Maud in Action: Applying Batch Analysis Codes

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ESM499

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Introduction

Introduction to X-Ray Diffraction (XRD)

X-ray diffraction (XRD) is a powerful non-destructive test method used to analyze the crystal structure of materials by measuring the diffraction patterns of X-rays as they interact with a material, XRD can provide detailed information about the atomic or molecular structure of a material.

Basic Principle

The working principle of XRD is based on the phenomenon that X-rays interact with the atomic lattice in a material. When an X-ray beam hits a crystalline material, the X-rays are scattered by the atoms in the material. If the crystal has a regular lattice structure, the scattered X-rays will be intensified at specific angles, forming an interference pattern. This phenomenon follows Bragg's law ($n\lambda = 2d \sin\theta$), where λ is the wavelength of the X-rays, d is the lattice spacing, θ is half of the angles of incidence and reflection, and n is an integer.

Data Analysis

The data generated from the XRD experiment consisted mainly of the diffraction angle (2θ) and the corresponding intensity (I). These data were used to generate an XRD map showing the intensity distribution for different values of 2θ. Each peak in the map corresponds to a specific lattice plane, the position of the peaks (2θ values) provides information about the lattice spacing, and the shape and width of the peaks can reveal the crystal size, stress state, and other structural defects of the material. In addition, error analysis is essential to determine the reliability and accuracy of the data.

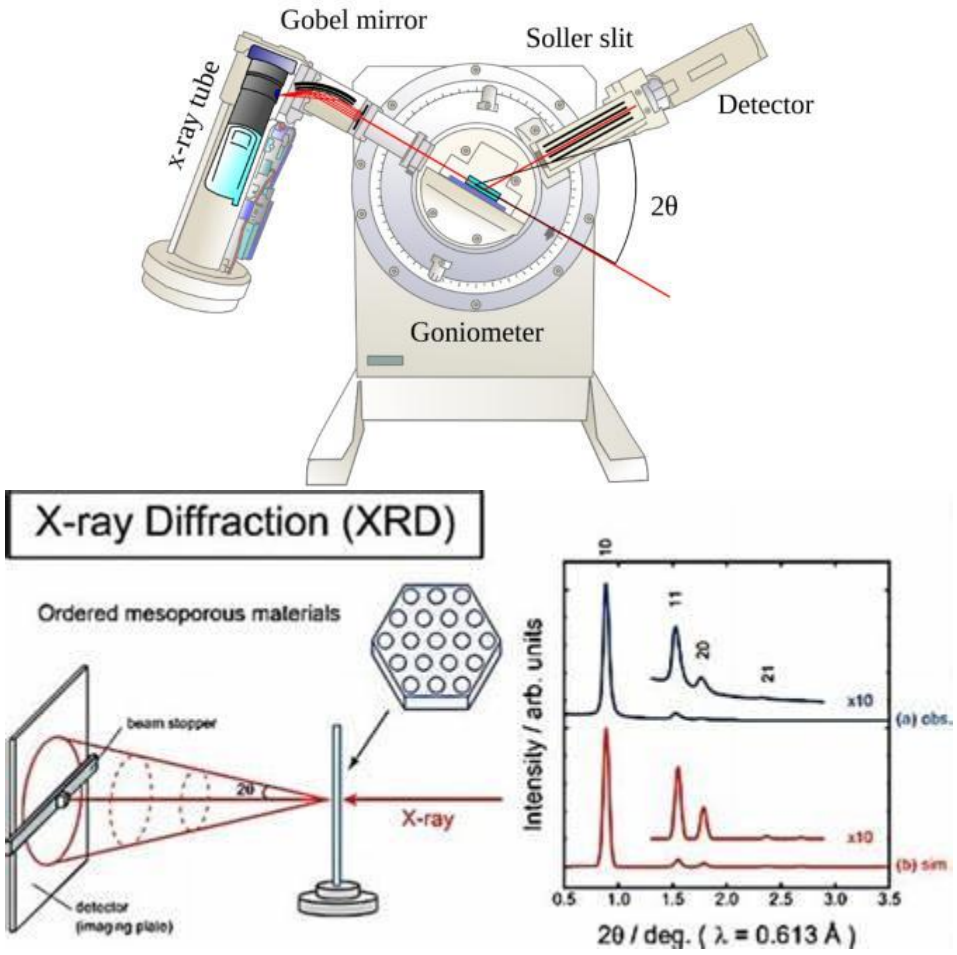

Fig1.1 XRD schematic diagram

Maud program

The precise crystallographic data analysis helps in understanding structural properties of materials. Maud is a software based on the Rietveld method that is very effective in refining diffraction data obtained from X-ray or neutron sources. The refinement includes structural parameters. Maud is used to make the fit with experimental data optimal, such as lattice constants, atomic positions, and thermal parameters that characterize properly the material under study.

However, each chi file often requires individual refinement based on the same par file to figure out subtle changes in sample characteristics or experimental conditions not reflected in the initial parameter file settings. This individual refinement process, while necessary to achieve high accuracy, is time-consuming and labor-intensive. It involves complex adjustments and reassessments of the fit between computed and observed data, often requiring considerable time and judgment.

Maud's feature allows processing multiple chi files using a single parameter file (par file) can prove very useful for situations where several experiments have been conducted under unchanged instrumental and experimental conditions. Researchers by making use of a uniform set of parameters ensure uniformity across different samples analyzed during comparative studies which are otherwise essential for keeping consistency when dealing with similar experiments conducted under similar conditions.

In this report, I will discuss the process of using Maud for batch analysis of chi files, focusing on the codes which are used to efficiently do batch analysis.

Software Requirements for XRD Data Batch Analysis

To effectively handle and analyze X-ray diffraction (XRD) data, several software tools and programming environments are essential. Here's a breakdown of the software requirements:

Strawberry Perl:

Strawberry Perl is a Perl environment for Windows that includes a Perl language interpreter, a compiler, and a large number of essential libraries and tools. It is particularly useful for scripting and automating data processing tasks. Perl scripts are often used for manipulating large datasets, formatting data, and interfacing with other software tools.

MAUD (Materials Analysis Using Diffraction):

MAUD operates on Java, thus requiring a compatible Java Runtime Environment (JRE).

Python Environment:

Essential Python libraries for XRD analysis include NumPy for numerical operations, Matplotlib for plotting, and SciPy for more advanced scientific computations.

Additional Scripts and Codes:

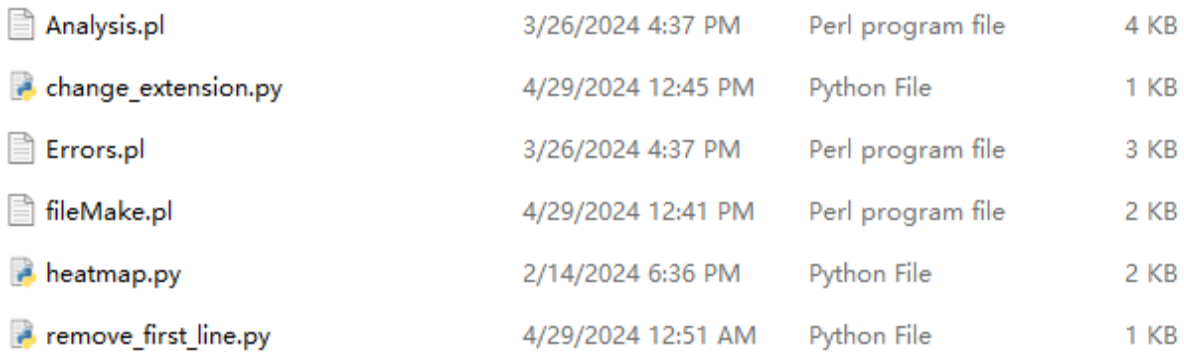

Fig 1.2 code

1. Analysis file

   The main purpose of this code is to automate the processing of experimental data and save the results in a structured format to an Excel file for further analysis and reporting. By automating the process, a lot of time can be saved in manual data organization and human errors can be reduced.

2. Change extension

   This file is used to change the file with the extension .xye to a chi file for maud for batch analysis.

3. Errors

   The main purpose of this Perl code is to extract specific error information from a .par file and save this information to a text file.

4. fileMake file

   The main purpose of this code is to automate the processing of .chi files and generate the required script files for batch analysis.

5. Remove first line file

   Usually XRD data are present in the first line of text 2θ, INTENSITY and ERROR. This file is used to remove the first line of text to facilitate the processing of data in later lines.

Experiment Process

1. First, create a results folder and place the "Analysis.pl" program inside of it.
2. Place the initial .par file with the .chi files that you want to analyze, and name the file "initial.par". (Make sure that the .par file does not contain datasets)

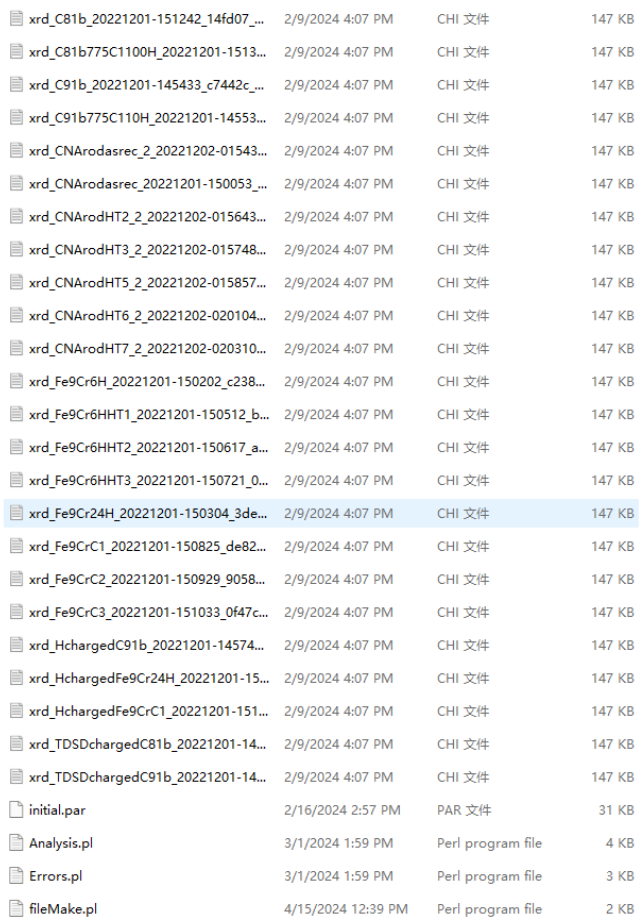

Fig 2.1 chi files

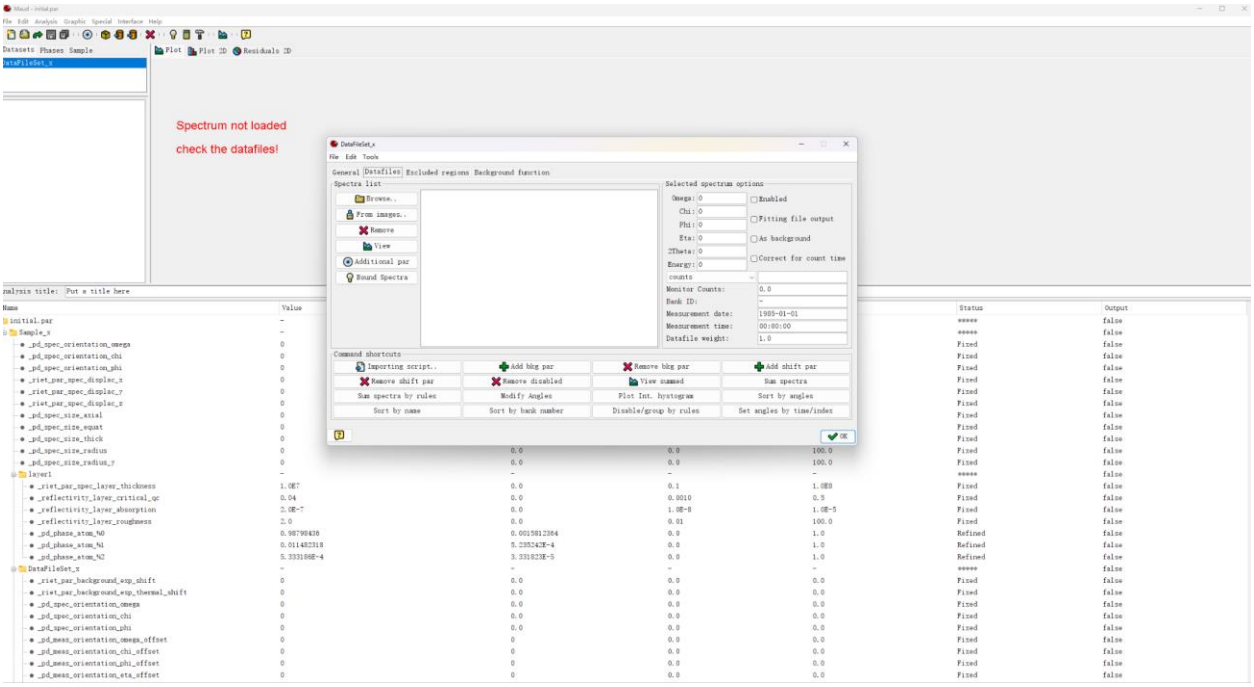

Fig 2.2 no data in dataset

1. Place the "FileMake.pl" program into the same folder as the "initial.par" and the .chi files and run the program. The program will ask for the path to "initial.par". Copy paste the path into the program and remove the quotation marks around the path name. Make sure that the path has "/initial.par" at the end of it. This program will output "script.ins" and "names.txt" files. Place "names.txt" into the results folder.

Fig 2.3 FileMake.pl

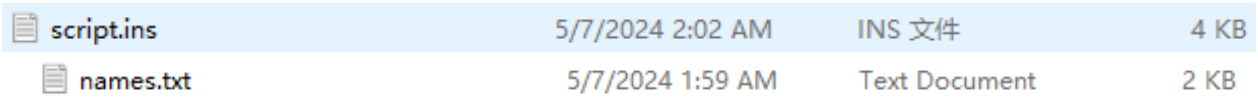

Fig 2.4 Script and names

4. Run the batch analysis with the script.ins file. To do this, go to the menu bar in MAUD and select the "special" dropdown. Then select "Refine in Batch". This will give a pop up window. Select the "script.ins" file. This will run the batch analysis and output a "results.txt" file. You can select the "interference" dropdown. Then select "console visible" to check the analysis process.

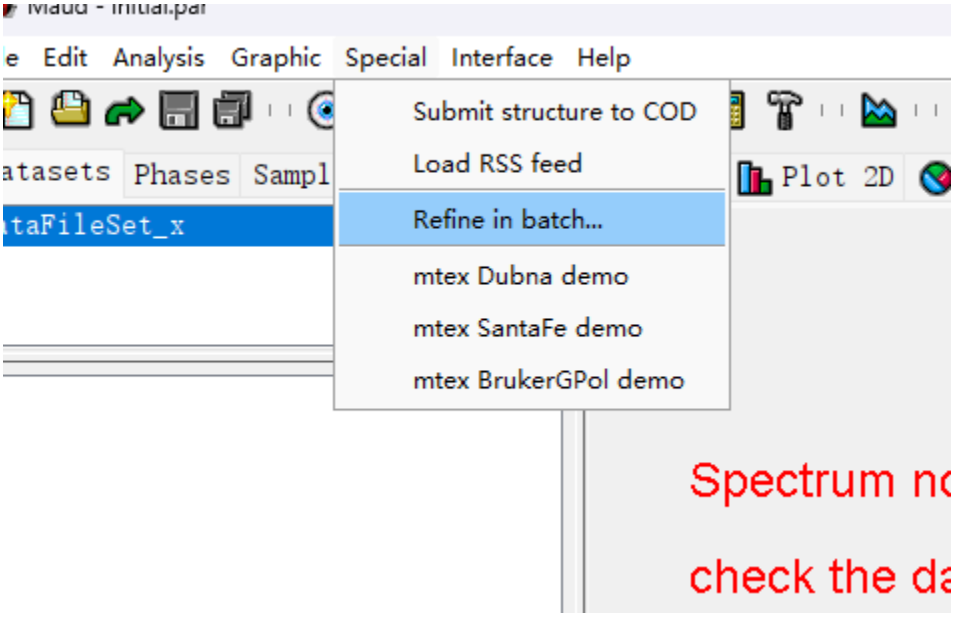

Fig 2.5 Refine in batch

名称	修改日期	类型	大小
Analysis.pl	3/1/2024 1:59 PM	Perl program file	4 KB
Errors.pl	3/1/2024 1:59 PM	Perl program file	3 KB
fileMake.pl	4/15/2024 12:39 PM	Perl program file	2 KB
initial.par	2/16/2024 2:57 PM	PAR 文件	31 KB
names.txt	5/7/2024 1:59 AM	Text Document	2 KB
script.ins	5/7/2024 2:02 AM	INS 文件	4 KB
xrd_C81b_20221201-151242_14fd07_primary-...	2/9/2024 4:07 PM	CHI 文件	147 KB
xrd_C81b775C1100H_20221201-151347_0bde...	2/9/2024 4:07 PM	CHI 文件	147 KB
xrd_C91b_20221201-145433_c7442c_primary-...	2/9/2024 4:07 PM	CHI 文件	147 KB
xrd_C91b775C110H_20221201-145535_b414c...	2/9/2024 4:07 PM	CHI 文件	147 KB
xrd_CNArodasrec_2_20221202-015437_80429...	2/9/2024 4:07 PM	CHI 文件	147 KB
xrd_CNArodasrec_20221201-150053_8d267e_...	2/9/2024 4:07 PM	CHI 文件	147 KB

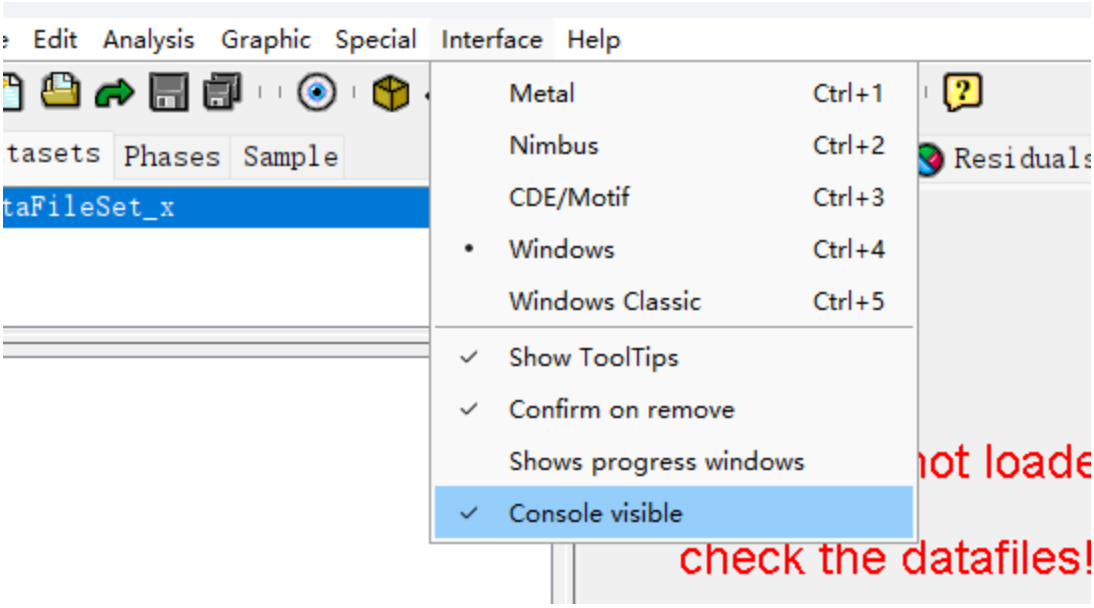

Fig 2.5 Console visible

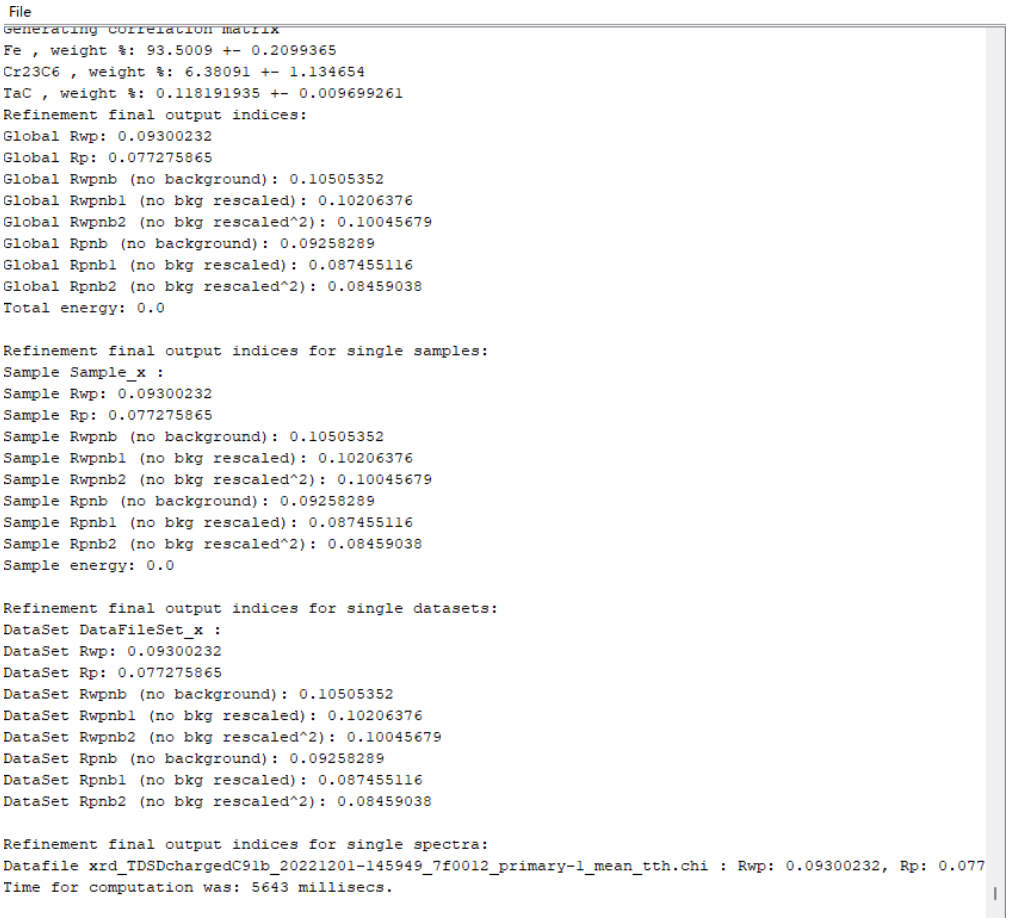

Fig 2.6 batch analysis process

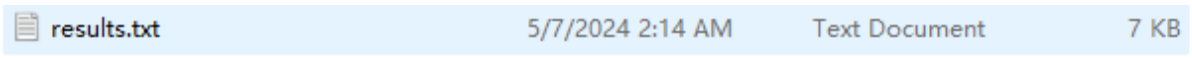

Fig 2.7 results

5. Run the error and Analysis file, and you will get an excel of the result and error. It should be noted that the analysis file default is for 3 phases to generate excel tables, for other quantities of phases, you need to modify the parameters to prevent excel sorting errors.

