3DSOC V1.0
Documentation

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Contents

1 Introduction

1.1 Objective

3DSOC (3DSrainOrientationCalculator) is a 3D diffraction data analysis tool for single crystal substructure information extraction.

To fulfil the requirement of neutron diffraction characterization of single crystal, 3DSOC enables an accurate and automatic extraction of single crystal substructure information including lattice strain and orientation of subgrains for the measurements on monochromatic neutron source. The output is an *.txt file of diffraction parameters of subgrains. This software has been successfully tested on HETU and RSND diffractometers from CMRR. SiC SC and Ni-based SC superalloy samples measured on HETU and RSND diffractometers in CMRR are successfully testes.

1.2 Hardware and software environment

CPU: Any Intel x86-64 processor

Hard disk: 2GB or more

Memory: 2GB or more

OS: Windows 10 or higher version

Software: MATLAB Runtime 9.1 or higher version

1.3 Software function and features

3DSOC is a data analysis software written by MATLAB R2018 language, built by App Designer and based on MATLAB environment.

This software can automatically obtain the experimental parameters and neutron diffraction intensity matrix by reading the head file of the detector. Based on neutron diffraction geometry, diffraction intensity matrix is transformed pixel by pixel. One-

dimensional diffraction curve and rocking curve are obtained by 2-D data reduction methods. Mixed Gaussian function model is used to fit and analyze the rocking curve, to realize the separation of subgrain diffraction peaks. For certain subgrain diffraction peak, two-dimensional Gaussian function is used for fitting analysis to extract the crystal plane spacing and orientation information.

3DSOC makes a great improvement in the following aspects:

a) Optimization of data input and output process. 3DSOC can automatically extract detector head files (*. txt) and output *. txt files containing single crystal substructure parameters and uncertainty.

b) Optimization of fitting procedure. 3DSOC only requires users to provide necessary parameters such as diffraction peak width as the initial values of fitting analysis. The remaining initial values will be automatically provided by the algorithm.

c) Improvement in analysis accuracy. 3DSOC is based on the analysis of two-dimensional diffraction data, avoiding the impact of step size on the results during the data dimensionality reduction process.

2 Installation and startup

After downloading 3DSOC, open Matlab and click on the "APP Menu" to enter APP selection interface. Click on 'Install App' and select the *APP_3DSOC.mlapinstall* installation package.

After installation is completed, click *APP_ 3DSOC* on the app menu. and enter the app selection menu. Click 3DSOC to enter the initial interface. To facilitate user analysis operations, 3DSOC has pre-set some parameters, which can be modified in subsequent operations. 3DSOC is divided into three parts according to the operation process: Load data, RC Analysis and Subgrain Separation, and 2D Gaussian Fitting.

