0	17	33	-2	100	0	0	0	1	0	10	24	0	
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
14	-7	4	0	0	0	0	2	20	-4	1	0	0	0	100	0	93	0	0	
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
16	-10	-16	0	0	0	0	29	20	10	10	0	0	0	93	0	100	-6	0	
17	51	77	0	0	0	0	-50	15	-25	24	0	0	0	0	0	-6	100	0	
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	

Final Parameters

Old Value	New Value(esd)	Description
13600.	13594.(53)	Scale Factor
2777.	2776.(24)	Background Constant
0.000	0.00000	Background S
0.000	0.00000	Background S**2
0.000	0.00000	Background S**3
0.000	0.00000	Background S**4
761.	760.(18)	Background 1/S
2.451	2.4511(7)	A, In plane Cell constant (Angstroms)
3.482	3.4827(8)	002, Interlayer Spacing (Angstroms)
15.7	15.7(1)	La, Coherence Length in the AB Plane
50.664	50.66446	M, Total Number of Layers
2.000	2.00000	SM, Width of M Distribution
0.000	0.00001	DAB, In plane strain
0.962	0.962(7)	del, Inter Plane Strain
0.990	0.99000	Pr, Probability of Random Stacking
0.405	0.405(6)	Pt, Probability of 3R stacking / g in 1 layer model
1.14	1.15(6)	Debye Waller (Temperature) Factor (Angstroms**2)
0.000	0.00088	PO, Preferred Orientation Factor

Lc = 176.4(0.0)

In one layer model, this is g


KS900 - Pitch heated to 900C
DATA - Solid
Theory - Dash
Using CARBONXS ON THICK SAMPLE
COUNTS
100000
80000
60000
40000
20000
0
10
30
50
70
90
110
130
SCATTERING ANGLE (DEG)