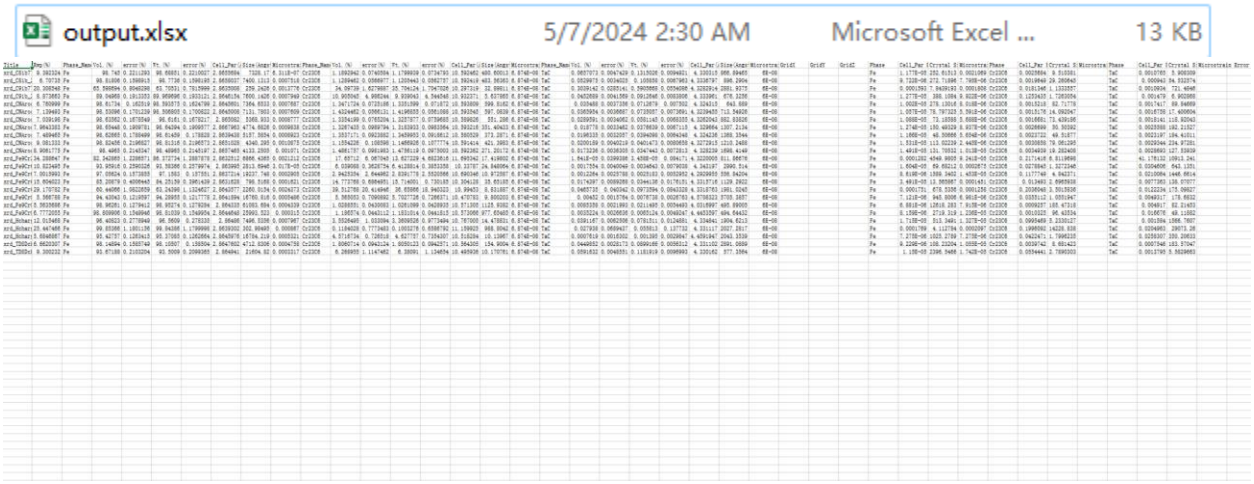

Fig 2.5 excel of output

The following parameters are output

Title - The title or identifier of the data set or sample.

Rwp(%) - Percentage of weighted profile factor, often used as a measure of how well X-ray powder diffraction data fits.

Phase_Name - The name of a specific phase in the sample.

Vol.(%) - The percentage of phase volume relative to the total sample volume.

error(%) - The percentage error associated with the volume percentage.

Wt.(%) - The weight percentage of the phase.

Cell_Par(Angstrom) - the cell parameter of the crystal in Ångström.

Size(Angstrom) - Grain size in Angstrom.

Microstrain - Microscopic strain, usually associated with lattice distortion.

GridX, GridY, GridZ - may indicate the position of the sample in some coordinate system or device.

Phase, Cell_Par Error, Crystal Size Error, Microstrain Error - Repeated list of phase names with errors in each parameter (cell parameter, grain size, microstrain).

6. Modify the analysis file based the amount of phases（ take 2 and 3 phases as examples ）

1. Modify the order of split

```
26  {
27      my $str = $_;
28      my @segments = (split '\t', $str)[0..25];
29      push (@cLines, @segments);
30  }
31
```

Fig 2.6 split code of 3 phases

```
26  {
27      my $str = $_;
28      my @segments = (split '\t', $str)[0..17];
29      push (@cLines, @segments);
30  }
```

Fig 2.7 split code of 2 phases

When expanding from processing data from two phases to three phases, it usually means that the number of data fields contained in each row increases, since each phase may have its own set of specific parameters. That's why when processing more phases in Perl code, you need to extract more columns from the data, i.e. adjust the range of the array index after the split function.

Here is an example, if each phase contains the following parameters:

Phase Name

Volume (%)

Error (%)

Weight (%)

Error (%)

Cell Parameter (Angstrom)

Size (Angstrom)

Microstrain

For two-phase data, you may need to extract to the 17th field of each row. And when increasing to three phases, each phase may add at least 8 fields (if the number of parameters of each phase is the same), so more fields need to be extracted to contain all the data of the third phase, which is the index The origin of 0.25.

2. Changing the write order of excel

```
84  $row = 0;
85  my $countMod = 0;
86  while(<fh>)
87  {
88      print $_;
89      $row++ if ($countMod % 3 == 0);
90      $worksheet->write($row, $col, "$_") if ($countMod % 3 == 0);
91      $worksheet->write($row, $col+1, "$_") if ($countMod % 3 == 1);
92      $worksheet->write($row, $col+2, "$_") if ($countMod % 3 == 2);
93      $countMod++;
94  }
```

Fig 2.8 excel code of 3 phases

Here, whenever $countMod is divisible by 3 (that is, 0, 3, 6, ...)), a new data point is written to the first position of the new row, and the row number $row is incremented; then, as $countMod increases, the next two data points fill the second ($col+1) and third ($col+2) positions of the row, respectively. In this way, every third data point fills three columns of a row.

```
86  while(<fh>)
87  {
88      print $_;
89      $row++ if ($countMod % 2 == 0);
90      $worksheet->write($row, $col, "$_") if ($countMod % 2 == 0);
91      $worksheet->write($row, $col+1, "$_") if ($countMod % 2 == 1);
92      $countMod++;
93  }
94
95  close(fh);
```

Fig 2.9 excel code of 2 phases

In this code, $countMod controls the position of the rows and columns. If $countMod is an even number (that is, 0, 2, 4, ...) is even (that is, 0, 2, 4, ...), the data is written to the first position ($col) of the current row and the row number $row is incremented in preparation for the next data point to be written. If $countMod is an odd number (1, 3, 5, ...) , then the data is written to the second position ($col+1) in the same row. This means that every two data points fill two columns of a row.

3. Modify the numbers of phase names, unit cell parameter errors, grain size errors, and microstrain errors that need to be displayed.

The main function of this code is to read a text file (ListOfErrors.txt) containing error data and write the data into an Excel worksheet. The columns of each worksheet correspond to different error types, and the error data is written into the corresponding columns according to specific rules. The code mainly contains two parts: setting the column headers of the Excel worksheet and writing error data.

```
114
115   $worksheet->write(0, $col, "Phase");
116   $worksheet->write(0, $col+1, "Cell_Par Error");
117   $worksheet->write(0, $col+2, "Crystal Size Error");
118   $worksheet->write(0, $col+3, "Microstrain Error");
119   $worksheet->write(0, $col+4, "Phase");
120   $worksheet->write(0, $col+5, "Cell_Par Error");
121   $worksheet->write(0, $col+6, "Crystal Size Error");
122   $worksheet->write(0, $col+7, "Microstrain Error");
123   $worksheet->write(0, $col+8, "Phase");
124   $worksheet->write(0, $col+9, "Cell_Par Error");
125   $worksheet->write(0, $col+10, "Crystal Size Error");
126   $worksheet->write(0, $col+11, "Microstrain Error");
127
128
129   #Add errors
130   open(fh, "ListOfErrors.txt");
131
132   $row = 0;
133   my $countMod = 0;
134   while(<fh>)
135   {
136       print $_;
137       $row++ if ($countMod % 12 == 0);
138       $worksheet->write($row, $col, "$_") if ($countMod % 12 == 0);
139       $worksheet->write($row, $col+1, "$_") if ($countMod % 12 == 1);
140       $worksheet->write($row, $col+2, "$_") if ($countMod % 12 == 2);
141       $worksheet->write($row, $col+3, "$_") if ($countMod % 12 == 3);
142       $worksheet->write($row, $col+4, "$_") if ($countMod % 12 == 4);
143       $worksheet->write($row, $col+5, "$_") if ($countMod % 12 == 5);
144       $worksheet->write($row, $col+6, "$_") if ($countMod % 12 == 6);
145       $worksheet->write($row, $col+7, "$_") if ($countMod % 12 == 7);
146       $worksheet->write($row, $col+8, "$_") if ($countMod % 12 == 8);
147       $worksheet->write($row, $col+9, "$_") if ($countMod % 12 == 9);
148       $worksheet->write($row, $col+10, "$_") if ($countMod % 12 == 10);
149       $worksheet->write($row, $col+11, "$_") if ($countMod % 12 == 11);
150       $countMod++;
151   }
152
153   close(fh);
154
155
156
157   $workbook->close;
```

Fig 3.1 code of listing errors of 3 phases

```
109
110   $col++;
111   $col++;
112   $col++;
113
114   $worksheet->write(0, $col, "Phase");
115   $worksheet->write(0, $col+1, "Cell_Par Error");
116   $worksheet->write(0, $col+2, "Crystal Size Error");
117   $worksheet->write(0, $col+3, "Microstrain Error");
118   $worksheet->write(0, $col+4, "Phase");
119   $worksheet->write(0, $col+5, "Cell_Par Error");
120   $worksheet->write(0, $col+6, "Crystal Size Error");
121   $worksheet->write(0, $col+7, "Microstrain Error");
122
123
124
125   #Add errors
126   open(fh, "ListOfErrors.txt");
127
128   $row = 0;
129   my $countMod = 0;
130   while(<fh>)
131   {
132       print $_;
133       $row++ if ($countMod % 8 == 0);
134       $worksheet->write($row, $col, "$_") if ($countMod % 8 == 0);
135       $worksheet->write($row, $col+1, "$_") if ($countMod % 8 == 1);
136       $worksheet->write($row, $col+2, "$_") if ($countMod % 8 == 2);
137       $worksheet->write($row, $col+3, "$_") if ($countMod % 8 == 3);
138       $worksheet->write($row, $col+4, "$_") if ($countMod % 8 == 4);
139       $worksheet->write($row, $col+5, "$_") if ($countMod % 8 == 5);
140       $worksheet->write($row, $col+6, "$_") if ($countMod % 8 == 6);
141       $worksheet->write($row, $col+7, "$_") if ($countMod % 8 == 7);
142       $countMod++;
143   }
144
145   close(fh);
146
147
148
149   $workbook->close;
150
```

Fig 3.2 code of listing errors of 2 phases

For the 3 phases code, write one line for every 18 columns of data, and for the 4 phases code, write one line for every 24 columns of data.

The number of columns written is different: 18 columns for 3 phases and 24 columns for 4 phases.

7. Modify the code to increase the amount of output data

While processing ATR2_RR data, Mingxi discovered that my output only included the error rate for crystal size and not the actual crystal size. Thus, it seems some values are missing from my output. I found that in some special phases like Cohenite, there is more than one cell length that should be exported. This will take up three rows in Excel and cause the crystal size and Microstrain to not show up. I have changed the code to export the crystal size and Microstrain.

> When I was checking the results, I found some weird issues:
>
> 1. In the IVAR output, all the crystal sizes of BCC are constant, which need to be refined (the fixed value is very large).
> 2. I can't find the crystal size for the cohenite in the ATR2_RR, but there is Crystal Size Error in the Excel file. I think he failed to export it during the analysis.
>
> Can you send these to Shukun and ask him to fix these issues?
>
> Thanks,
> Mingxi

Fig 3.3 Mingxi's email

```
# Reading the file till FH reaches EOF
while(<fh>)
{
    #Cell Parameter (a) Error
    push (@cellParError1, $_) if (/_cell_length_a/i);
    #Cell Parameter (b) Error
    push (@cellParError2, $_) if (/_cell_length_b/i);
    #Cell Parameter (c) Error
    push (@cellParError3, $_) if (/_cell_length_c/i);
    #Crystal Size Error
    push (@crystalSizeError, $_) if (/_riet_par_cryst_size/i);
    #Microstrain Error
    push (@microstrainError, $_) if (/_riet_par_rs_microstrain/i);
    #Phase Names
    push (@phaseNames, $_) if (/_pd_phase_name/i);
}
```

Fig 3.4 Modified codes of error.pl

```
$worksheet->write(0, $col, "Phase");
$worksheet->write(0, $col+1, "Cell_Par Error");
$worksheet->write(0, $col+2, "Cell_Par Error");
$worksheet->write(0, $col+3, "Cell_Par Error");
$worksheet->write(0, $col+4, "Crystal Size Error");
$worksheet->write(0, $col+5, "Microstrain Error");
$worksheet->write(0, $col+6, "Phase");
$worksheet->write(0, $col+7, "Cell_Par Error");
$worksheet->write(0, $col+8, "Cell_Par Error");
$worksheet->write(0, $col+9, "Cell_Par Error");
$worksheet->write(0, $col+10, "Crystal Size Error");
$worksheet->write(0, $col+11, "Microstrain Error");
$worksheet->write(0, $col+12, "Phase");
$worksheet->write(0, $col+13, "Cell_Par Error");
$worksheet->write(0, $col+14, "Cell_Par Error");
$worksheet->write(0, $col+15, "Cell_Par Error");
$worksheet->write(0, $col+16, "Crystal Size Error");
$worksheet->write(0, $col+17, "Microstrain Error");


#Add errors
open(fh, "ListOfErrors.txt");

$row = 0;
my $countMod = 0;
while(<fh>)
{
    print $_;
    $row++ if ($countMod % 18 == 0);
    $worksheet->write($row, $col, "$_") if ($countMod % 18 == 0);
    $worksheet->write($row, $col+1, "$_") if ($countMod % 18 == 1);
    $worksheet->write($row, $col+2, "$_") if ($countMod % 18 == 2);
    $worksheet->write($row, $col+3, "$_") if ($countMod % 18 == 3);
    $worksheet->write($row, $col+4, "$_") if ($countMod % 18 == 4);
    $worksheet->write($row, $col+5, "$_") if ($countMod % 18 == 5);
    $worksheet->write($row, $col+6, "$_") if ($countMod % 18 == 6);
    $worksheet->write($row, $col+7, "$_") if ($countMod % 18 == 7);
    $worksheet->write($row, $col+8, "$_") if ($countMod % 18 == 8);
    $worksheet->write($row, $col+9, "$_") if ($countMod % 18 == 9);
    $worksheet->write($row, $col+10, "$_") if ($countMod % 18 == 10);
    $worksheet->write($row, $col+11, "$_") if ($countMod % 18 == 11);
    $worksheet->write($row, $col+12, "$_") if ($countMod % 18 == 12);
    $worksheet->write($row, $col+13, "$_") if ($countMod % 18 == 13);
    $worksheet->write($row, $col+14, "$_") if ($countMod % 18 == 14);
    $worksheet->write($row, $col+15, "$_") if ($countMod % 18 == 15);
    $worksheet->write($row, $col+16, "$_") if ($countMod % 18 == 16);
    $worksheet->write($row, $col+17, "$_") if ($countMod % 18 == 17);
```

Fig 3.5 Modified codes of analysis.pl

Due to the fact that there are three crystal sizes in the Cohenite phase, namely lengths a, b, and c, the error output code should output errors for all three crystal sizes. In the analysis, two additional columns should be added for lengths b and c. This way, other data will not be overwritten.

Practical applications of batch

Professor David Sprouster and his lab member Mingxi Ouyang provided me with the XRD experimental data obtained during the beam time at BNL. First, I need to refine one par file from a set using MAUD to obtain a parameter file suitable for the entire dataset, and then proceed with batch analysis.

The results include: Title, Rwp(%), Vol.(%), error(%), Wt.(%), Cell_Par(Angstrom), size(Angstrom), MicrostrainGridX, GridY, GridZPhase, Cell_Par Error, Crystal Size Error, Microstrain Error.

Most of the Rwp values are as expected, and only a few files with Rwp values greater than 10 need manual refinement, significantly reducing the time required.

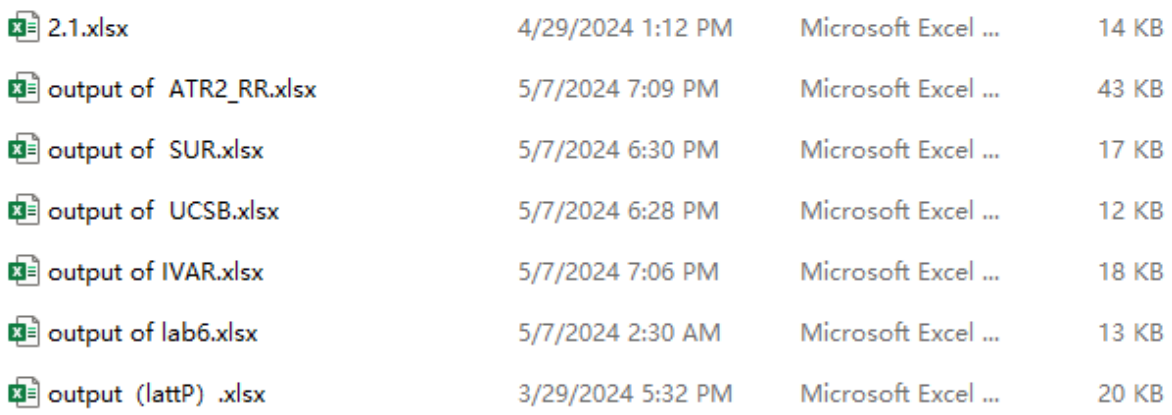

Fig 4.1 excel of output

Appendix (processed data)

1.practice sample

Title	Rwp(%)	Phase Na	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(A	Cell Par E	Size(Angst	Crystal Siz	Microstrai	Microstrai
xrd C81b775C11(	9.392324	Fe	98.745	0.221129	98.68851	0.221003	2.865568	1.18E-05	7328.17	252.6151	6.31E-07	0.002107
xrd C81b 202212	6.70735	Fe	98.81806	0.159891	98.7736	0.15982	2.865804	9.72E-06	7400.131	272.719	0.000752	7.79E-06
xrd C91b775C11(	20.30855	Fe	65.59869	0.80483	63.70531	0.7816	2.863501	0.000159	259.2426	7.843919	0.001378	0.000181
xrd C91b 202212	8.873663	Fe	89.04968	0.191335	89.9697	0.193312	2.864615	1.28E-05	7600.143	388.1084	0.000795	9.92E-06
xrd CNArodasrec	6.760999	Fe	98.61734	0.162519	98.59358	0.16248	2.86456	1E-05	7364.653	278.1302	0.000769	8.02E-06
xrd CNArodasrec	7.139493	Fe	98.53096	0.170124	98.50681	0.170082	2.864501	1.06E-05	7131.78	78.79733	0.000761	5.59E-06
xrd CNArodHT2	7.039198	Fe	98.63562	0.167855	98.6161	0.167822	2.865082	1.09E-05	5368.933	73.18588	0.000878	5.69E-06
xrd CNArodHT3	7.964338	Fe	98.65448	0.190978	98.64394	0.190958	2.866796	1.27E-05	4774.683	150.4933	0.000984	8.94E-06
xrd CNArodHT5	7.489465	Fe	98.62665	0.17885	98.61459	0.178828	2.863944	1.17E-05	5157.585	48.50666	0.000892	5.65E-06
xrd CNArodHT6	9.081333	Fe	98.82456	0.219683	98.81316	0.219657	2.865103	1.53E-05	4340.295	113.0224	0.001088	2.45E-06
xrd CNArodHT7	8.906178	Fe	98.4965	0.214535	98.48965	0.21452	2.865747	1.49E-05	4133.251	131.7053	0.001071	1.01E-05
xrd Fe9Cr24H 20	34.28865	Fe	82.34287	1.228657	86.37273	1.288788	2.863251	0.000128	6866.437	4549.981	0.002121	9.24E-05
xrd Fe9Cr6HHT1	10.8235	Fe	93.95916	0.259033	93.58366	0.257997	2.863995	1.6E-05	2813.695	69.68212	3.02E-05	0.000267
xrd Fe9Cr6HHT2	7.001599	Fe	97.05624	0.157386	97.1583	0.157551	2.863721	8.62E-06	19237.75	1589.34	0.00029	1.45E-05
xrd Fe9Cr6HHT3	15.60402	Fe	85.20879	0.400645	84.25159	0.396144	2.863163	3.49E-05	798.5168	13.56587	0.000162	0.000145
xrd Fe9Cr6H 202	29.17078	Fe	60.44066	1.082266	63.24398	1.132463	2.864358	0.000175	2260.015	678.5356	0.002437	0.000126
xrd Fe9CrC1 202	5.566788	Fe	94.43043	0.12196	94.28955	0.121778	2.864189	7.12E-06	16760.82	945.8006	0.000549	6.98E-06
xrd Fe9CrC2 202	5.563569	Fe	98.96261	0.127941	98.95274	0.127928	2.864335	6.88E-06	61083.68	12618.28	0.000434	7.92E-06
xrd Fe9CrC3 202	6.777206	Fe	98.80991	0.154995	98.81039	0.154995	2.864465	8.16E-06	25993.52	2719.319	0.000315	1.24E-05
xrd HchargedC91	12.01547	Fe	96.40823	0.277895	96.5609	0.278335	2.86486	1.71E-05	7496.536	513.3491	0.000797	1.33E-05
xrd HchargedFe9	25.44747	Fe	99.85366	1.180116	99.84386	1.18	2.86393	0.000177	302.985	4.112784	0.000867	0.00021
xrd HchargedFe9	5.684687	Fe	95.42757	0.126341	95.37085	0.126266	2.864598	7.27E-06	16784.22	1025.279	0.000532	7.28E-06
xrd_TDSDcharged	6.662031	Fe	98.14894	0.158575	98.10507	0.158504	2.86476	9.23E-06	4712.831	108.232	0.000476	1.05E-05

Fig 5.1.1 Fe phase

Title	Phase Na	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(A	Cell Par Er	Size(Angst	Crystal Siz	Microstrai	Microstrai
xrd C81b7	Cr23C6	1.189294	0.074058	1.179994	0.073479	10.59246	0.002568	480.6001	9.510381	6.87E-08	
xrd C81b	Cr23C6	1.128946	0.056698	1.120544	0.056276	10.59242	0.001965	483.5636	29.26065	6.87E-08	
xrd C91b7	Cr23C6	34.09739	1.627989	35.70412	1.704703	10.29732	0.018135	32.89811	1.133356	6.87E-08	
xrd C91b	Cr23C6	10.90505	4.986244	9.939043	4.544548	10.93237	0.125343	5.637865	1.726305	6.87E-08	
xrd CNArc	Cr23C6	1.347172	0.072519	1.33516	0.071872	10.59381	0.001522	599.8162	82.71778	6.87E-08	
xrd CNArc	Cr23C6	1.432446	0.056613	1.419686	0.056109	10.59355	0.001518	597.0839	14.09205	6.87E-08	
xrd CNArc	Cr23C6	1.33542	0.07652	1.325788	0.075968	10.58983	0.001668	551.286	73.43919	6.87E-08	
xrd CNArc	Cr23C6	1.326744	0.098979	1.318393	0.098356	10.59322	0.00267	351.4043	50.50392	6.87E-08	
xrd CNArc	Cr23C6	1.353717	0.092388	1.345995	0.091861	10.58053	0.002372	373.2871	49.51877	6.87E-08	
xrd CNArc	Cr23C6	1.155423	0.108598	1.146693	0.107777	10.59141	0.003086	421.3983	79.0613	6.87E-08	
xrd CNArc	Cr23C6	1.486176	0.098198	1.475612	0.0975	10.59236	0.003494	271.2017	19.28241	6.87E-08	
xrd Fe9Cr	Cr23C6	17.65712	6.067045	13.62723	4.682362	11.69534	0.217142	17.4198	6.81197	6.87E-08	
xrd Fe9Cr	Cr23C6	6.039088	0.362875	6.412881	0.385336	10.33787	0.027884	24.84806	1.327235	6.87E-08	
xrd Fe9Cr	Cr23C6	2.942535	2.644962	2.839178	2.552057	10.69035	0.117775	10.97259	4.842371	6.87E-08	
xrd Fe9Cr	Cr23C6	14.77377	0.686495	15.714	0.730185	10.30413	0.013493	35.65185	2.696594	6.87E-08	
xrd Fe9Cr	Cr23C6	39.51277	20.41495	36.65866	18.94032	10.99453	0.203605	8.831887	3.501584	6.87E-08	
xrd Fe9Cr	Cr23C6	5.565053	0.709089	5.702773	0.726637	10.47078	0.035511	9.800203	1.055195	6.87E-08	
xrd Fe9Cr	Cr23C6	1.028855	0.043008	1.02611	0.042894	10.57131	0.000926	1125.938	185.4732	6.87E-08	
xrd Fe9Cr	Cr23C6	1.186574	0.044311	1.183101	0.044181	10.57307	0.001032	977.6549	96.43534	6.87E-08	
xrd Hchar	Cr23C6	3.55265	1.033094	3.360953	0.977349	10.76701	0.099547	14.47883	5.233013	6.87E-08	
xrd Hchar	Cr23C6	0.118403	0.777348	0.100328	0.658679	11.15992	0.199609	988.8042	14228.84	6.87E-08	
xrd Hchar	Cr23C6	4.571673	0.726518	4.627757	0.735431	10.51828	0.042247	10.13967	1.799624	6.87E-08	

Fig 5.1.2 Cr23C6 phase

Title	Phase Na	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(A	Cell Par Er	Size(Angs	Crystal Siz	Microstrai	Microstrai
xrd C81b7	TaC	0.065707	0.004743	0.131503	0.009492	4.330315	0.001076	866.8947	5.908309	6E-08	
xrd C81b	TaC	0.052997	0.003403	0.105858	0.006796	4.33368	0.000943	896.2904	54.53257	6E-08	
xrd C91b7	TaC	0.303914	0.028514	0.590567	0.055409	4.328291	0.001093	2881.938	721.4846	6E-08	
xrd C91b	TaC	0.045269	0.004157	0.091265	0.008381	4.333961	0.001479	676.3256	6.902868	6E-08	
xrd CNArc	TaC	0.035488	0.003736	0.071268	0.007502	4.324315	0.001742	643.889	89.84669	6E-08	
xrd CNArc	TaC	0.036595	0.003669	0.073506	0.007369	4.323946	0.001676	713.5493	17.4006	6E-08	
xrd CNArc	TaC	0.028959	0.003406	0.058114	0.006835	4.326204	0.001814	882.8383	118.9204	6E-08	
xrd CNArc	TaC	0.018778	0.003346	0.037664	0.006712	4.329664	0.002559	1307.213	192.2153	6E-08	
xrd CNArc	TaC	0.019633	0.003206	0.03941	0.006435	4.324236	0.00232	1368.354	184.4101	6E-08	
xrd CNArc	TaC	0.020019	0.004022	0.040147	0.008066	4.327292	0.002934	1210.249	234.9728	6E-08	
xrd CNArc	TaC	0.017324	0.00363	0.034744	0.007281	4.328239	0.002869	1698.415	127.5394	6E-08	
xrd Fe9Cr	TaC	1.64E-05	0.039939	3.46E-05	0.084171	4.322001	41.17613	811.8668	10913.24	6E-08	
xrd Fe9Cr	TaC	0.001755	0.004005	0.003464	0.007904	4.343197	0.030461	2990.514	643.1351	6E-08	
xrd Fe9Cr	TaC	0.001226	0.002579	0.002518	0.005295	4.292996	0.021006	556.842	1446.661	6E-08	
xrd Fe9Cr	TaC	0.01744	0.008927	0.034414	0.017615	4.331572	0.007736	1129.292	138.0708	6E-08	
xrd Fe9Cr	TaC	0.046574	0.040342	0.097359	0.084333	4.331876	0.012223	1981.025	175.0983	6E-08	
xrd Fe9Cr	TaC	0.00452	0.001576	0.007674	0.002676	4.570832	0.004932	5705.386	178.6832	6E-08	
xrd Fe9Cr	TaC	0.008536	0.002199	0.02115	0.005449	4.0317	0.004917	495.8901	82.21453	6E-08	
xrd Fe9Cr	TaC	0.003522	0.002664	0.006512	0.004925	4.44536	0.016676	494.6443	49.11882	6E-08	
xrd Hchar	TaC	0.039117	0.006251	0.078151	0.012488	4.334841	0.001584	1904.621	1566.761	6E-08	
xrd Hchar	TaC	0.027938	0.068944	0.055813	0.137732	4.331117	0.020496	2027.282	29073.26	6E-08	
xrd Hchar	TaC	0.000762	0.00163	0.001395	0.002985	4.459195	0.025831	2043.354	350.2063	6E-08	
xrd TDSD	TaC	0.044985	0.002817	0.089917	0.005631	4.331102	0.000755	2891.089	183.5705	6E-08	

Fig 5.1.3 TaC phase

2. Second sets of data

Title	Rwp(%)	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
xrd KI276	15.02712	Iron- alpha	40.34332	0.576829	39.94726	0.571167	2.87554	0.000126	2748.954	313.9277	0.000872	5.6E- 05
xrd KI314	13.27217	Iron- alpha	28.06402	0.438878	27.69234	0.433065	2.87513	0.000121	2582.078	322.2231	0.001035	5.43E- 05
xrd KI318	11.61818	Iron- alpha	36.71874	0.286852	36.34222	0.28391	2.87583	0.000101	2192.691	16.54635	0.000954	3.2E- 05
xrd KI321	12.6234	Iron- alpha	33.95254	0.444862	33.59604	0.440191	2.875578	0.000113	1876.14	146.1836	0.001014	5.01E- 05
xrd KI322	15.83001	Iron- alpha	37.13502	0.585004	36.75243	0.578977	2.876322	0.000138	2609.626	300.2583	0.000907	6.12E- 05
xrd KI327	10.12082	Iron- alpha	38.19008	0.384612	37.79364	0.38062	2.876254	8.68E- 05	1670.802	84.41656	0.000873	4.02E- 05
xrd KI330	10.30008	Iron- alpha	34.10378	0.334835	33.7505	0.331367	2.874703	0.000114	732.4085	26.78488	0.001637	4.97E- 05
xrd KI1 01	10.48494	Iron- alpha	32.18122	0.379532	31.82601	0.375343	2.877776	9.97E- 05	1233.502	59.16574	0.000873	4.99E- 05
xrd KI1 10	11.31243	Iron- alpha	37.93419	0.433449	37.52909	0.428821	2.877554	0.000111	1263.584	62.01959	0.001074	4.54E- 05
xrd KI1 13	11.48782	Iron- alpha	34.15893	0.432765	33.7892	0.428081	2.876432	0.000113	1313.719	75.77752	0.001113	4.83E- 05
xrd KI1 18	11.69488	Iron- alpha	39.04123	0.470268	38.6371	0.4654	2.876765	0.000108	1259.977	61.75798	0.000861	4.94E- 05
xrd KI1 31	9.923027	Iron- alpha	39.06535	0.386705	38.65251	0.382618	2.875861	9.85E- 05	1242.341	52.02436	0.001079	3.96E- 05
xrd KI1 35	9.990195	Iron- alpha	30.98361	0.347542	30.63171	0.343595	2.876894	0.000102	1023.61	38.44283	0.001119	4.9E- 05
xrd KI1 37	11.33353	Iron- alpha	39.26129	0.452559	38.85008	0.447819	2.875298	0.000104	1208.168	40.53526	0.000775	3.97E- 06
xrd KI1 50	12.72503	Iron- alpha	33.51311	0.456851	33.14444	0.451826	2.877385	0.000119	1152.356	62.7091	0.000924	5.59E- 05
xrd KI1 53	9.46133	Iron- alpha	31.04782	0.334159	30.69747	0.330389	2.878623	9.38E- 05	912.7029	31.5572	0.000962	4.93E- 05
xrd KI1 57	9.388589	Iron- alpha	35.61132	0.386135	35.22643	0.381962	2.877769	9.74E- 05	809.7889	24.22515	0.000785	6.06E- 05
xrd KI1 70	10.47861	Iron- alpha	40.71528	0.441288	40.30201	0.436809	2.875492	9.97E- 05	1220.72	48.24007	0.000896	4.83E- 05
xrd KI1 73	8.456536	Iron- alpha	39.24355	0.324298	38.83957	0.320959	2.876509	8.18E- 05	1550.277	64.61289	0.00111	3.1E- 05
xrd KI1 77	11.26567	Iron- alpha	30.19643	0.39263	29.85482	0.388188	2.874627	0.000113	1158.081	62.25256	0.001124	5.15E- 05
xrd KI2 00	8.875178	Iron- alpha	32.75642	0.322549	32.39347	0.318975	2.875523	8.52E- 05	1023.615	35.93336	0.00098	4.2E- 05
xrd KI2 05	12.94762	Iron- alpha	36.66565	0.472514	36.27587	0.467491	2.876247	0.000127	1249.92	69.81088	0.001111	5.08E- 05
xrd KI2 07	11.53383	Iron- alpha	35.18016	0.447981	34.80669	0.443225	2.879247	0.000122	1012.811	42.38529	0.001228	5.67E- 05
xrd KI2 20	8.943566	Iron- alpha	34.26008	0.339908	33.88292	0.336166	2.8744	8.75E- 05	1189.749	48.48904	0.001025	3.98E- 05
xrd KI2 26	15.16319	Iron- alpha	38.3273	0.608106	37.9333	0.601855	2.875226	0.000163	1339.628	97.20384	0.001324	6.35E- 05
xrd KI2 27	12.12177	Iron- alpha	32.41587	0.45989	32.06504	0.454912	2.875068	0.000131	850.2044	47.22788	0.001063	6.72E- 05
xrd KI2 40	12.82829	Iron- alpha	38.66371	0.502008	38.27875	0.49701	2.877452	0.00013	1102.131	55.53396	0.001076	5.56E- 05
xrd KI2 43	10.71713	Iron- alpha	40.06318	0.42772	39.64923	0.423301	2.875744	0.000109	1303.243	61.87257	0.001201	4.14E- 05
xrd KI2 49	12.72862	Iron- alpha	36.03932	0.479519	35.65044	0.474345	2.876674	0.000136	1076.219	58.15288	0.001383	5.42E- 05
xrd KI2 60	11.24747	Iron- alpha	33.36809	0.407024	32.94718	0.401889	2.877343	0.000111	1144.476	54.41108	0.000972	5.14E- 05
xrd KI2 63	9.356222	Iron- alpha	40.28653	0.377044	39.85843	0.373037	2.876542	9.05E- 05	1261.876	50.57353	0.001063	3.74E- 05
xrd KI2 68	10.41379	Iron- alpha	39.61754	0.406794	39.19965	0.402503	2.877892	0.000105	1241.173	54.78254	0.001186	4E- 05
xrd KI2 70	10.45001	Iron- alpha	33.64114	0.389021	33.26698	0.384695	2.876542	0.000102	1275.06	62.48771	0.000926	4.96E- 05
xrd KI2 78	9.928652	Iron- alpha	32.17584	0.356375	31.80318	0.352247	2.878018	9.53E- 05	1215.575	55.88695	0.000954	4.46E- 05
xrd KI2 81	11.221	Iron- alpha	36.82135	0.430327	36.43228	0.42578	2.876111	0.000102	1515.189	75.46086	0.00093	4.83E- 05
xrd KI2 85	11.40008	Iron- alpha	31.42986	0.287079	31.07116	0.283803	2.877142	0.000117	1000.998	44.68419	0.000937	4.73E- 05
xrd KI2 88	9.374949	Iron- alpha	30.04227	0.317542	29.69738	0.313897	2.877165	9.57E- 05	989.8413	40.13268	0.001096	4.49E- 05
xrd KI2 92	8.629328	Iron- alpha	30.81696	0.308266	30.42093	0.304305	2.877007	8.81E- 05	979.6197	34.38751	0.000991	4.39E- 05
xrd KI2 99	15.0625	Iron- alpha	22.75192	0.328604	22.42871	0.323936	2.874481	0.000172	850.2331	56.57789	0.000859	8.99E- 05
xrd KI3 13	13.27522	Iron- alpha	31.16047	0.454311	30.75832	0.448448	2.879063	0.000134	1091.012	45.5665	0.001037	3.8E- 06

Fig 5.2.1 Iron-alpha phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
xrd KI276	Iron	59.65669	0.709441	60.05274	0.714151	3.603103	0.000151	5444.286	928.4957	0.000892	4.1E-05
xrd KI314	Iron	71.93598	0.721161	72.30766	0.724887	3.600184	0.00014	4897.593	648.596	0.000994	3.36E-05
xrd KI318	Iron	63.28126	0.576895	63.65778	0.580328	3.603759	0.000121	4806.512	541.9581	0.000931	3.07E-05
xrd KI321	Iron	66.04746	0.650255	66.40396	0.653764	3.603804	0.00013	4008.176	413.4784	0.000867	3.43E-05
xrd KI322	Iron	62.86498	0.778431	63.24757	0.783169	3.604153	0.00016	6065.97	1047.057	0.000899	4.19E-05
xrd KI327	Iron	61.80991	0.419435	62.20636	0.422125	3.603582	0.000102	2989.93	172.4582	0.000796	2.87E-05
xrd KI330	Iron	65.89622	0.516539	66.2495	0.519308	3.602922	0.00012	2788.915	161.1038	0.000888	2.81E-05
xrd KI1 01	Iron	67.81879	0.567006	68.17399	0.569975	3.606097	0.000118	2421.112	139.1873	0.000995	2.94E-05
xrd KI1 10	Iron	62.06582	0.5749	62.47091	0.578652	3.604714	0.000136	1965.623	109.9396	0.001092	3.43E-05
xrd KI1 13	Iron	65.84107	0.615943	66.2108	0.619402	3.60422	0.000135	2165.192	131.26	0.001031	3.38E-05
xrd KI1 18	Iron	60.95877	0.598479	61.3629	0.602447	3.604	0.000131	1789.62	11.28436	0.000885	2.76E-05
xrd KI1 31	Iron	60.93465	0.495853	61.34749	0.499212	3.602432	0.00012	1977.897	98.86723	0.001152	2.96E-05
xrd KI1 35	Iron	69.01639	0.552263	69.36829	0.555079	3.604768	0.000123	2345.034	139.2827	0.001152	2.83E-05
xrd KI1 37	Iron	60.73871	0.570201	61.14992	0.574061	3.601847	0.000123	1842.108	91.91372	0.000862	3.55E-05
xrd KI1 50	Iron	66.48689	0.508186	66.85555	0.511004	3.605284	0.000143	1885.65	112.515	0.000857	4.17E-05
xrd KI1 53	Iron	68.95218	0.517545	69.30253	0.520175	3.607045	0.000111	2148.679	98.53722	0.001025	2.74E-05
xrd KI1 57	Iron	64.38868	0.511473	64.77358	0.51453	3.605482	0.000114	1795.935	77.58254	0.000983	2.94E-05
xrd KI1 70	Iron	59.28472	0.523226	59.69799	0.526874	3.602243	0.000119	1907.976	97.69534	0.000966	3.22E-05
xrd KI1 73	Iron	60.75645	0.379085	61.16044	0.381605	3.603726	0.000101	2164.935	81.86411	0.001137	2.25E-05
xrd KI1 77	Iron	69.80357	0.501829	70.14519	0.504285	3.602227	0.000131	2469.527	152.7107	0.001035	3.08E-05
xrd KI2 00	Iron	67.24358	0.360234	67.60653	0.362178	3.60303	0.0001	2383.824	109.7145	0.001004	2.52E-05
xrd KI2 05	Iron	63.33435	0.667102	63.72413	0.671207	3.603579	0.000158	2601.763	219.4494	0.001253	3.68E-05
xrd KI2 07	Iron	64.81984	0.602067	65.19331	0.605536	3.607826	0.000139	2016.601	117.0027	0.001082	3.34E-05
xrd KI2 20	Iron	65.73993	0.307004	66.11708	0.308765	3.601305	0.000101	2111.693	95.06806	0.000983	2.7E-05
xrd KI2 26	Iron	61.6727	0.778632	62.0667	0.783606	3.602446	0.000188	2921.222	335.7387	0.001217	4.33E-05
xrd KI2 27	Iron	67.58413	0.445796	67.93496	0.44811	3.603019	0.000144	2290.358	142.0412	0.00107	3.35E-05
xrd KI2 40	Iron	61.33629	0.492249	61.72125	0.495339	3.605763	0.000153	2344.748	184.5926	0.001097	3.85E-05
xrd KI2 43	Iron	59.93682	0.52905	60.35077	0.532704	3.602414	0.000134	2153.246	128.2493	0.001221	3.18E-05
xrd KI2 49	Iron	63.96068	0.668817	64.34956	0.672883	3.604009	0.000159	2817.469	252.8648	0.001219	3.61E-05
xrd KI2 60	Iron	66.63191	0.589995	67.05283	0.593722	3.602348	0.000131	1887.73	94.29763	0.00101	3.34E-05
xrd KI2 63	Iron	59.71347	0.463923	60.14157	0.467249	3.602743	0.000107	1900.495	84.27186	0.000965	2.9E-05
xrd KI2 68	Iron	60.38246	0.525509	60.80035	0.529146	3.604826	0.000131	1934.852	104.6848	0.001227	3.2E-05
xrd KI2 70	Iron	66.35886	0.546873	66.73303	0.549956	3.603968	0.000118	2859.263	186.959	0.001033	2.88E-05
xrd KI2 78	Iron	67.82417	0.409061	68.19682	0.411309	3.605431	0.000114	2407.002	134.5816	0.001018	2.95E-05
xrd KI2 81	Iron	63.17865	0.581013	63.56772	0.584591	3.603483	0.000123	2287.662	139.183	0.000955	3.29E-05
xrd KI2 85	Iron	68.57014	0.564094	68.92884	0.567045	3.604853	0.000137	2542.072	126.8281	0.001043	2.79E-05
xrd KI2 88	Iron	69.95773	0.444598	70.30262	0.446789	3.60516	0.000109	3325.149	215.9709	0.001048	2.45E-05
xrd KI2 92	Iron	69.18304	0.464231	69.57907	0.466888	3.602346	0.000101	2268.102	101.7169	0.001062	2.4E-05
xrd KI2 99	Iron	77.24809	0.782298	77.57129	0.785571	3.599375	0.000182	2281.114	132.6717	0.001086	3.53E-05
xrd KI3 13	Iron	68.83953	0.609809	69.24168	0.613371	3.604714	0.000151	2589.011	169.3771	0.001034	3.32E-05
xrd KI3 26	Iron	66.38842	0.390061	66.75933	0.39224	3.602937	0.000116	1917.408	85.17968	0.000943	2.9E-05

Fig 5.2.2 Iron phase

3. To get Lattice Parameter for Second sets of data

Title	Rwp(%)	Phase_Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell_Par(A	Cell_Par Er	Size(Angstr	Crystal Size	Microstrain	Microstrain
xrd_K1276	11.143988	BCC	69.61401	0.6778659	69.2628	0.6744459	2.874631	8.924E-05	2514.594	151.7606	0.0007718	3.435E-05
xrd_K1314	11.986854	BCC	69.52602	0.7613442	69.13137	0.7570226	2.8743012	0.0001076	2220.7036	19.27733	0.0009891	3.402E-05
xrd_K1318	8.774734	BCC	72.77929	0.5599425	72.455536	0.5574516	2.8749435	7.583E-05	2017.3043	90.73508	0.0009304	2.885E-05
xrd_K1321	9.307289	BCC	73.77394	0.7579325	73.4635	0.7547431	2.8747213	7.988E-05	1772.1056	97.293724	0.0009548	3.589E-05
xrd_K1322	10.069211	BCC	69.47966	0.7373053	69.128586	0.7335798	2.8753548	8.123E-05	2300.8413	151.9213	0.0007868	3.774E-05
xrd_K1327	8.69538	BCC	73.72105	0.6673985	73.39272	0.6644262	2.875415	7.361E-05	1588.2815	67.71397	0.0008326	3.511E-05
xrd_K1330	8.721075	BCC	79.62748	0.7792826	79.37016	0.7767643	2.87374	9.502E-05	727.04834	23.184378	0.0016301	4.277E-05
xrd_KI1_01	7.33962	BCC	37.461372	0.3303666	37.078926	0.3269938	2.876837	6.917E-05	1226.3944	39.15806	0.0008165	3.395E-05
xrd_KI1_10	6.849005	BCC	36.19168	0.2627581	35.793472	0.259867	2.8766115	6.483E-05	1249.9081	36.13872	0.0009894	2.718E-05
xrd_KI1_13	7.787527	BCC	45.597923	0.3746589	45.190544	0.3713117	2.8754687	7.838E-05	1292.8395	45.616577	0.0010315	3.137E-05
xrd_KI1_18	10.455277	BCC	43.89388	0.4795421	43.471966	0.4749327	2.8760138	0.0001033	1240.0431	54.69159	0.0009926	4.048E-05
xrd_KI1_31	6.886564	BCC	39.814	0.2572766	39.398563	0.254592	2.8748934	6.758E-05	1214.8218	25.271837	0.0009992	9.575E-06
xrd_KI1_35	7.295691	BCC	41.00322	0.3428123	40.603504	0.3394705	2.8757844	6.813E-05	1240.102	42.53436	0.0009926	2.906E-05
xrd_KI1_37	8.409289	BCC	43.918514	0.401481	43.493763	0.3975982	2.8742917	7.5E-05	1200.4276	39.99376	0.0007059	4.013E-05
xrd_KI1_50	7.058265	BCC	38.917187	0.3191302	38.52302	0.3158979	2.8765287	6.447E-05	1130.4673	33.74621	0.0008722	3.13E-05
xrd_KI1_53	8.3027935	BCC	39.27796	0.3847222	38.89075	0.3809295	2.8775234	8.488E-05	1239.9788	50.211697	0.0009926	3.661E-05
xrd_KI1_57	7.3141623	BCC	51.566685	0.442673	51.146095	0.4390625	2.876914	7.428E-05	827.4964	20.3111	0.0007146	4.531E-05
xrd_KI1_70	7.519621	BCC	50.63849	0.4102134	50.21	0.4067423	2.8746068	7.051E-05	1200.9703	36.103436	0.0008239	3.384E-05
xrd_KI1_73	5.888843	BCC	37.06512	0.2237022	36.668816	0.2213104	2.8756437	5.598E-05	1498.3519	42.319736	0.001045	2.17E-05
xrd_KI1_77	7.712143	BCC	36.962364	0.3472165	36.584267	0.3436647	2.8736563	7.424E-05	1145.8485	41.434296	0.0010551	3.43E-05
xrd_KI2_00	6.505446	BCC	44.44302	0.3406892	44.035316	0.3375638	2.874611	6.207E-05	1015.4089	27.14319	0.0009322	3.099E-05
xrd_KI2_05	7.359008	BCC	39.112026	0.2198243	38.711166	0.2175713	2.8753214	8.403E-05	1240.1652	47.17476	0.0009927	3.513E-05
xrd_KI2_07	8.194078	BCC	39.990395	0.3875626	39.59796	0.3837593	2.878366	8.368E-05	1049.6467	37.537086	0.0012236	3.585E-05
xrd_KI2_20	6.7214584	BCC	43.83992	0.344348	43.426468	0.3411005	2.8735163	6.519E-05	1177.6354	36.328533	0.0009825	3.028E-05
xrd_KI2_26	8.735613	BCC	49.69297	0.4446573	49.272808	0.4408976	2.8743002	8.738E-05	1257.1443	50.22112	0.0011767	3.388E-05
xrd_KI2_27	9.432569	BCC	42.350792	0.5054528	41.957214	0.5007555	2.874115	0.0001005	893.1579	34.81681	0.0011312	4.9E-05
xrd_KI2_40	6.7813034	BCC	39.33283	0.2975316	38.94322	0.2945844	2.8765907	6.547E-05	1081.9366	28.54771	0.0009617	2.924E-05
xrd_KI2_43	7.0584135	BCC	39.84692	0.2850457	39.43361	0.282089	2.8747613	6.947E-05	1280.1307	38.540245	0.0011246	2.658E-05
xrd_KI2_49	8.364666	BCC	47.467377	0.4007561	47.044403	0.397185	2.8757513	8.657E-05	1048.8154	35.686394	0.0012748	3.387E-05
xrd_KI2_60	8.30697	BCC	33.502544	0.2898662	33.079918	0.2862097	2.8764505	8.023E-05	1117.3536	36.273262	0.0008824	3.691E-05
xrd_KI2_63	6.9223804	BCC	41.821373	0.3054179	41.387096	0.3022465	2.8757076	6.592E-05	1228.4824	35.872986	0.0010034	2.801E-05
xrd_KI2_68	6.756642	BCC	41.896015	0.2549211	41.470276	0.2523307	2.8769379	6.77E-05	1224.844	30.423737	0.0011152	2.326E-05
xrd_KI2_70	7.261526	BCC	39.483624	0.3177016	39.083958	0.3144857	2.8754756	6.961E-05	1253.8167	38.534256	0.0008507	3.241E-05
xrd_KI2_78	6.8787804	BCC	44.107414	0.3616839	43.684498	0.358216	2.8771856	6.598E-05	1164.9799	34.815945	0.0008903	3.126E-05
xrd_KI2_81	10.193259	BCC	39.112026	0.2198243	38.711166	0.2175713	2.8753214	8.403E-05	1240.1652	47.17476	0.0009927	3.513E-05
xrd_KI2_85	6.565733	BCC	40.905624	0.3007153	40.502148	0.2977492	2.876266	6.294E-05	1073.2313	27.873861	0.0010104	2.719E-05
xrd_KI2_88	9.120785	BCC	38.830914	0.4182604	38.446793	0.4141229	2.876126	9.425E-05	1239.9946	55.30943	0.0009925	4.221E-05
xrd_KI2_92	7.269846	BCC	40.302635	0.3398577	39.85442	0.3360781	2.8761241	7.41E-05	1040.8859	31.282272	0.0010089	3.404E-05
xrd_KI2_99	14.181191	BCC	33.794308	0.705146	33.38095	0.696521	2.8735964	0.0001574	873.3327	57.52971	0.0009318	9.366E-05
xrd_KI3_13	7.771137	BCC	33.83067	0.3183189	33.41146	0.3143745	2.8780603	7.329E-05	1083.0637	35.606403	0.0008984	3.722E-05

Fig 5.3.3 BCC phase

Title	Phase_Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell_Par(A	Cell_Par Er	Size(Angstr	Crystal Size	Microstrain	Microstrain
xrd_K1276	FCC	30.38598	0.2637248	30.7372	0.2667731	3.6018825	0.0001129	4972.4355	260.45795	0.0008461	2.256E-05
xrd_K1314	FCC	30.47398	0.2715758	30.868631	0.2750928	3.5990577	0.0001278	3547.0781	256.73862	0.0009219	2.883E-05
xrd_K1318	FCC	27.22071	0.1818873	27.544466	0.1840506	3.6025963	9.221E-05	3454.2617	123.24491	0.0008527	1.863E-05
xrd_K1321	FCC	26.226063	0.1895877	26.536503	0.1918318	3.602675	9.651E-05	3801.0828	272.1958	0.0008453	2.574E-05
xrd_K1322	FCC	30.520338	0.2356434	30.871416	0.238354	3.602846	0.0001023	5383.0415	275.40137	0.0008424	2.034E-05
xrd_K1327	FCC	26.278957	0.1820418	26.607277	0.1843162	3.6024692	8.893E-05	2906.2598	156.44452	0.000787	2.588E-05
xrd_K1330	FCC	20.372519	0.1412703	20.629837	0.1430546	3.6016808	0.0001029	2602.3247	116.7559	0.0008452	2.096E-05
xrd_KI1_01	FCC	62.53863	0.2952606	62.921074	0.2970662	3.6048772	8.384E-05	2379.0996	91.9107	0.0009717	2.068E-05
xrd_KI1_10	FCC	63.80832	0.3174101	64.20653	0.319391	3.6034813	8.299E-05	1971.546	55.251762	0.0010723	1.908E-05
xrd_KI1_13	FCC	54.40208	0.3360538	54.809456	0.3385703	3.603071	0.0001002	2493.4175	111.66615	0.0011803	2.172E-05
xrd_KI1_18	FCC	56.10612	0.4913999	56.528034	0.4950952	3.6028943	0.000141	2438.9856	154.99033	0.0012111	3.104E-05
xrd_KI1_31	FCC	60.186	0.3137762	60.601437	0.315942	3.6012294	8.513E-05	2331.6104	88.31836	0.0012084	1.898E-05
xrd_KI1_35	FCC	58.99678	0.3302099	59.396496	0.3324471	3.6033297	8.877E-05	2438.7986	97.56483	0.001211	1.945E-05
xrd_KI1_37	FCC	56.081486	0.3904015	56.506237	0.3933584	3.600601	9.149E-05	1802.9827	65.07248	0.0008121	2.717E-05
xrd_KI1_50	FCC	61.082817	0.350207	61.47698	0.3524669	3.604186	8.145E-05	1809.2928	54.345764	0.0008653	2.252E-05
xrd_KI1_53	FCC	60.72204	0.3892299	61.10925	0.3917119	3.6058512	0.0001067	2438.065	112.30045	0.0012107	2.234E-05
xrd_KI1_57	FCC	48.433315	0.2996886	48.853905	0.3022911	3.6043997	8.887E-05	1780.7772	59.150112	0.0009819	2.293E-05
xrd_KI1_70	FCC	49.36151	0.3157668	49.79	0.3185079	3.6011431	8.537E-05	2223.0176	95.53301	0.0010328	2.203E-05
xrd_KI1_73	FCC	62.93488	0.2756879	63.331184	0.2774239	3.6025789	7.141E-05	2138.4119	53.905113	0.0011386	1.558E-05
xrd_KI1_77	FCC	63.037636	0.3155385	63.415733	0.3174311	3.6010072	8.979E-05	2430.6914	98.00538	0.0010163	2.104E-05
xrd_KI2_00	FCC	55.556976	0.2932294	55.964684	0.2953812	3.6018846	7.44E-05	2258.272	72.79389	0.0009804	1.878E-05
xrd_KI2_05	FCC	60.887974	0.2786293	61.288834	0.2804636	3.602371	0.0001104	2438.9824	131.50914	0.0012111	2.567E-05
xrd_KI2_07	FCC	60.009605	0.2823741	60.40204	0.2842207	3.6067672	9.859E-05	2318.5637	108.36195	0.0011318	2.306E-05
xrd_KI2_20	FCC	56.16008	0.3128905	56.573532	0.315194	3.6001732	7.819E-05	2062.828	68.1749	0.0009775	1.984E-05
xrd_KI2_26	FCC	50.30703	0.334236	50.727192	0.3370275	3.6011581	0.0001094	2562.6333	137.01721	0.0011391	2.488E-05
xrd_KI2_27	FCC	57.64921	0.2891793	58.042786	0.2911535	3.6017277	0.0001142	2160.5337	104.57638	0.0010302	2.675E-05
xrd_KI2_40	FCC	60.667175	0.3409761	61.05678	0.3431658	3.604571	8.271E-05	2206.006	81.870544	0.0010741	2.014E-05
xrd_KI2_43	FCC	60.15308	0.3507154	60.56639	0.3531252	3.6011767	8.827E-05	2137.5732	83.22894	0.0012031	2.112E-05
xrd_KI2_49	FCC	52.532623	0.3416103	52.955597	0.3443608	3.602782	0.0001062	2458.0518	114.99891	0.0011585	2.295E-05
xrd_KI2_60	FCC	66.49746	0.4133114	66.92008	0.4159381	3.6011841	9.833E-05	1796.9614	60.14904	0.000976	2.436E-05
xrd_KI2_63	FCC	58.17863	0.3366149	58.612904	0.3391275	3.6016405	8.042E-05	1821.8783	56.76892	0.0009411	2.178E-05
xrd_KI2_68	FCC	58.103985	0.2915518	58.529724	0.2936881	3.6036148	8.68E-05	1906.5969	53.93831	0.0011952	1.906E-05
xrd_KI2_70	FCC	60.516376	0.3221389	60.916042	0.3242664	3.602693	8.332E-05	2789.1143	118.18493	0.0010093	1.925E-05
xrd_KI2_78	FCC	55.892586	0.2480889	56.315502	0.2499661	3.6043355	8.068E-05	2320.367	85.862465	0.001014	1.963E-05
xrd_KI2_81	FCC	60.887974	0.2786293	61.288834	0.2804636	3.602371	0.0001104	2438.9824	131.50914	0.0012111	2.567E-05
xrd_KI2_85	FCC	59.094376	0.2947238	59.497852	0.2967361	3.6037307	7.78E-05	2512.4968	86.61421	0.0010422	1.751E-05
xrd_KI2_88	FCC	61.16909	0.4240263	61.553207	0.426689	3.6041749	0.0001157	2438.7644	119.20583	0.001211	2.4E-05
xrd_KI2_92	FCC	59.697365	0.3148094	60.14558	0.3171731	3.6012156	8.691E-05	2373.095	89.10896	0.0010806	1.93E-05
xrd_KI2_99	FCC	66.20569	0.6365262	66.61905	0.6405003	3.5982096	0.0001726	2216.1206	119.39904	0.0010657	3.336E-05
xrd_KI3_13	FCC	66.169334	0.3941203	66.58854	0.3966172	3.6034951	8.949E-05	2456.6904	103.01489	0.001018	2.136E-05

Fig 5.3.4 FCC phase

4. Third set of data

Title	Rwp(%)	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrair	Microstrair	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrair	Microstrain Error
xrd K1276	16.33748	Iron- alpha	40.83619	0.431433	40.43874	0.427234	2.876861	7.33E- 05	2734.396	318.7264	0.000849	6.4E- 05	Iron	59.16381	0.508235	59.56126	0.51165	3.604766	7.07E- 05	5391.255	1006.548	0.000893	4.63E- 05
xrd K1314	16.27853	Iron- alpha	30.74673	0.401202	30.35253	0.396059	2.876607	9.5E- 05	2434.414	351.7281	0.000989	8.17E- 05	Iron	69.25327	0.564103	69.64748	0.567314	3.601921	6.89E- 05	4775.879	761.5571	0.000979	4.3E- 05
xrd K1318	14.19612	Iron- alpha	38.89289	0.366705	38.50609	0.363058	2.877257	6.95E- 05	2147.395	188.3181	0.00091	6.05E- 05	Iron	61.10712	0.439258	61.49391	0.442038	3.605468	6.18E- 05	5083.739	125.7208	0.000945	2.35E- 05
xrd K1321	15.99759	Iron- alpha	35.93966	0.40848	35.57135	0.404294	2.877181	8.64E- 05	1812.176	167.17	0.000911	7.81E- 05	Iron	64.06033	0.515304	64.42866	0.518267	3.605698	6.91E- 05	4110.045	121.5202	0.000872	2.59E- 05

Fig 5.4.1 Iron-alpha phase

5. ATR2_RR

Title	Rwp(%)	Phase_Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell_Par(Ar	Cell_Par Er	Size(Angst	Crystal Siz	Microstrain
LaB6_C	88.43797	Iron FCC	34.21388	33.97007	47.28253	46.9456	3.60091	0.010923	604.8585	1679.514	1.52E-08
R10ATR2 a	8.956888	Iron FCC	8.498858	2.708637	7.217593	2.300291	3.830606	0.031109	6.344948	1.024619	1.52E-08
R10unirr a	11.48104	Iron FCC	0.118338	0.039872	0.118572	0.039951	3.597692	0.006525	305.0967	20.69824	1.52E-08
R11ATR2 a	10.41145	Iron FCC	0.720142	0.072472	0.724266	0.072887	3.595807	0.001881	176.7421	27.71878	1.52E-08
R11unirr a	7.550715	Iron FCC	0.186312	0.035408	0.186853	0.035511	3.60292	0.002341	349.1002	129.0789	1.52E-08
R13ATR2 a	11.14649	Iron FCC	0.704143	0.080814	0.707592	0.081209	3.595958	0.00213	177.8393	31.97101	1.52E-08
R13unirr a	10.4106	Iron FCC	0.71244	0.066906	0.715678	0.06721	3.597181	0.001599	208.7259	32.17065	1.52E-08
R14ATR2 a	9.637147	Iron FCC	7.751358	2.823014	6.442057	2.346171	3.869752	0.033613	6.541453	1.286434	1.52E-08
R14unirr a	9.094402	Iron FCC	0.133023	0.042579	0.132863	0.042528	3.607673	0.003874	352.9253	217.9313	1.52E-08
R15ATR2 a	9.192183	Iron FCC	0.198721	0.06265	0.199074	0.062762	3.600695	0.005901	169.3152	79.91118	1.52E-08
R15unirr a	7.283204	Iron FCC	0.158016	0.034275	0.158133	0.0343	3.604031	0.00265	350.7553	147.6084	1.52E-08
R16ATR2 a	7.373287	Iron FCC	8.954893	2.072681	7.657438	1.772375	3.822886	0.02236	6.46605	0.801588	1.52E-08
R16unirr a	10.03033	Iron FCC	2.856254	0.533555	2.676489	0.499974	3.686464	0.017667	13.28279	2.24875	1.52E-08
R17ATR2 a	7.778843	Iron FCC	8.586639	2.246729	7.332339	1.918537	3.818952	0.025714	6.343308	0.877282	1.52E-08
R17unirr a	8.789688	Iron FCC	0.332763	0.052279	0.333784	0.052439	3.599256	0.002597	212.164	54.61713	1.52E-08
R18ATR2 a	8.912221	Iron FCC	1.000027	0.113555	1.001785	0.113755	3.602854	0.004677	61.03757	8.525903	1.52E-08
R18unirr a	7.717035	Iron FCC	0.63014	0.062807	0.630159	0.062809	3.603398	0.002416	122.9532	17.29245	1.52E-08
R1ATR2 av	11.41673	Iron FCC	5.880473	2.841503	5.026995	2.429094	3.8147	0.04642	6.751036	1.813922	1.52E-08
R1unirr av	12.53121	Iron FCC	5.624554	2.917412	4.850936	2.516142	3.802368	0.049128	6.961333	2.220222	1.52E-08
R21ATR2 a	8.573923	Iron FCC	5.7734	1.893622	5.017088	1.645558	3.794543	0.031355	7.062332	1.342436	1.52E-08
R21unirr a	12.12547	Iron FCC	0.2766	2.555838	0.27433	2.534864	3.617726	0.968025	6.259345	34.37314	1.52E-08
R22ATR2 a	8.94157	Iron FCC	7.80206	2.6054	6.593522	2.201824	3.838786	0.03255	6.26212	1.094576	1.52E-08
R22unirr a	7.523181	Iron FCC	0.0832	0.0344	0.082673	0.034182	3.612249	0.004995	360.9478	286.0501	1.52E-08
R24ATR2 a	11.21678	Iron FCC	7.629416	3.139259	6.515906	2.681086	3.820705	0.041076	6.312927	1.373063	1.52E-08
R24unirr a	8.906373	Iron FCC	2.228632	0.410024	2.110856	0.388356	3.67042	0.017652	14.21302	2.451721	1.52E-08
R25ATR2 a	12.70572	Iron FCC	0.674727	0.067156	0.681847	0.067865	3.59741	0.001395	293.6075	53.23449	1.52E-08
R25unirr a	12.73196	Iron FCC	0.771385	0.049415	0.777631	0.049815	3.596989	0.001183	308.8896	13.98309	1.52E-08
R26ATR2 a	6.960313	Iron FCC	7.551526	2.018168	6.433507	1.719374	3.829349	0.026122	6.349771	0.894373	1.52E-08
R26unirr a	6.428339	Iron FCC	7.320622	2.059379	6.140549	1.72741	3.842142	0.027474	6.235894	0.838228	1.52E-08
R27ATR2 a	9.663356	Iron FCC	6.716641	2.336315	5.822081	2.025152	3.808502	0.033577	6.698806	1.28731	1.52E-08
R27unirr a	9.44897	Iron FCC	3.505618	0.959674	3.187917	0.872703	3.732061	0.024364	9.871014	2.031575	1.52E-08
R28ATR2 a	9.600985	Iron FCC	7.63859	2.88214	6.458224	2.436772	3.83216	0.036873	6.342997	1.256272	1.52E-08
R28unirr a	14.45728	Iron FCC	1.957765	0.464682	1.874247	0.444859	3.656799	0.024168	17.31318	4.577708	1.52E-08
R29ATR2 a	10.52835	Iron FCC	0.361657	0.065439	0.362429	0.065579	3.603467	0.003252	187.3963	52.76832	1.52E-08
R29unirr a	12.2458	Iron FCC	0.56547	0.064117	0.567726	0.064373	3.602377	0.001608	293.0572	60.37026	1.52E-08
R2ATR2 av	13.39212	Iron FCC	0.351922	1.181487	0.282466	0.948307	3.882593	0.290428	12.6106	33.31802	1.52E-08
R2unirr av	16.75313	Iron FCC	3.124015	1.277471	2.847474	1.164388	3.724433	0.040585	10.67139	3.919099	1.52E-08
R30ATR2 a	9.729699	Iron FCC	5.59863	2.225233	4.819933	1.915732	3.809122	0.037729	6.97639	1.581051	1.52E-08
R30unirr a	8.136072	Iron FCC	0.117413	0.036953	0.116536	0.036677	3.614395	0.003719	369.6944	228.5607	1.52E-08
R31ATR2 a	8.173783	Iron FCC	0.093106	0.039599	0.092611	0.039388	3.610278	0.005435	315.6006	245.6965	1.52E-08
R31unirr a	6.85592	Iron FCC	0.101485	0.031287	0.100877	0.031099	3.612787	0.003628	370.4464	224.4151	1.52E-08
R32ATR2 a	10.46362	Iron FCC	2.365843	0.282196	2.329609	0.277874	3.624564	0.011601	19.60922	2.644049	1.52E-08
R32unirr a	8.126671	Iron FCC	0.552122	0.046033	0.554487	0.04623	3.598132	0.00122	266.6326	39.46589	1.52E-08
R33ATR2 a	7.850479	Iron FCC	7.035912	2.036207	6.024995	1.743646	3.820796	0.02779	6.636388	1.056186	1.52E-08
R33unirr a	8.139206	Iron FCC	5.234768	1.453627	4.559421	1.266091	3.78874	0.027365	7.544386	1.403221	1.52E-08
R34ATR2 a	8.672145	Iron FCC	6.745786	2.30298	5.714679	1.950965	3.831552	0.032878	6.607324	1.228162	1.52E-08
R34unirr a	10.46149	Iron FCC	6.323658	2.725094	5.34295	2.302472	3.8299	0.040894	6.797312	1.62904	1.52E-08
R35ATR2 a	9.929754	Iron FCC	0.32824	0.828613	0.256624	0.647824	3.915195	0.225431	12.99297	26.24775	1.52E-08
R35unirr a	11.88662	Iron FCC	0.073508	0.054896	0.072861	0.054413	3.613777	0.008755	371.1879	543.4661	1.52E-08
R36ATR2 a	10.91401	Iron FCC	5.265914	2.225821	4.592939	1.941365	3.79433	0.039593	7.350218	1.844484	1.52E-08
R36unirr a	12.74973	Iron FCC	4.31931	1.631965	3.853903	1.45612	3.758603	0.036911	8.357078	2.673614	1.52E-08
R37ATR2 a	12.0756	Iron FCC	7.040986	3.487178	5.887421	2.915854	3.850449	0.048751	6.326866	1.640439	1.52E-08
R37unirr a	14.37885	Iron FCC	0.430784	0.098741	0.430798	0.098745	3.601943	0.00435	172.0815	60.07499	1.52E-08
R38ATR2 a	11.93981	Iron FCC	3.664233	1.322084	3.317456	1.196964	3.739579	0.032738	9.272917	2.579728	1.52E-08
R38unrr av	11.03097	Iron FCC	1.642571	0.221641	1.617626	0.218275	3.627139	0.011002	26.61985	3.815252	1.52E-08
R39ATR2 a	9.575704	Iron FCC	0.34499	0.787155	0.28145	0.642178	3.861658	0.196015	13.13991	24.0707	1.52E-08
R39unirr a	11.17651	Iron FCC	0.080869	0.050647	0.080416	0.050363	3.612359	0.007441	363.159	442.0684	1.52E-08
R40ATR2 a	16.46109	Iron FCC	6.718622	4.466842	5.674013	3.772339	3.837892	0.064325	6.520647	2.330392	1.52E-08
R40unirr a	8.397553	Iron FCC	0.07794	0.038808	0.077368	0.038523	3.614973	0.006178	338.8531	318.1435	1.52E-08
R41ATR2 a	9.074718	Iron FCC	6.554479	2.335168	5.560363	1.980994	3.829624	0.034199	6.690342	1.31353	1.52E-08
R41unirr a	9.486341	Iron FCC	0.07281	0.043227	0.072261	0.042901	3.614699	0.006997	371.4616	433.596	1.52E-08
R43ATR2 a	7.643929	Iron FCC	6.137697	1.907529	5.232987	1.626355	3.822368	0.029661	6.788152	1.175028	1.52E-08
R43unirr a	12.72285	Iron FCC	0.077599	0.058727	0.07711	0.058357	3.613227	0.008974	365.6827	539.096	1.52E-08
R44ATR2 a	7.539533	Iron FCC	7.018989	2.099906	5.931604	1.774588	3.838188	0.029461	6.361803	1.005909	1.52E-08
R44unirr a	9.239126	Iron FCC	0.088256	0.04345	0.087749	0.0432	3.612402	0.006117	334.6056	308.1441	1.52E-08
R47ATR2 a	9.792538	Iron FCC	7.097176	2.561488	6.049073	2.18321	3.824777	0.036342	6.478157	1.435228	1.52E-08
R47unirr a	9.051991	Iron FCC	6.955436	2.697753	5.846806	2.267756	3.844189	0.037595	6.385311	1.305758	1.52E-08
R48ATR2 a	7.488773	Iron FCC	6.819599	1.969675	5.841639	1.687215	3.815785	0.027019	6.761907	1.086942	1.52E-08
R48unirr a	6.853718	Iron FCC	6.581237	1.912943	5.517272	1.603684	3.840838	0.027366	6.571311	1.036491	1.52E-08
R49ATR2 a	7.973427	Iron FCC	6.44873	1.90877	5.559559	1.645583	3.804265	0.028472	6.828142	1.135384	1.52E-08
R49unirr a	8.577701	Iron FCC	0.097207	0.041586	0.096994	0.041494	3.60815	0.005445	319.4862	251.3451	1.52E-08
R4ATR2 av	21.80405	Iron FCC	0.33363	1.523678	0.270345	1.234661	3.86716	0.368228	14.94852	57.57951	1.52E-08
R4unirr av	14.62514	Iron FCC	1.758749	0.303948	1.666639	0.288029	3.669233	0.015457	25.57459	4.694839	1.52E-08
R50ATR2 a	7.748114	Iron FCC	0.116391	0.036171	0.115829	0.035996	3.612296	0.003781	349.1233	207.688	1.52E-08
R50unirr a	9.010006	Iron FCC	0.12173	0.041769	0.121174	0.041579	3.611307	0.004059	368.3679	248.2463	1.52E-08
R5ATR2 av	9.761727	Iron FCC	5.580596	2.194019	4.841369	1.903391	3.799278	0.037729	7.036724	1.595909	1.52E-08
R5unirr av	16.17482	Iron FCC	2.77313	1.15518	2.555087	1.064351	3.709478	0.037928	11.68865	4.104936	1.52E-08
R6ATR2 av	13.79704	Iron FCC	6.294044	3.305392	5.424549	2.848767	3.806523	0.051439	6.706383	2.210762	1.52E-08
R6unirr av	8.255617	Iron FCC	1.339824	0.133505	1.269031	0.126451	3.671081	0.005886	39.75198	4.618716	1.52E-08
R8ATR2 av	11.67287	Iron FCC	3.770746	1.37991	3.409678	1.247777	3.739453	0.032011	9.298286	2.461952	1.52E-08
R8unirr av	15.69528	Iron FCC	3.14519	1.441321	2.856842	1.309182	3.732494	0.042389	10.36257	3.634617	1.52E-08
R9ATR2 av	10.90612	Iron FCC	3.869689	1.180461	3.513637	1.071846	3.734911	0.026875	9.586333	2.165543	1.52E-08
R9unirr av	10.51655	Iron FCC	2.548295	0.644028	2.361157	0.596733	3.701699	0.023045	12.49954	2.702751	1.52E-08
RHAATR2	11.16508	Iron FCC	6.037634	2.608009	5.200803	2.246532	3.809984	0.041089	6.969461	1.718548	1.52E-08
RHAunirr a	12.94133	Iron FCC	1.572645	0.545163	1.445704	0.501158	3.707829	0.032268	15.8798	5.117399	1.52E-08
RX10ATR2	11.45402	Iron FCC	6.768796	2.862036	5.715004	2.416463	3.832696	0.040045	6.767135	1.581862	1.52E-08
RX10unirr	16.06894	Iron FCC	5.384748	3.622008	4.495957	3.02417	3.846699	0.060342	7.381569	2.897336	1.52E-08

Fig 5.5.1 IronFCC phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Siz	Microstrain	Microstrain
LaB6_C	IronBCC	58.68772	2.63E+08	2.312381	10363997	9.355441	32523578	5570.87	3.77E+10	3.918535	5629412
R10ATR2 a	IronBCC	88.54358	0.183204	89.51473	0.185214	2.868725	1.52E-05	5194.108	231.3496	0.001105	1.3E-05
R10unirr a	IronBCC	98.39523	0.262466	97.17874	0.259221	2.869242	2.03E-05	5803.411	374.8893	0.001313	1.58E-05
R11ATR2 a	IronBCC	97.64824	0.235444	96.68916	0.233131	2.868855	1.78E-05	4616.081	211.6754	0.001115	1.54E-05
R11unirr a	IronBCC	98.00918	0.168156	97.29281	0.166927	2.869411	1.26E-05	6036.722	239.3337	0.001135	1.05E-05
R13ATR2 a	IronBCC	97.88922	0.255663	96.86658	0.252992	2.868791	1.88E-05	5316.85	300.5214	0.001047	1.72E-05
R13unirr a	IronBCC	98.11274	0.237057	97.16632	0.23477	2.868657	1.78E-05	5320.956	280.8567	0.001137	1.53E-05
R14ATR2 a	IronBCC	87.92657	0.194974	89.61534	0.198719	2.869468	1.62E-05	4971.512	214.3426	0.001058	1.43E-05
R14unirr a	IronBCC	97.6826	0.203667	96.92361	0.202084	2.869718	1.53E-05	6037.419	302.2067	0.001147	1.29E-05
R15ATR2 a	IronBCC	97.49038	0.207842	96.50855	0.205749	2.86923	1.55E-05	5653.921	279.5877	0.001108	1.36E-05
R15unirr a	IronBCC	97.89443	0.163529	97.06725	0.162147	2.869329	1.24E-05	6017.185	245.6277	0.001202	1.02E-05
R16ATR2 a	IronBCC	88.42049	0.149741	89.42058	0.151434	2.8692	1.23E-05	5088.282	169.8144	0.001055	1.09E-05
R16unirr a	IronBCC	96.35409	0.221609	95.75464	0.22023	2.869192	1.67E-05	6002.407	318.8999	0.001074	1.45E-05
R17ATR2 a	IronBCC	89.7506	0.15871	90.38426	0.159831	2.868944	1.33E-05	4806.267	111.1907	0.001145	1.39E-06
R17unirr a	IronBCC	98.2533	0.197304	97.27673	0.195343	2.869186	1.49E-05	5872.872	272.8606	0.001166	1.22E-05
R18ATR2 a	IronBCC	96.65999	0.200526	95.87646	0.198901	2.869036	1.53E-05	4867.581	206.2225	0.001144	1.32E-05
R18unirr a	IronBCC	97.73065	0.173761	96.8056	0.172116	2.869129	1.3E-05	5856.873	247.0386	0.001137	1.11E-05
R1ATR2 av	IronBCC	91.40588	0.238772	91.87576	0.239999	2.868623	1.87E-05	7257.553	512.7523	0.001049	1.63E-05
R1unirr av	IronBCC	91.54739	0.264396	91.96815	0.265611	2.868311	2.06E-05	6836.816	505.1675	0.001042	1.81E-05
R21ATR2 a	IronBCC	91.2608	0.17845	91.752	0.17941	2.86888	1.4E-05	8553.428	529.0798	0.001073	1.19E-05
R21unirr a	IronBCC	96.72758	0.270563	96.21923	0.269141	2.868548	2E-05	9510.901	968.155	0.001104	1.69E-05
R22ATR2 a	IronBCC	88.6389	0.182591	89.70084	0.184779	2.869211	1.51E-05	5670.378	260.9902	0.001131	1.27E-05
R22unirr a	IronBCC	97.14577	0.168112	96.33173	0.166703	2.869019	1.28E-05	6055.626	253.7834	0.001167	1.06E-05
R24ATR2 a	IronBCC	89.48486	0.230942	90.28836	0.233015	2.868583	1.91E-05	5338.128	289.1807	0.001148	1.58E-05
R24unirr a	IronBCC	96.53127	0.19804	95.74291	0.196423	2.868795	1.56E-05	5429.937	250.4979	0.001274	1.22E-05
R25ATR2 a	IronBCC	96.84116	0.28193	96.49706	0.280929	2.868676	2.08E-05	8257.243	720.4592	0.001077	1.8E-05
R25unirr a	IronBCC	97.75409	0.284932	97.13936	0.28314	2.868644	2.09E-05	8298.758	768.7808	0.001112	1.76E-05
R26ATR2 a	IronBCC	88.4659	0.141426	89.59506	0.143231	2.869128	1.18E-05	6908.252	299.6855	0.001198	9.46E-06
R26unirr a	IronBCC	90.14055	0.132607	90.77798	0.133545	2.869215	1.1E-05	6974.574	267.5828	0.001218	8.7E-06
R27ATR2 a	IronBCC	90.46821	0.197628	91.73743	0.200401	2.868816	1.58E-05	8680.271	601.2098	0.001119	1.29E-05
R27unirr a	IronBCC	94.94804	0.203054	95.02438	0.203218	2.869039	1.54E-05	10722.79	899.2548	0.001121	1.25E-05
R28ATR2 a	IronBCC	89.75315	0.199075	90.4447	0.200609	2.868726	1.67E-05	5287.724	252.4327	0.001235	1.33E-05
R28unirr a	IronBCC	96.61922	0.325795	95.81043	0.323067	2.868557	2.49E-05	5088.01	352.7035	0.001139	2.12E-05
R29ATR2 a	IronBCC	98.4734	0.23422	97.80418	0.232628	2.868621	1.76E-05	7128.697	324.5561	0.001163	1.94E-06
R29unirr a	IronBCC	98.27934	0.27492	97.7157	0.273343	2.868499	2.03E-05	6239.492	420.2184	0.001081	1.75E-05
R2ATR2 av	IronBCC	97.47763	0.299278	97.01313	0.297851	2.868424	2.14E-05	7234.771	583.0788	0.00092	2.04E-05
R2unirr av	IronBCC	94.9433	0.365923	94.75725	0.365206	2.868025	2.63E-05	11670.95	1632.486	0.000879	2.55E-05
R30ATR2 a	IronBCC	91.47242	0.202528	92.13045	0.203985	2.869218	1.59E-05	6696.399	367.2553	0.00104	1.39E-05
R30unirr a	IronBCC	97.7808	0.17986	97.02989	0.178478	2.868944	1.35E-05	6043.21	176.9246	0.001107	7.3E-07
R31ATR2 a	IronBCC	97.81733	0.183223	96.90784	0.18152	2.869305	1.35E-05	6024.992	265.5285	0.001057	1.2E-05
R31unirr a	IronBCC	97.60022	0.152644	96.84733	0.151466	2.86913	1.16E-05	6037.221	221.7726	0.001187	9.41E-06
R32ATR2 a	IronBCC	97.16959	0.236207	96.44213	0.234438	2.869235	1.77E-05	4491.124	226.3666	0.001048	1.58E-05
R32unirr a	IronBCC	98.23395	0.184387	97.28169	0.1826	2.869211	1.39E-05	5437.335	226.8971	0.001153	1.17E-05
R33ATR2 a	IronBCC	89.53834	0.159493	90.53533	0.161269	2.869148	1.3E-05	7975.678	292.7699	0.001102	9.86E-07
R33unirr a	IronBCC	92.26097	0.171418	92.5349	0.171927	2.868972	1.35E-05	8724.844	504.0449	0.00114	1.09E-05
R34ATR2 a	IronBCC	90.36605	0.179126	91.17266	0.180724	2.869005	1.44E-05	7080.34	371.3357	0.001111	1.2E-05
R34unirr a	IronBCC	91.55435	0.219806	92.01894	0.220922	2.868901	1.74E-05	8121.068	588.7581	0.001118	1.44E-05
R35ATR2 a	IronBCC	96.52837	0.221244	95.93128	0.219876	2.868645	1.65E-05	6541.433	381.4973	0.001085	1.43E-05
R35unirr a	IronBCC	97.48745	0.264664	96.60468	0.262267	2.868495	1.97E-05	6047.829	259.2358	0.001042	1.86E-06
R36ATR2 a	IronBCC	92.29153	0.228503	93.13386	0.230588	2.868681	1.77E-05	8430.217	634.6747	0.001052	1.51E-05
R36unirr a	IronBCC	93.96584	0.273218	94.30341	0.2742	2.868531	2.06E-05	8920.001	803.1874	0.001041	1.78E-05
R37ATR2 a	IronBCC	89.5119	0.249051	90.53068	0.251886	2.868315	2.05E-05	5709.546	352.4124	0.001131	1.71E-05
R37unirr a	IronBCC	97.54585	0.326585	96.60378	0.323431	2.868158	2.44E-05	5038.658	340.4809	0.001071	2.17E-05
R38ATR2 a	IronBCC	94.73324	0.255808	94.96446	0.256433	2.869022	1.91E-05	7347.177	523.1962	0.000993	1.7E-05
R38unrr av	IronBCC	97.51719	0.244886	97.0482	0.243708	2.868821	1.79E-05	7668.287	559.0587	0.001058	1.56E-05
R39ATR2 a	IronBCC	96.75398	0.213435	96.27011	0.212368	2.868719	1.58E-05	6608.349	369.9258	0.001049	1.39E-05
R39unirr a	IronBCC	97.68975	0.249485	96.99548	0.247712	2.868585	1.85E-05	6066.27	359.1751	0.001067	1.61E-05
R40ATR2 a	IronBCC	90.16435	0.341716	91.15739	0.345479	2.868801	2.73E-05	6223.01	546.1966	0.001041	2.39E-05
R40unirr a	IronBCC	97.64358	0.186116	96.96127	0.184815	2.868864	1.4E-05	6083.671	263.482	0.001113	1.17E-05
R41ATR2 a	IronBCC	90.51038	0.188627	91.33019	0.190336	2.868771	1.5E-05	6388.419	321.1722	0.001045	1.3E-05
R41unirr a	IronBCC	97.74139	0.210939	96.98885	0.209314	2.869143	1.56E-05	6049.805	285.5108	0.001031	1.36E-05
R43ATR2 a	IronBCC	90.80913	0.158355	91.55368	0.159654	2.868942	1.28E-05	6582.398	286.2918	0.001115	1.06E-05
R43unirr a	IronBCC	97.52561	0.28316	96.82108	0.281114	2.86871	2.12E-05	6064.2	281.579	0.001063	3.26E-06
R44ATR2 a	IronBCC	89.7699	0.154226	90.82486	0.156039	2.868957	1.26E-05	6866.97	304.9299	0.001128	1.03E-05
R44unirr a	IronBCC	97.71106	0.206399	96.98291	0.204861	2.868804	1.55E-05	6093.774	305.4452	0.001125	1.31E-05
R47ATR2 a	IronBCC	89.32002	0.201786	90.22142	0.203822	2.868645	1.63E-05	6899.759	400.0985	0.001088	1.38E-05
R47unirr a	IronBCC	89.40723	0.185644	90.41837	0.187744	2.868786	1.51E-05	7111.168	396.5571	0.001116	1.26E-05
R48ATR2 a	IronBCC	89.93304	0.15148	90.61913	0.152635	2.869012	1.26E-05	6370.286	0.96574	0.001139	7.04E-06
R48unirr a	IronBCC	90.89767	0.143482	91.41333	0.144296	2.869036	1.17E-05	6584.457	270.8763	0.001192	9.45E-06
R49ATR2 a	IronBCC	91.22357	0.166227	91.68525	0.167069	2.868921	1.34E-05	6326.169	283.8962	0.001149	1.1E-05
R49unirr a	IronBCC	97.5745	0.192277	96.84593	0.190841	2.868851	1.46E-05	6012.076	286.4749	0.001177	1.21E-05
R4ATR2 av	IronBCC	97.2119	0.49833	96.56061	0.494991	2.867962	3.62E-05	6658.244	861.1743	0.001006	3.28E-05
R4unirr av	IronBCC	97.15579	0.326544	96.37207	0.32391	2.86825	2.36E-05	7477.597	682.8929	0.000958	2.18E-05
R50ATR2 a	IronBCC	97.67795	0.173256	96.97343	0.172007	2.869377	1.3E-05	6017.554	254.3434	0.001134	1.1E-05
R50unirr a	IronBCC	98.09185	0.203085	97.35798	0.201566	2.869097	1.51E-05	6033.281	296.8691	0.001125	1.29E-05
R5ATR2 av	IronBCC	91.09282	0.203616	91.77225	0.205135	2.868872	1.57E-05	10261.19	856.1702	0.001023	1.38E-05
R5unirr av	IronBCC	94.98483	0.354732	94.66161	0.353525	2.868191	2.58E-05	12718.62	2137.155	0.000955	2.35E-05
R6ATR2 av	IronBCC	90.71064	0.288372	91.36359	0.290448	2.868301	2.23E-05	8235.963	771.2131	0.000983	2.01E-05
R6unirr av	IronBCC	97.29377	0.184363	96.54092	0.182936	2.868909	1.36E-05	6613.182	321.406	0.001078	1.19E-05
R8ATR2 av	IronBCC	93.04938	0.24846	93.19315	0.248844	2.868599	1.87E-05	11604.37	1298.609	0.001006	1.64E-05
R8unirr av	IronBCC	93.59052	0.339736	93.6889	0.340093	2.868029	2.52E-05	9516.982	1187.473	0.000955	2.33E-05
R9ATR2 av	IronBCC	92.96291	0.231566	93.12945	0.231981	2.86883	1.74E-05	9956.593	892.1992	0.000984	1.57E-05
R9unirr av	IronBCC	95.40907	0.22948	94.96938	0.228422	2.868698	1.7E-05	9553.978	805.3172	0.001025	1.49E-05
RHAATR2	IronBCC	90.56306	0.231714	91.38752	0.233823	2.868594	1.8E-05	8785.729	720.3088	0.000992	1.61E-05
RHAunirr a	IronBCC	97.40799	0.289236	96.6901	0.287105	2.868557	2.11E-05	6852.593	518.9555	0.000993	1.92E-05
RX10ATR2	IronBCC	92.30116	0.239118	92.93525	0.240761	2.868611	1.88E-05	6180.371	367.0232	0.001069	1.59E-05
RX10unirr	IronBCC	93.44262	0.342805	94.02123	0.344927	2.869041	2.61E-05	8241.114	897.4739	0.00103	2.26E-05

Fig 5.5.2 IronBCC phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
LaB6_C	Cohenite	7.098396	103.5829	50.40509	735.5331	5.11941	0.025628	6.729665	0.029476	4.538464	0.025027	379.7914	385.769	0.0006	
R10ATR2 a	Cohenite	2.957568	0.763966	3.26768	0.84407	5.081672	0.001244	6.753004	0.002119	4.526094	0.001045	777.6503	87.05393	0.0006	
R10unirr a	Cohenite	1.486429	0.133531	2.702683	0.242792	5.083102	0.001979	6.753318	0.003381	4.524177	0.0017	354.8312	4.075948	0.0006	
R11ATR2 a	Cohenite	1.631621	0.340434	2.586578	0.539683	5.083977	0.001784	6.755092	0.003086	4.526914	0.001564	442.7789	38.17429	0.0006	
R11unirr a	Cohenite	1.804511	0.139766	2.52034	0.19521	5.081863	0.001236	6.754699	0.002108	4.524071	0.001054	576.2302	26.5509	0.0006	
R13ATR2 a	Cohenite	1.406634	0.921455	2.425833	1.589109	5.083728	0.001885	6.75574	0.003244	4.526999	0.001647	461.8989	44.70315	0.0006	
R13unirr a	Cohenite	1.174822	0.767824	2.118005	1.384257	5.083152	0.001738	6.754929	0.003002	4.525679	0.001518	504.0124	48.92641	0.0006	
R14ATR2 a	Cohenite	4.32207	0.451547	3.942602	0.411902	5.082007	0.001438	6.752007	0.002423	4.526146	0.001213	696.6456	80.16942	0.0006	
R14unirr a	Cohenite	2.184378	0.217546	2.943532	0.293151	5.081907	0.001357	6.755138	0.002297	4.524039	0.001146	572.8704	48.06015	0.0006	
R15ATR2 a	Cohenite	2.310906	0.217858	3.29237	0.310384	5.083084	0.001676	6.756108	0.00285	4.525316	0.001451	351.1277	22.1661	0.0006	
R15unirr a	Cohenite	1.947556	0.140425	2.774625	0.20006	5.082779	0.001126	6.754606	0.001921	4.524407	0.000961	538.4324	34.30134	0.0006	
R16ATR2 a	Cohenite	2.62462	0.220832	2.921986	0.245852	5.082114	0.001101	6.753325	0.001868	4.527329	0.000927	795.1396	80.93329	0.0006	
R16unirr a	Cohenite	0.789654	0.089892	1.568874	0.178597	5.081358	0.00155	6.753477	0.002676	4.526802	0.001317	751.4803	104.8748	0.0006	
R17ATR2 a	Cohenite	1.662755	0.157607	2.283401	0.216436	5.082105	0.001131	6.752689	0.001933	4.526832	0.000958	844.1793	95.60936	0.0006	
R17unirr a	Cohenite	1.413935	0.227846	2.389489	0.385051	5.082821	0.001409	6.754599	0.002423	4.525258	0.001221	482.7097	21.78402	0.0006	
R18ATR2 a	Cohenite	2.339984	0.933168	3.121755	1.244932	5.081771	0.001474	6.754783	0.002504	4.527108	0.001262	478.985	38.52083	0.0006	
R18unirr a	Cohenite	1.639212	0.662052	2.564241	1.035657	5.082326	0.001257	6.754349	0.002136	4.525817	0.001076	489.4559	31.34858	0.0006	
R1ATR2 av	Cohenite	2.713648	0.408983	3.097249	0.466796	5.082756	0.001521	6.750853	0.002577	4.526339	0.001256	834.4564	122.1313	0.0006	
R1unirr av	Cohenite	2.828057	0.403009	3.180919	0.453293	5.081928	0.001696	6.7508	0.00287	4.524882	0.001397	813.3064	130.0738	0.0006	
R21ATR2 a	Cohenite	2.965797	0.332885	3.230917	0.362643	5.081534	0.001043	6.750786	0.001754	4.525244	0.00086	1063.093	132.8541	0.0006	
R21unirr a	Cohenite	2.995828	1.429988	3.506441	1.673717	5.080277	0.001664	6.751094	0.002793	4.523298	0.001376	652.8857	85.39172	0.0006	
R22ATR2 a	Cohenite	3.559037	0.684717	3.705635	0.71292	5.0816	0.001123	6.752489	0.001895	4.525905	0.000929	837.7635	93.04956	0.0006	
R22unirr a	Cohenite	2.771026	0.197338	3.585605	0.255347	5.080536	0.000971	6.753723	0.001625	4.523341	0.000805	595.1788	36.75645	0.0006	
R24ATR2 a	Cohenite	2.885718	0.35135	3.195734	0.389096	5.081957	0.00153	6.751317	0.002599	4.527031	0.001272	817.7138	119.7344	0.0006	
R24unirr a	Cohenite	1.240097	0.100148	2.146231	0.173326	5.080579	0.001304	6.751818	0.00224	4.526174	0.001096	638.7063	64.20206	0.0006	
R25ATR2 a	Cohenite	2.484109	0.269657	2.821098	0.306238	5.081883	0.003474	6.753858	0.005851	4.52719	0.003066	321.7015	42.48435	0.0006	
R25unirr a	Cohenite	1.474524	1.151609	2.083007	1.626836	5.081604	0.003632	6.754235	0.00615	4.527009	0.003211	321.7702	33.58082	0.0006	
R26ATR2 a	Cohenite	3.982567	0.299266	3.971428	0.298429	5.081658	0.000845	6.751611	0.001416	4.526135	0.000695	869.2568	72.41029	0.0006	
R26unirr a	Cohenite	2.53883	0.278306	3.081475	0.337791	5.081645	0.000764	6.751443	0.001285	4.525193	0.000627	981.164	86.90692	0.0006	
R27ATR2 a	Cohenite	2.815148	0.482489	2.440483	0.418275	5.081162	0.002096	6.750462	0.003548	4.525531	0.001761	811.9448	155.743	0.0006	
R27unirr a	Cohenite	1.546346	0.645213	1.787709	0.745921	5.080838	0.002089	6.751133	0.003576	4.525153	0.00176	773.3062	149.0865	0.0006	
R28ATR2 a	Cohenite	2.608261	0.444272	3.097072	0.527533	5.082466	0.001297	6.751647	0.00221	4.526817	0.001079	777.0295	92.38123	0.0006	
R28unirr a	Cohenite	1.423018	0.210088	2.315323	0.341824	5.081491	0.001931	6.751751	0.00331	4.526686	0.001622	792.8064	140.8735	0.0006	
R29ATR2 a	Cohenite	1.164946	0.107183	1.83339	0.168684	5.081055	0.0031	6.753994	0.005222	4.526375	0.002701	326.2523	35.13912	0.0006	
R29unirr a	Cohenite	1.155183	0.980609	1.716574	1.457162	5.081688	0.003301	6.753233	0.005688	4.528143	0.002915	420.5696	64.12461	0.0006	
R2ATR2 av	Cohenite	2.170445	1.455873	2.704407	1.814039	5.082094	0.002254	6.753803	0.003866	4.526106	0.001879	589.3126	94.14689	0.0006	
R2unirr av	Cohenite	1.932687	0.683328	2.395277	0.846883	5.080522	0.002522	6.75019	0.00427	4.524535	0.002081	916.8778	261.6205	0.0006	
R30ATR2 a	Cohenite	2.928949	0.381708	3.049623	0.397435	5.083075	0.001359	6.752273	0.002304	4.525769	0.001125	938.3881	136.1929	0.0006	
R30unirr a	Cohenite	2.101786	0.177545	2.853575	0.241051	5.081859	0.001175	6.753538	0.001963	4.52336	0.000974	620.955	47.51442	0.0006	
R31ATR2 a	Cohenite	2.089563	0.172895	2.999556	0.24819	5.083019	0.001251	6.755933	0.002129	4.525177	0.001055	480.0144	30.89135	0.0006	
R31unirr a	Cohenite	2.298292	0.130733	3.051791	0.173594	5.082435	0.000972	6.75408	0.001644	4.523991	0.000808	608.7639	25.31641	0.0006	
R32ATR2 a	Cohenite	0.464559	0.051898	1.228262	0.137215	5.082169	0.001766	6.754981	0.003094	4.529458	0.001541	625.9174	71.31112	0.0006	
R32unirr a	Cohenite	1.213927	0.19607	2.163822	0.349494	5.082807	0.00141	6.755632	0.002431	4.525731	0.001237	468.8846	34.08297	0.0006	
R33ATR2 a	Cohenite	3.42575	0.845737	3.439671	0.849173	5.082581	0.001006	6.751703	0.001668	4.526388	0.000832	998.5848	119.7811	0.0006	
R33unirr a	Cohenite	2.504263	0.273184	2.905674	0.316973	5.082006	0.001029	6.750471	0.001736	4.524967	0.000849	1022.023	125.1008	0.0006	
R34ATR2 a	Cohenite	2.888158	0.339145	3.112658	0.365507	5.082542	0.00113	6.7516	0.001908	4.526233	0.000932	1018.2	132.6411	0.0006	
R34unirr a	Cohenite	2.121995	0.30614	2.638115	0.3806	5.082246	0.001322	6.750373	0.002227	4.525024	0.001085	1161.407	183.0724	0.0006	
R35ATR2 a	Cohenite	3.143384	1.178426	3.812093	1.429118	5.081418	0.001257	6.752301	0.002133	4.524743	0.001043	603.1287	54.10685	0.0006	
R35unirr a	Cohenite	2.439044	0.279774	3.322464	0.381108	5.080633	0.001497	6.752909	0.002486	4.522959	0.001235	642.0615	64.22244	0.0006	
R36ATR2 a	Cohenite	2.442555	0.566237	2.273203	0.526978	5.081929	0.002316	6.74976	0.003928	4.526139	0.001938	861.5547	195.8378	0.0006	
R36unirr a	Cohenite	1.714843	0.687668	1.842683	0.738933	5.08115	0.002956	6.749655	0.005053	4.525635	0.002486	789.898	219.0292	0.0006	
R37ATR2 a	Cohenite	3.447114	0.538948	3.581904	0.560022	5.082222	0.001554	6.750343	0.002625	4.525667	0.001281	867.2409	133.8662	0.0006	
R37unirr a	Cohenite	2.023366	0.488225	2.965428	0.715539	5.082091	0.001997	6.752232	0.003409	4.524253	0.001694	581.9694	73.7516	0.0006	
R38ATR2 a	Cohenite	1.602527	0.629519	1.718087	0.674914	5.08257	0.00284	6.749856	0.004855	4.527503	0.002409	837.7468	230.1009	0.0006	
R38unrr av	Cohenite	0.840243	0.776873	1.334182	1.23356	5.080499	0.00272	6.752061	0.004682	4.529869	0.002335	599.8145	118.1455	0.0006	
R39ATR2 a	Cohenite	2.90103	1.134884	3.448442	1.349031	5.081499	0.00138	6.752707	0.002352	4.524947	0.001148	581.4122	54.9899	0.0006	
R39unirr a	Cohenite	2.229386	0.278039	2.924109	0.364681	5.08094	0.001623	6.752709	0.002744	4.523075	0.001352	626.2398	68.58447	0.0006	
R40ATR2 a	Cohenite	3.117032	0.701955	3.168596	0.713568	5.08222	0.002285	6.751172	0.003864	4.525351	0.001889	972.1236	243.8388	0.0006	
R40unirr a	Cohenite	2.278482	0.174925	2.96136	0.227352	5.081753	0.001196	6.753503	0.002014	4.523758	0.000987	649.0098	36.88154	0.0006	
R41ATR2 a	Cohenite	2.935137	0.332475	3.109443	0.35222	5.082084	0.001216	6.751196	0.002059	4.525428	0.001006	982.0174	121.4994	0.0006	
R41unirr a	Cohenite	2.185801	0.173118	2.938885	0.232764	5.081938	0.001339	6.754469	0.002247	4.523945	0.001102	646.3174	20.14957	0.0006	
R43ATR2 a	Cohenite	3.053171	0.30498	3.213335	0.320978	5.08216	0.001006	6.751436	0.001703	4.52558	0.000831	971.177	107.6833	0.0006	
R43unirr a	Cohenite	2.396783	0.305496	3.101805	0.395358	5.081684	0.001759	6.752909	0.002934	4.523587	0.001457	659.5756	78.23716	0.0006	
R44ATR2 a	Cohenite	3.211116	0.314138	3.243533	0.317309	5.082295	0.00102	6.751073	0.001721	4.52548	0.000843	968.3218	104.8478	0.0006	
R44unirr a	Cohenite	2.200686	0.20852	2.929341	0.277562	5.081738	0.001351	6.752647	0.002283	4.523535	0.001123	604.483	53.0504	0.0006	
R47ATR2 a	Cohenite	3.582808	0.408223	3.72951	0.424938	5.081605	0.001127	6.751212	0.001898	4.525403	0.000926	1013.318	128.4976	0.0006	
R47unirr a	Cohenite	3.637327	0.363097	3.734832	0.37283	5.081898	0.001046	6.750442	0.001753	4.524619	0.000858	1046.419	114.8166	0.0006	
R48ATR2 a	Cohenite	3.247356	0.258554	3.539233	0.281793	5.080645	0.000923	6.752585	0.001527	4.525762	0.000758	901.0515	83.9822	0.0006	
R48unirr a	Cohenite	2.521096	0.58456	3.069395	0.711692	5.08084	0.000834	6.751781	0.00141	4.524654	0.000688	938.6602	89.38701	0.0006	
R49ATR2 a	Cohenite	2.327695	0.354693	2.755189	0.419834	5.081305	0.001189	6.750821	0.002021	4.524517	0.000993	755.2575	80.01023	0.0006	
R49unirr a	Cohenite	2.328293	0.204839	3.057077	0.268957	5.081575	0.001384	6.751925	0.002331	4.523055	0.001164	499.8345	36.79158	0.0006	
R4ATR2 av	Cohenite	2.454473	1.042308	3.16905	1.345758	5.082739	0.003553	6.752704	0.006072	4.525928	0.002964	495.2897	101.6886	0.0006	
R4unirr av	Cohenite	1.085464	0.263152	1.96129	0.475481	5.082365	0.002058	6.752831	0.003483	4.524869	0.001681	756.874	74.11127	0.0006	
R50ATR2 a	Cohenite	2.205664	0.177372	2.910733	0.234071	5.083787	0.001355	6.753369	0.002284	4.524183	0.001136	470.5631	30.05159	0.0006	
R50unirr a	Cohenite	1.786418	0.18813	2.520849	0.265475	5.083433	0.001483	6.751649	0.002503	4.52348	0.001242	577.3059	53.53493	0.0006	
R5ATR2 av	Cohenite	3.326586	1.103462	3.386385	1.123298	5.082395	0.001232	6.750903	0.00206	4.525954	0.001011	1032.324	159.8087	0.0006	
R5unirr av	Cohenite	2.242045	0.659458	2.783303	0.81866	5.080599	0.002075	6.750069	0.003482	4.523924	0.001704	1018.515	248.0777	0.0006	
R6ATR2 av	Cohenite	2.995316	0.569931	3.211857	0.611133	5.081941	0.001788	6.750044	0.003018	4.525899	0.001475	949.2537	182.5128	0.0006	
R6unirr av	Cohenite	1.366408	0.202528	2.190056	0.324609	5.082755	0.001233	6.753112	0.002073	4.52532	0.001003	696.5965	67.64269	0.0006	
R8ATR2 av	Cohenite	3.179879	0.428874	3.397171	0.458181	5.082101	0.001538	6.751558	0.002582	4.52633	0.001265	847.6716	126.3953	0.0006	
R8unirr av	Cohenite	3.264289	0.57214	3.454263	0.605438	5.081995	0.002203	6.750536	0.003696	4.52506	0.001811	764.3619	147.5594	0.0006	
R9ATR2 av	Cohenite	3.167399	0.596936	3.356918	0.632654	5.082386	0.001482	6.751711	0.002489	4.526905	0.001225	814.0178	113.2725	0.0006	
R9unirr av	Cohenite	2.042633	0.245626	2.669462	0.321001	5.080692	0.001473	6.750695	0.002478	4.524893	0.001214	781.0198	104.8264	0.0006	
RHAATR2	Cohenite	3.39931	1.217969	3.411681	1.222402	5.083299	0.001414	6.751805	0.002388	4.52527	0.00117	1037.271	184.7125	0.0006	

Fig 5.5.3 Cohenite phase

6. ATR2_UCSB

Title	Rwp(%)	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain
17 LJ03-0(	7.795087	Cohenite	2.16236	0.11884	2.109692	0.115946	5.083397	0.002228	6.761617	0.003865	4.530305	0.002037	589.0188	87.93825	0.0006
20 LJ BL-0	8.670251	Cohenite	2.213329	0.137082	2.159721	0.133761	5.083216	0.002403	6.761677	0.004148	4.529008	0.002189	594.6952	99.15333	0.0006
29 LG01-0	7.842006	Cohenite	2.393822	0.112527	2.334526	0.10974	5.086141	0.001582	6.764152	0.00276	4.529263	0.001386	968.8966	160.3861	0.0006
2 WA BL-(	9.800974	Cohenite	1.289188	0.115564	1.256663	0.112649	5.085082	0.004109	6.769443	0.007302	4.526866	0.003612	716.5923	135.0675	0.0006
2 WA BL-(	9.348998	Cohenite	1.31313	0.13808	1.279962	0.134592	5.084852	0.003974	6.769982	0.007104	4.526789	0.003527	663.9312	200.5627	0.0006
39 LD02-0	7.967835	Cohenite	2.982986	0.114319	2.907584	0.111429	5.084551	0.001827	6.767323	0.003168	4.531364	0.001675	537.1429	38.58313	0.0006
46 CM6 4-	10.99331	Cohenite	2.997373	0.283617	2.794319	0.264404	4.88434	0.098305	6.970807	0.132595	4.798824	0.081327	29.81173	5.784958	0.0006
4 LI03-00(	9.397326	Cohenite	2.567583	0.140662	2.504546	0.137208	5.08492	0.002159	6.76487	0.003785	4.52898	0.001942	590.994	84.60945	0.0006
54 LH03-0	8.939767	Cohenite	2.777543	0.127816	2.709093	0.124666	5.084552	0.00202	6.764121	0.003512	4.529341	0.001821	534.9096	40.11639	0.0006
56 LB BL-(	11.74011	Cohenite	2.621104	0.19407	2.556192	0.189263	5.082641	0.003699	6.769517	0.006384	4.526504	0.003355	373.1933	58.9973	0.0006
57 LB03 C	7.502475	Cohenite	2.129057	0.089324	2.076217	0.087107	5.084166	0.001905	6.763409	0.003331	4.529123	0.001698	715.6819	28.94832	0.0006
57 WA03	8.569508	Cohenite	1.375154	0.11219	1.340952	0.109399	5.08383	0.003781	6.765619	0.006732	4.528116	0.003443	564.4184	96.06281	0.0006
65 LD BL-(	7.982783	Cohenite	2.244108	0.0932	2.189992	0.090952	5.086031	0.001605	6.763192	0.002798	4.526753	0.001403	1030.916	66.93318	0.0006
75 LC03-0	7.972867	Cohenite	2.585973	0.133934	2.520244	0.130529	5.082065	0.002594	6.770213	0.004457	4.533255	0.002393	385.5774	43.33627	0.0006
LC LTTA B	9.397618	Cohenite	3.056326	0.183337	2.977069	0.178583	5.076948	0.004298	6.781518	0.006694	4.538769	0.00379	254.2131	29.78294	0.0006

Fig 5.6.1 Cohenite phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Microstrain
17 LJ03-0(	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
20 LJ BL-0	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
29 LG01-0	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
2 WA BL-(	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
2 WA BL-(	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
39 LD02-0	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
46 CM6 4-	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
4 LI03-00(	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
54 LH03-0	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
56 LB BL-(	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
57 LB03 C	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
57 WA03	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
65 LD BL-(	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
75 LC03-0	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006
LC LTTA B	IronFCC	0	0	0	0	3.595892	0.001512	350	0.0006

Fig 5.6.2 IronFCC phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
17 LJ03-0(	FeBCC	97.6665	0.221077	97.68735	0.221125	2.869261	1.47E-05	5311.605	156.2951	0.000783	1.76E-06
20 LJ BL-0	FeBCC	97.6127	0.24744	97.63431	0.247494	2.869087	1.59E-05	9011.473	647.3974	0.000773	1.38E-05
29 LG01-0	FeBCC	97.47997	0.222571	97.51569	0.222652	2.869363	1.45E-05	6446.494	299.0245	0.000773	1.25E-05
2 WA BL-(	FeBCC	98.62179	0.279803	98.63704	0.279847	2.869158	1.82E-05	8589.531	620.9362	0.000773	1.54E-05
2 WA BL-(	FeBCC	98.59864	0.268356	98.61462	0.2684	2.869138	1.73E-05	8735.075	646.1724	0.000773	1.49E-05
39 LD02-0	FeBCC	96.85404	0.225977	96.89851	0.22608	2.86937	1.47E-05	7417.309	397.0681	0.000735	1.3E-05
46 CM6 4-	FeBCC	96.90276	0.307707	97.08751	0.308293	2.870145	1.89E-05	10539.75	1040.485	0.000661	1.76E-05
4 LI03-00(	FeBCC	97.27788	0.26452	97.31181	0.264613	2.869407	1.69E-05	5249.291	239.0317	0.000731	1.5E-05
54 LH03-0	FeBCC	97.09734	0.250869	97.14227	0.250985	2.869108	1.6E-05	7083.29	398.9583	0.000747	1.35E-05
56 LB BL-(	FeBCC	97.27972	0.332591	97.32616	0.33275	2.86878	2.08E-05	12260.75	1612.039	0.000759	1.8E-05
57 LB03 C	FeBCC	97.75945	0.211027	97.79125	0.211096	2.86885	1.38E-05	6022	186.6065	0.000742	1.58E-06
57 WA03	FeBCC	98.5381	0.244001	98.55529	0.244044	2.868978	1.59E-05	5809.37	260.5651	0.000762	1.39E-05
65 LD BL-	FeBCC	97.61305	0.224619	97.64069	0.224683	2.869399	1.45E-05	6972.046	347.8688	0.000785	1.21E-05
75 LC03-0	FeBCC	97.29898	0.226103	97.34303	0.226205	2.869578	1.47E-05	5694.88	245.0187	0.000752	1.3E-05
LC LTTA B	FeBCC	96.83926	0.271206	96.89913	0.271374	2.87071	1.76E-05	10700.52	1016.468	0.00085	1.44E-05

Fig 5.6.3 FeBCC phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Size(Angst	Microstrain
17 LJ03-0(	Mo2 C	0.171139	0.014531	0.202963	0.017233	4.719903	0.006104	5.995471	0.007856	5.140561	0.007344	440	0.0006
20 LJ BL-0	Mo2 C	0.173968	0.016373	0.205974	0.019385	4.719304	0.006709	5.998488	0.008754	5.146325	0.008176	440	0.0006
29 LG01-0	Mo2 C	0.126208	0.014282	0.149789	0.016951	4.720515	0.008515	6.006322	0.009773	5.128103	0.009736	440	0.0006
2 WA BL-(	Mo2 C	0.089024	0.017592	0.106296	0.021005	4.717308	0.015852	6.006918	0.016679	5.098071	0.016878	440	0.0006
2 WA BL-(	Mo2 C	0.088231	0.016843	0.105418	0.020124	4.717496	0.015243	6.005738	0.01605	5.095454	0.016189	440	0.0006
39 LD02-0	Mo2 C	0.162977	0.015408	0.193913	0.018333	4.725704	0.006903	5.993928	0.008202	5.120747	0.007963	440	0.0006
46 CM6 4-	Mo2 C	0.09987	0.018854	0.118172	0.022308	4.727306	0.013221	5.999779	0.017828	5.154021	0.016429	440	0.0006
4 LI03-00(	Mo2 C	0.154545	0.016769	0.183638	0.019926	4.71936	0.007836	6.001204	0.009372	5.127822	0.009122	440	0.0006
54 LH03-0	Mo2 C	0.125121	0.015572	0.148634	0.018498	4.719276	0.009045	6.00067	0.01074	5.12876	0.010507	440	0.0006
56 LB BL-(	Mo2 C	0.099174	0.020361	0.117642	0.024153	4.719899	0.015108	5.996992	0.018694	5.136855	0.017987	440	0.0006
57 LB03 C	Mo2 C	0.111485	0.013221	0.132529	0.015717	4.719774	0.008963	6.001011	0.010224	5.122181	0.010215	440	0.0006
57 WA03	Mo2 C	0.086746	0.014857	0.103754	0.01777	4.716742	0.013588	5.998852	0.014544	5.095938	0.014779	440	0.0006
65 LD BL-	Mo2 C	0.142843	0.014356	0.169313	0.017016	4.721108	0.007441	6.009987	0.008543	5.13073	0.008536	440	0.0006
75 LC03-0	Mo2 C	0.115048	0.013979	0.136729	0.016614	4.722246	0.008921	5.990715	0.011341	5.134223	0.010575	440	0.0006
LC LTTA B	Mo2 C	0.104406	0.018076	0.123802	0.021434	4.750299	0.013205	5.983356	0.016291	5.128618	0.014952	440	0.0006

Fig 5.6.4 Mo2 C phase

7. IVAR

Title	Rwp(%)	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Siz	Microstrair
CM6 BL-0	9.972408	Cohenite	2.453713	0.332475	2.286017	0.309752	5.141396	0.129092	6.423576	0.130335	4.930219	0.108531	28.79873	6.642446	0.0006
G1 CM6-0	10.44902	Cohenite	1.776782	0.135593	1.730876	0.132089	5.079815	0.001898	6.76345	0.003396	4.52566	0.00166	2068.848	848.1854	0.0006
G1 LC-000	11.73923	Cohenite	2.879709	0.192949	2.810064	0.188282	5.07727	0.003064	6.755584	0.005258	4.524302	0.002812	440.3367	56.58534	0.0006
G1 LC-000	10.93884	Cohenite	2.46628	0.158058	2.406073	0.1542	5.077607	0.002322	6.758634	0.004021	4.524469	0.002117	694.0988	110.2397	0.0006
G1 LG-000	11.18281	Cohenite	2.936149	0.192252	2.86385	0.187518	5.077306	0.003143	6.757652	0.005276	4.52413	0.002721	397.7869	52.19357	0.0006
G3 LD-000	11.88992	Cohenite	2.874108	0.1822	2.802476	0.177659	5.077761	0.002231	6.757479	0.003839	4.525876	0.00207	671.6979	106.2394	0.0006
G4 LD-000	10.93964	Cohenite	2.790181	0.155191	2.720897	0.151338	5.078661	0.00172	6.75705	0.002977	4.524799	0.001577	934.056	167.8112	0.0006
G5-LC-000	9.239042	Cohenite	2.449502	0.152967	2.38983	0.149241	5.078688	0.002542	6.756707	0.004347	4.524506	0.002281	483.8819	65.0704	0.0006
G5-LD-000	11.37246	Cohenite	2.786884	0.171565	2.718015	0.167326	5.079422	0.002141	6.758711	0.003675	4.526172	0.00197	691.3212	110.425	0.0006
G5-LI-000	11.16555	Cohenite	2.656917	0.156082	2.59327	0.152343	5.079186	0.001821	6.758538	0.003125	4.52336	0.001598	938.0076	175.408	0.0006
LC BL-000	10.65018	Cohenite	2.571573	0.273881	2.38147	0.253634	5.14068	0.103871	6.398226	0.108137	4.981812	0.08601	31.76699	4.335451	0.0006
LC BL 2-0	11.73645	Cohenite	2.270615	0.179969	2.219403	0.17591	5.074072	0.003186	6.754298	0.005381	4.521563	0.002848	551.3137	92.35787	0.0006
LD BL-000	8.550262	Cohenite	3.112983	0.114178	3.043305	0.111622	5.075306	0.001997	6.754783	0.003329	4.519644	0.001784	445.4847	13.74319	0.0006
LD GI-000	8.380768	Cohenite	3.26337	0.127622	3.182532	0.124461	5.079652	0.001419	6.758678	0.002453	4.524051	0.001299	652.3146	66.4063	0.0006
LG BL-000	11.08884	Cohenite	2.671887	0.161948	2.61292	0.158374	5.07402	0.002161	6.752553	0.003623	4.519416	0.001855	733.1491	113.7154	0.0006
LH BL-000	12.78932	Cohenite	2.985992	0.193763	2.918065	0.189355	5.076349	0.002639	6.75406	0.004469	4.521167	0.002312	560.3477	82.47805	0.0006
LH GI-000	13.12088	Cohenite	3.378699	0.20548	3.296596	0.200487	5.077915	0.003029	6.759023	0.005168	4.521874	0.002725	398.082	50.93759	0.0006
LI BL-0000	10.95567	Cohenite	2.145929	0.113836	2.099857	0.111392	5.073543	0.001808	6.752327	0.003063	4.519659	0.001535	1634.117	115.4694	0.0006
LI GI-0000	9.181023	Cohenite	2.922153	0.134072	2.85041	0.13078	5.079286	0.001638	6.759422	0.002823	4.52302	0.001448	669.121	81.53873	0.0006
T14 LD-00	10.5703	Cohenite	2.615005	0.159586	2.551034	0.155682	5.079173	0.001718	6.753934	0.002918	4.524178	0.001523	1131.65	255.7995	0.0006
T15 LD-00	9.911072	Cohenite	2.680381	0.142368	2.614272	0.138856	5.079382	0.001591	6.754108	0.002697	4.524458	0.001404	1028.258	190.3458	0.0006
T18 CM6-	11.33362	Cohenite	1.03015	0.145726	1.003908	0.142014	5.076772	0.003949	6.759182	0.007047	4.528179	0.003511	1156.689	617.1799	0.0006
TU-CM6-0	11.2144	Cohenite	1.608006	0.169091	1.565898	0.164664	5.078021	0.003958	6.763126	0.007047	4.530047	0.003708	553.2911	135.5062	0.0006
TU-LC-000	9.469064	Cohenite	2.807836	0.156459	2.739708	0.152663	5.077829	0.002384	6.753647	0.004065	4.525137	0.002192	459.0519	53.97079	0.0006
TU-LD-000	10.62121	Cohenite	3.511091	0.172965	3.423211	0.168636	5.079738	0.002226	6.76133	0.003808	4.526642	0.002076	438.5153	45.90926	0.0006
TU-LG-000	12.34168	Cohenite	2.890317	0.19277	2.820244	0.188097	5.077342	0.002544	6.756624	0.004321	4.52387	0.002253	556.8157	84.23528	0.0006
TU-LH-000	12.94281	Cohenite	3.076162	0.208099	3.002169	0.203094	5.077645	0.002664	6.757405	0.00458	4.523828	0.002414	525.0357	83.99679	0.0006
TU-LI-000	9.934315	Cohenite	3.001685	0.159485	2.928871	0.155617	5.078376	0.002061	6.757638	0.003536	4.524488	0.001872	551.9439	64.26849	0.0006

Fig 5.7.1 Cohenite phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Microstrain
CM6 BL- 0(	IronFCC	0.19519	0.035617	0.199304	0.036368	3.588476	0.002932	350	0.0006
G1 CM6- 0	IronFCC	0.132285	0.034283	0.133471	0.03459	3.60099	0.004507	350	0.0006
G1 LC- 00(	IronFCC	0.223858	0.04219	0.226827	0.042749	3.595559	0.003161	350	0.0006
G1 LC- 00(	IronFCC	0.24245	0.038079	0.244906	0.038464	3.59966	0.002668	350	0.0006
G1 LG- 00(	IronFCC	0.084618	0.03723	0.082096	0.036121	3.647776	0.007547	350	0.0006
G3 LD- 00(	IronFCC	0.716645	0.049018	0.726788	0.049711	3.594468	0.001086	350	0.0006
G4 LD- 00(	IronFCC	0.652029	0.0436	0.661125	0.044208	3.594672	0.00107	350	0.0006
G5- LC- 00(	IronFCC	0.289358	0.032749	0.291584	0.033001	3.602544	0.001912	350	0.0006
G5- LD- 00(	IronFCC	0.623011	0.045328	0.630134	0.045847	3.598637	0.001165	350	0.0006
G5- LI- 000	IronFCC	0.134034	0.035704	0.134984	0.035958	3.603901	0.004608	350	0.0006
LC BL- 000	IronFCC	0.242419	0.038394	0.247555	0.039207	3.588716	0.002497	350	0.0006
LC BL 2- 0(	IronFCC	0.341997	0.042864	0.345895	0.043352	3.598063	0.002111	350	0.0006
LD BL- 000	IronFCC	0.336416	0.030368	0.340935	0.030775	3.595733	0.001507	350	0.0006
LD GI- 000	IronFCC	0.470921	0.031627	0.476572	0.032007	3.597379	0.001107	350	0.0006
LG BL- 000	IronFCC	0.08304	0.03539	0.083422	0.035553	3.605861	0.007536	350	0.0006
LH BL- 000	IronFCC	0.122164	0.042098	0.123353	0.042508	3.600185	0.005948	350	0.0006
LH GI- 000	IronFCC	0.099136	0.041317	0.099839	0.04161	3.602862	0.007093	350	0.0006
LI BL- 000(	IronFCC	0.111831	0.033066	0.106552	0.031505	3.670729	0.005645	350	0.0006
LI GI- 000(	IronFCC	0.114876	0.028542	0.115523	0.028703	3.605001	0.0043	350	0.0006
T14 LD- 0(	IronFCC	0.550614	0.042597	0.556751	0.043072	3.597849	0.001277	350	0.0006
T15 LD- 0(	IronFCC	0.428678	0.037403	0.433686	0.03784	3.597121	0.001453	350	0.0006
T18 CM6-	IronFCC	0.091176	0.034508	0.091091	0.034475	3.612475	0.006691	350	0.0006
TU- CM6- (	IronFCC	0.387786	0.040853	0.393405	0.041445	3.594686	0.001724	350	0.0006
TU- LC- 00(	IronFCC	0.257793	0.03342	0.260579	0.033781	3.598381	0.002184	350	0.0006
TU- LD- 00(	IronFCC	0.538801	0.040798	0.546063	0.041348	3.596491	0.001224	350	0.0006
TU- LG- 00(	IronFCC	0.095243	0.039518	0.092542	0.038398	3.64619	0.00705	350	0.0006
TU- LH- 00(	IronFCC	0.082389	0.042269	0.08303	0.042598	3.60252	0.00869	350	0.0006
TU- LI- 000	IronFCC	0.088414	0.032241	0.089064	0.032478	3.603165	0.006375	350	0.0006

Fig 5.7.2 IronFCC phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain Error
CM6 BL- 0(	FeBCC	97.27712	0.274653	97.42718	0.275077	2.866575	1.53E- 05	45222.91	12302.1	0.000923	9.18E- 06
G1 CM6- 0	FeBCC	97.95403	0.286423	97.97292	0.286478	2.866434	1.4E- 05	23872972	14818105	0.000477	1.06E- 05
G1 LC- 00(	FeBCC	96.79449	0.321381	96.84155	0.321538	2.865895	1.7E- 05	45092.58	5711.793	0.00073	9.68E- 06
G1 LC- 00(	FeBCC	97.1714	0.297931	97.20546	0.298036	2.866332	1.54E- 05	482845	95782.75	0.000677	8.94E- 06
G1 LG- 00(	FeBCC	96.87962	0.304897	96.93608	0.305075	2.865636	1.73E- 05	49393.74	6448.256	0.000925	8.58E- 06
G3 LD- 00(	FeBCC	96.24731	0.322344	96.2771	0.322444	2.866033	1.63E- 05	72600.93	11648.54	0.00057	2.62E- 06
G4 LD- 00(	FeBCC	96.39538	0.295253	96.4239	0.29534	2.866017	1.49E- 05	571246	103146.7	0.000586	9.51E- 06
G5- LC- 00(	FeBCC	97.13605	0.252663	97.16989	0.252751	2.866323	1.4E- 05	42207.96	5593.139	0.000851	7.62E- 06
G5- LD- 00(	FeBCC	96.43071	0.307893	96.46124	0.307991	2.866782	1.55E- 05	85447	13493.68	0.000553	1.03E- 05
G5- LI- 000	FeBCC	97.07774	0.302769	97.11488	0.302885	2.866798	1.52E- 05	154157.4	28894.47	0.000581	9.8E- 06
LC BL- 000	FeBCC	97.11193	0.292426	97.28334	0.292942	2.866658	1.58E- 05	287389.8	519827.3	0.000837	1.11E- 05
LC BL 2- 0(	FeBCC	97.26147	0.32192	97.28501	0.321998	2.866361	1.78E- 05	55189.55	9113.381	0.000817	9.65E- 06
LD BL- 000	FeBCC	96.37636	0.229918	96.40887	0.229995	2.866333	1.3E- 05	43161.76	1453.609	0.000871	6.39E- 06
LD GI- 000	FeBCC	96.10948	0.226257	96.15449	0.226363	2.86617	1.17E- 05	202215.1	39397.45	0.000631	7.08E- 06
LG BL- 000	FeBCC	97.12192	0.302183	97.1573	0.302293	2.866007	1.69E- 05	6594772	3883650	0.000853	8.58E- 06
LH BL- 000	FeBCC	96.76936	0.347207	96.8131	0.347364	2.866282	1.89E- 05	2700412	1802641	0.000825	9.75E- 06
LH GI- 000	FeBCC	96.41653	0.352755	96.4781	0.352981	2.865731	2.03E- 05	112833.3	14799.49	0.000976	9.35E- 06
LI BL- 0000	FeBCC	97.60101	0.299363	97.62579	0.299439	2.866628	1.68E- 05	43493.02	19.66302	0.000854	8.64E- 06
LI GI- 0000	FeBCC	96.84122	0.247408	96.88913	0.24753	2.866179	1.31E- 05	125167.5	15384.93	0.000735	7.16E- 06
T14 LD- 00	FeBCC	96.68384	0.290022	96.71333	0.290111	2.865894	1.59E- 05	157329.8	35641.34	0.000789	8.6E- 06
T15 LD- 00	FeBCC	96.70802	0.269658	96.73525	0.269734	2.865843	1.44E- 05	586735.5	109652.3	0.000719	8.12E- 06
T18 CM6-	FeBCC	98.71938	0.310688	98.71636	0.310678	2.866359	1.53E- 05	1111835	4357732	0.000555	1.11E- 05
TU- CM6- (	FeBCC	97.86812	0.30603	97.87904	0.306064	2.866711	1.5E- 05	1034329	7351312	0.000534	1.32E- 05
TU- LC- 00(	FeBCC	96.82156	0.258555	96.86515	0.258672	2.86586	1.39E- 05	40364.75	7251.483	0.000755	8.72E- 06
TU- LD- 00(	FeBCC	95.79959	0.285706	95.85107	0.285859	2.86679	1.43E- 05	47482.56	4866.003	0.000546	9.51E- 06
TU- LG- 00(	FeBCC	96.897	0.334265	96.9464	0.334435	2.865884	1.68E- 05	48107.26	7061.552	0.000586	1.09E- 05
TU- LH- 00(	FeBCC	96.72917	0.352858	96.78008	0.353044	2.866213	1.8E- 05	52470.64	7871.244	0.000628	1.11E- 05
TU- LI- 000	FeBCC	96.78632	0.270351	96.83403	0.270484	2.866355	1.37E- 05	41278.29	4907.174	0.000575	9.14E- 06

Fig 5.7.1 FeBCC phase

8. IVAR

Title	Rwp(%)	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain
73W irr-00	14.11833	Cohenite	1.901764	0.142273	1.851034	0.138478	5.084081	0.00286	6.766594	0.00512	4.5292	0.002499	838.136	29.89569	0.0006
73W unirr-	14.46931	Cohenite	2.030576	0.168195	1.975941	0.16367	5.084245	0.002877	6.766494	0.005159	4.528743	0.002532	891.3002	111.8639	0.0006
A18 irr-00	12.55747	Cohenite	2.039786	0.20691	1.988226	0.20168	5.085685	0.002183	6.763302	0.003902	4.530192	0.001939	1593.722	690.8076	0.0006
A24 unirr-	10.98259	Cohenite	2.714376	0.178587	2.642149	0.173835	5.085083	0.002067	6.765498	0.003669	4.530192	0.001889	664.236	119.9469	0.0006
B12 irr-00	12.26779	Cohenite	1.534357	0.129472	1.49491	0.126144	5.084071	0.002414	6.764436	0.004312	4.530264	0.002104	1298.897	247.9037	0.0006
B29 unirr-	12.72506	Cohenite	1.921229	0.169556	1.872157	0.165225	5.083669	0.002453	6.765604	0.004372	4.529666	0.002137	1227.236	284.8504	0.0006
C33 unirr-	11.61628	Cohenite	1.75259	0.156493	1.707515	0.152468	5.084376	0.002103	6.764809	0.003759	4.530156	0.001839	1566.791	527.2354	0.0006
CM6 AT u	10.0003	Cohenite	2.494138	0.17381	2.425925	0.169056	5.084172	0.002572	6.76919	0.00458	4.530124	0.002317	479.9352	65.35973	0.0006
CM6 irr-00	13.89357	Cohenite	2.69177	0.235357	2.615734	0.228708	5.085381	0.002777	6.776758	0.005088	4.531472	0.002533	646.1892	131.5467	0.0006
CM6 SR ui	11.89757	Cohenite	1.776698	0.195173	1.723971	0.189381	5.083901	0.003963	6.786595	0.007225	4.530118	0.00351	533.0895	110.206	0.0006
E21 irr-00	11.0005	Cohenite	1.589799	0.127495	1.54977	0.124284	5.084189	0.002238	6.763617	0.00401	4.53077	0.001958	1304.547	310.8173	0.0006
JRO irr-00	13.25865	Cohenite	3.054376	0.160979	2.97869	0.15699	5.084836	0.001485	6.764638	0.002616	4.527932	0.001294	1820.653	237.6449	0.0006
JRO unirr-	11.33476	Cohenite	2.988246	0.179366	2.912751	0.174835	5.085165	0.001398	6.765629	0.002465	4.52777	0.001222	1318.301	301.8437	0.0006
LC irr-000	13.9814	Cohenite	2.753352	0.22183	2.681431	0.216035	5.08572	0.002406	6.770494	0.004311	4.532492	0.002108	869.4312	161.1121	0.0006
LC unirr-0	11.86409	Cohenite	2.698568	0.181972	2.625412	0.177039	5.086199	0.002058	6.770337	0.003602	4.531009	0.001819	781.5314	128.4764	0.0006
LD irr-000	7.695387	Cohenite	2.489778	0.101554	2.422605	0.098815	5.08349	0.001242	6.76978	0.002235	4.53149	0.001128	732.5626	77.90269	0.0006
LD unirr-0	11.59395	Cohenite	3.335273	0.196224	3.244198	0.190866	5.084631	0.00184	6.774103	0.003274	4.528318	0.001661	677.9495	102.8758	0.0006
Midland ir	13.72625	Cohenite	3.531272	0.203581	3.446054	0.198668	5.083787	0.00144	6.763733	0.002517	4.526938	0.001253	1754.256	419.139	0.0006
Midland u	12.91583	Cohenite	1.887537	0.178404	1.837285	0.173654	5.083887	0.002523	6.76763	0.00451	4.529136	0.002201	907.9564	226.6233	0.0006
palisadesH	12.30508	Cohenite	2.748487	0.185682	2.680664	0.1811	5.084128	0.001748	6.764522	0.003082	4.529308	0.00153	1095.939	217.7065	0.0006
palisadesL	13.05171	Cohenite	2.506706	0.183868	2.450016	0.179709	5.084119	0.001592	6.763968	0.002795	4.528945	0.001361	1785.7	628.9857	0.0006
palisades u	14.03116	Cohenite	2.215252	0.210817	2.160173	0.205575	5.084158	0.002037	6.767001	0.003624	4.527706	0.001775	1819.172	781.7628	0.0006
plate02 irr	14.51115	Cohenite	4.256295	0.260763	4.153862	0.254488	5.084388	0.001504	6.762904	0.002611	4.526924	0.001309	1392.066	320.2523	0.0006
plate02 un	13.51451	Cohenite	3.838765	0.231907	3.743207	0.226134	5.083995	0.001509	6.764585	0.002635	4.526294	0.001309	1329.626	279.7284	0.0006
r Si stand-	35.33973	Cohenite	3.265445	0.488967	3.168989	0.474523	5.101447	0.008931	6.753752	0.012063	4.536305	0.008577	354.5758	94.31886	0.0006

Fig 5.8.1 Cohenite phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
73W irr-0(	IronFCC	0.792567	0.200953	0.784437	0.198892	3.625627	0.024091	33.34214	8.085213	0.0006	
73W unirr-	IronFCC	0.880483	0.145305	0.879371	0.145121	3.614322	0.010616	56.53729	7.092994	0.0006	
A18 irr-00	IronFCC	2.758	0.443867	2.651346	0.426702	3.662811	0.019082	18.72423	3.265506	0.0006	
A24 unirr-	IronFCC	0.62061	0.072185	0.62846	0.073098	3.598466	0.001669	260.0735	49.82457	0.0006	
B12 irr-00(	IronFCC	1.605248	0.264001	1.558552	0.256321	3.65002	0.015194	25.60642	4.53352	0.0006	
B29 unirr-(	IronFCC	2.121944	0.356896	2.059436	0.346383	3.650645	0.017457	22.83223	3.911824	0.0006	
C33 unirr-	IronFCC	1.853018	0.187526	1.795119	0.181667	3.652825	0.016157	24.08022	1.010888	0.0006	
CM6 AT u	IronFCC	0.623855	0.064799	0.629528	0.065388	3.602196	0.001421	264.5134	42.15848	0.0006	
CM6 irr-0(	IronFCC	0.485934	0.077263	0.493106	0.078403	3.596353	0.001761	394.2745	114.3179	0.0006	
CM6 SR u	IronFCC	0.780651	0.093367	0.784377	0.093812	3.607493	0.002081	187.0466	31.99719	0.0006	
E21 irr-00(	IronFCC	1.782518	0.274838	1.720131	0.265219	3.658137	0.014965	23.94204	4.123379	0.0006	
JRO irr-00	IronFCC	2.521186	0.453094	2.424968	0.435802	3.662218	0.023422	17.40589	3.29239	0.0006	
JRO unirr-	IronFCC	2.012013	0.190596	1.961129	0.185776	3.645633	0.014903	23.6608	0.856651	0.0006	
LC irr-000(	IronFCC	1.958521	0.389149	1.898278	0.377179	3.653683	0.021013	23.16971	4.206359	0.0006	
LC unirr-0(	IronFCC	1.926711	0.099504	1.936052	0.099986	3.608477	0.00256	80.73908	2.122505	0.0006	
LD irr-000	IronFCC	0.624527	0.03716	0.632617	0.037641	3.598376	0.000927	264.5841	23.64151	0.0006	
LD unirr-0	IronFCC	1.252644	0.073898	1.269364	0.074884	3.597702	0.000761	318.0057	34.46827	0.0006	
Midland ir	IronFCC	2.448234	0.431415	2.342441	0.412772	3.668775	0.0203	21.20631	3.873587	0.0006	
Midland u	IronFCC	0.893776	0.194662	0.886034	0.192976	3.623866	0.013	43.50968	10.32229	0.0006	
palisadesH	IronFCC	2.646744	0.480566	2.549135	0.462843	3.660898	0.022856	16.29429	2.868118	0.0006	
palisadesL	IronFCC	3.269902	1.063985	3.000373	0.976284	3.722914	0.0387	14.45141	3.61168	0.0006	
palisades u	IronFCC	2.154549	0.385581	2.07351	0.371078	3.661616	0.021522	20.56774	4.247987	0.0006	
plate02 irr	IronFCC	3.056023	0.590829	2.955535	0.571402	3.655739	0.023765	17.74099	3.736303	0.0006	
plate02 un	IronFCC	2.09035	0.306737	2.044922	0.300071	3.640808	0.013363	30.37917	4.792404	0.0006	
r Si stand-	IronFCC	0.752976	0.168332	0.761961	0.170341	3.599087	0.001942	728.9987	425.3477	0.0006	

Fig 5.8.1 IronFCC phase

Title	Phase Nan	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
73W irr-0(	FeBCC	96.91159	0.28794	96.88165	0.287851	2.868084	1.54E-05	9259.302	620.7771	0.000663	1.26E-05
73W unirr-	FeBCC	96.60684	0.292903	96.55244	0.292738	2.868021	1.6E-05	11936.34	1034.528	0.000731	1.21E-05
A18 irr-00	FeBCC	94.93775	0.247209	95.03793	0.24747	2.868198	1.35E-05	10889.96	757.9489	0.000691	1.07E-05
A24 unirr-	FeBCC	96.24673	0.221159	96.21899	0.221095	2.868372	1.21E-05	15269.25	1354.916	0.000798	8.86E-06
B12 irr-00(	FeBCC	96.60712	0.249114	96.63705	0.249191	2.868359	1.35E-05	10947.27	777.0232	0.000718	1.06E-05
B29 unirr-(	FeBCC	95.64853	0.254319	95.69221	0.254435	2.868346	1.36E-05	11944.39	928.4625	0.000654	1.12E-05
C33 unirr-	FeBCC	96.10723	0.233193	96.14716	0.23329	2.868336	1.25E-05	9771.738	583.3389	0.000688	9.88E-06
CM6 AT u	FeBCC	96.30586	0.199815	96.19659	0.199588	2.86879	1.11E-05	13272	931.9816	0.000798	8.18E-06
CM6 irr-0(	FeBCC	96.27805	0.283707	96.18639	0.283437	2.869313	1.64E-05	4222.01	149.0562	0.000739	1.35E-05
CM6 SR u	FeBCC	96.94343	0.241412	96.85003	0.24118	2.868739	1.36E-05	5554.726	205.1524	0.000757	1.03E-05
E21 irr-00(	FeBCC	96.37157	0.220481	96.41887	0.22059	2.868719	1.23E-05	8617.334	434.5476	0.000782	9.23E-06
JRO irr-00	FeBCC	94.11028	0.260598	94.21278	0.260882	2.868206	1.4E-05	10368.76	726.2972	0.000612	1.18E-05
JRO unirr-	FeBCC	94.66318	0.224798	94.71542	0.224922	2.868412	1.22E-05	10114.39	607.5198	0.000673	9.89E-06
LC irr-000(	FeBCC	94.92852	0.28031	94.98182	0.280468	2.86935	1.64E-05	4491.174	166.1456	0.000756	1.31E-05
LC unirr-0(	FeBCC	95.03916	0.23674	95.02765	0.236712	2.868787	1.32E-05	8630.569	478.4434	0.000724	1.05E-05
LD irr-000	FeBCC	96.49103	0.157494	96.46099	0.157445	2.86861	9.17E-06	4040.544	74.9661	0.000748	7.47E-06
LD unirr-0	FeBCC	94.91814	0.232365	94.88063	0.232273	2.868524	1.3E-05	6658.395	286.137	0.000712	1.06E-05
Midland ir	FeBCC	93.73175	0.269897	93.8585	0.270262	2.868054	1.46E-05	8807.778	555.6088	0.00061	1.27E-05
Midland u	FeBCC	96.84274	0.262908	96.81558	0.262834	2.868204	1.42E-05	10541.98	758.6147	0.000692	1.15E-05
palisadesH	FeBCC	94.34151	0.241512	94.44894	0.241788	2.868401	1.3E-05	14538.88	1293.612	0.000641	1.07E-05
palisadesL	FeBCC	94.13644	0.258148	94.42075	0.258927	2.868467	1.37E-05	12475.63	1033.979	0.00062	1.16E-05
palisades u	FeBCC	95.3508	0.279909	95.42564	0.280128	2.868573	1.45E-05	10720.86	821.6654	0.000584	1.28E-05
plate02 irr	FeBCC	92.36256	0.280501	92.49381	0.2809	2.868046	1.51E-05	11509.12	957.2092	0.00059	1.32E-05
plate02 un	FeBCC	93.67631	0.265317	93.73069	0.265472	2.868069	1.44E-05	8216.076	479.177	0.000609	1.26E-05
r Si stand-	FeBCC	95.47167	0.861672	95.40276	0.86105	2.868605	5.08E-05	5238.65	666.8734	0.000799	3.85E-05

Fig 5.8.2 FeBCC phase

Title	Phase Nar	Vol.(%)	error(%)	Wt.(%)	error(%)	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Cell Par(Ar	Cell Par Er	Size(Angst	Crystal Size	Microstrain	Microstrain
73W irr-00	Mo2 C	0.394077	0.056404	0.482882	0.069114	4.74701	0.033567	6.025727	0.034168	4.913426	0.038749	80.57708	8.923497	0.0006	
73W unirr-	Mo2 C	0.482095	0.058839	0.592254	0.072283	4.730861	0.021637	6.025806	0.021951	4.915912	0.023624	104.9152	18.43669	0.0006	
A18 irr-00	Mo2 C	0.264457	0.051977	0.322499	0.063385	4.739862	0.016523	6.049985	0.017224	4.932016	0.016936	207.4642	41.8583	0.0006	
A24 unirr-	Mo2 C	0.418289	0.04117	0.510407	0.050237	4.729061	0.013435	6.061373	0.014041	4.925238	0.014197	141.4857	19.81125	0.0006	
B12 irr-00	Mo2 C	0.253274	0.039002	0.30949	0.047659	4.751856	0.02166	6.026301	0.021671	4.926024	0.022579	141.1615	6.158085	0.0006	
B29 unirr-	Mo2 C	0.308302	0.057134	0.376199	0.069716	4.755556	0.023906	6.030224	0.023916	4.926621	0.024996	128.3717	25.44393	0.0006	
C33 unirr-	Mo2 C	0.28716	0.045647	0.350204	0.055668	4.742201	0.015064	6.048599	0.015471	4.927997	0.015567	183.5207	42.93107	0.0006	
CM6 AT u	Mo2 C	0.576156	0.085638	0.747952	0.111173	4.56324	0.056038	5.751724	0.191786	5.053951	0.161345	30.48982	5.97522	0.0006	
CM6 irr-0(	Mo2 C	0.54425	0.087444	0.704768	0.113234	4.592979	0.050178	5.889878	0.064957	4.919308	0.075244	40.0761	15.10935	0.0006	
CM6 SR u	Mo2 C	0.499227	0.074591	0.641623	0.095866	4.533896	0.042542	5.841552	2.925745	5.059471	2.537466	46.95969	9.246252	0.0006	
E21 irr-00	Mo2 C	0.256113	0.043166	0.311234	0.052456	4.784776	0.022782	6.003157	0.023108	4.940989	0.023978	137.068	14.01805	0.0006	
JRO irr-00	Mo2 C	0.314166	0.054115	0.383561	0.066068	4.734431	0.013486	6.0642	0.014365	4.920617	0.013665	199.4302	43.58983	0.0006	
JRO unirr-	Mo2 C	0.336563	0.039976	0.410701	0.048782	4.733694	0.012586	6.05595	0.013136	4.928959	0.012822	184.8751	24.20045	0.0006	
LC irr-000	Mo2 C	0.359607	0.058909	0.438473	0.071829	4.762777	0.026917	6.011668	0.027582	4.943749	0.028756	118.7541	5.572075	0.0006	
LC unirr-0(	Mo2 C	0.335556	0.04045	0.410891	0.049532	4.723789	0.013133	6.040904	0.013869	4.933112	0.013965	175.0454	28.15654	0.0006	
LD irr-000	Mo2 C	0.39467	0.023849	0.48379	0.029234	4.728432	0.009959	6.027176	0.010272	4.932394	0.010767	119.1844	8.654235	0.0006	
LD unirr-0	Mo2 C	0.493936	0.050949	0.605809	0.062488	4.720982	0.017682	6.052391	0.017928	4.915995	0.019545	110.6872	15.936	0.0006	
Midland ir	Mo2 C	0.288747	0.058024	0.353007	0.070937	4.739543	0.014775	6.045345	0.015392	4.92446	0.014911	229.6667	56.16398	0.0006	
Midland u	Mo2 C	0.375953	0.054724	0.461103	0.067119	4.736946	0.029658	6.027289	0.030077	4.918758	0.033768	85.46558	15.10397	0.0006	
palisadesH	Mo2 C	0.263259	0.053499	0.321264	0.065287	4.74243	0.020113	6.052502	0.020498	4.925275	0.020559	161.5052	34.42282	0.0006	
palisadesLI	Mo2 C	0.08695	0.71596	0.128867	1.06111	4.977287	1.203438	8.453995	1.802025	2.771824	0.892904	9.467252	5.083415	0.0006	
palisades u	Mo2 C	0.279399	0.061273	0.340679	0.074712	4.743206	0.017253	6.058166	0.017755	4.923073	0.017684	202.4315	59.1192	0.0006	
plate02 irr	Mo2 C	0.325116	0.067847	0.396791	0.082804	4.728125	0.014226	6.079154	0.015421	4.917592	0.014698	253.0837	56.20894	0.0006	
plate02 un	Mo2 C	0.394579	0.058778	0.481183	0.071678	4.724726	0.011428	6.077901	0.012496	4.922067	0.011856	224.2865	50.33977	0.0006	
r Si stand-	Mo2 C	0.509912	0.20886	0.666294	0.272914	4.758947	0.101923	5.840516	0.10424	4.742403	0.117437	66.15743	39.37952	0.0006	

Fig 5.8.3 Mo2 C phase

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