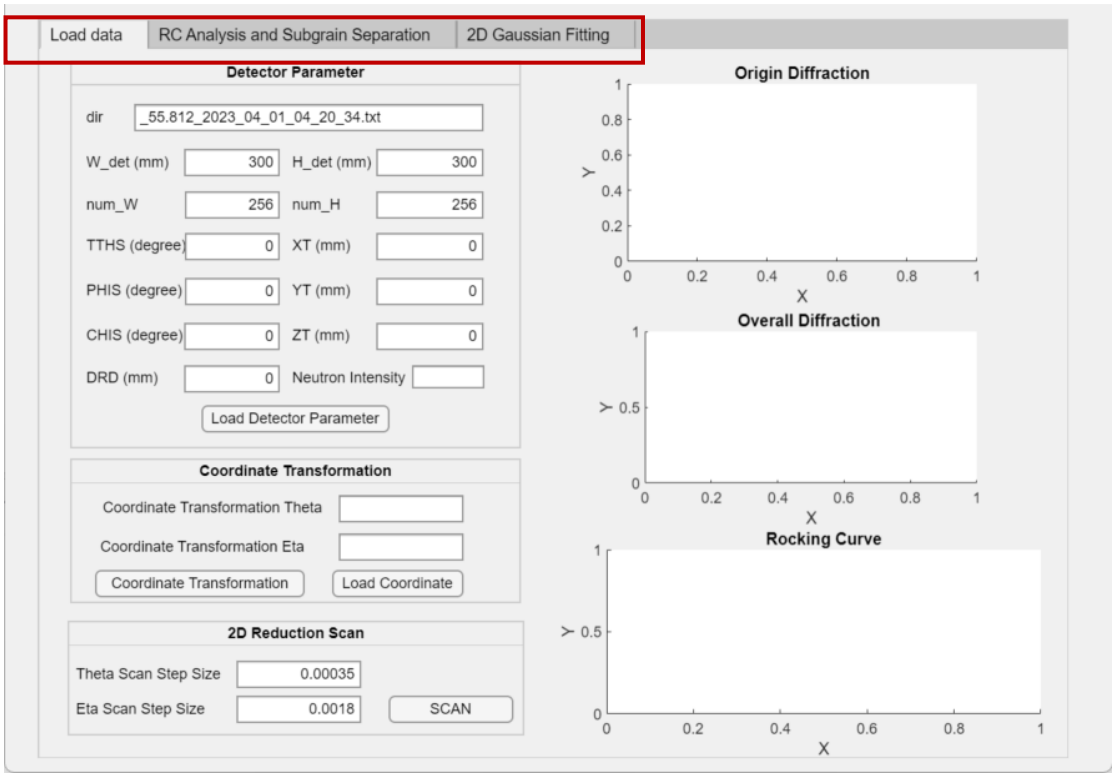

Figure 1. 3DSOC initial interface

3. Operation

3.1 Data loading and pre-processing

3.1.1 Data loading

Data loading operation is in the Detector Parameter panel. Place the original detector head file (*. txt) in the current file path of MATLAB. Enter the analyzed file name in dir and click Load Detector Parameter, then experimental parameters will be automatically imported, and diffraction signal will be shown in Origin Diffraction. Wherein, TTHS, PHIS and CHIS are the three rotation angles of the Euler ring, XT, YT and ZT are coordinates of the sample stage, DRD is the distance from the detector to the sample center, and Neutron Intensity is the neutron diffraction intensity matrix. W_ Det, H_ Det is the width and height of the detector, num_ W, num_ H is the number of pixels in the width and height of the detector.

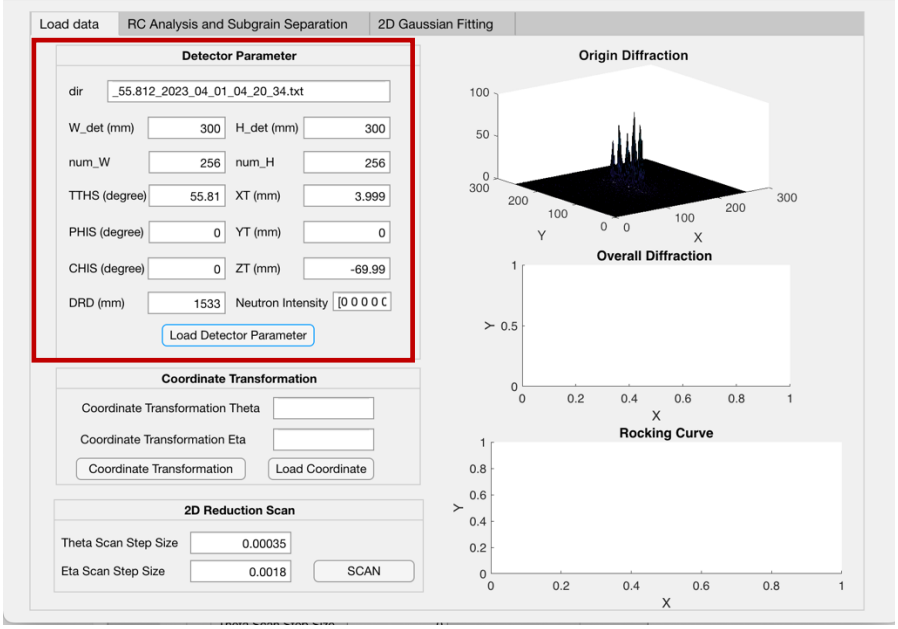

Figure 2. Data loading

3.1.2 Coordinate transformation

To accurately analyze diffraction data, it is necessary to calculate the polar coordinates of each pixel on two-dimensional detector, which is mainly performed in the Coordinate Transformation panel. Click on "Coordinate transformation" to start coordinate transformation. This process requires pixel by pixel calculation, so it takes about ten minutes. Two *. txt files containing polar coordinate matrices, *eta. txt* and *theta. txt*, will be output in the current MATLAB file path. If related experimental parameters are unchanged in subsequent analysis, then *eta. txt* and *theta. tx*t should be consistent. In this case, click the Load Coordinate button to import the *eta. txt* and *theta. txt* that already exist in the current MATLAB file path, thereby reducing calculation time. The operation is shown in Figure 3.

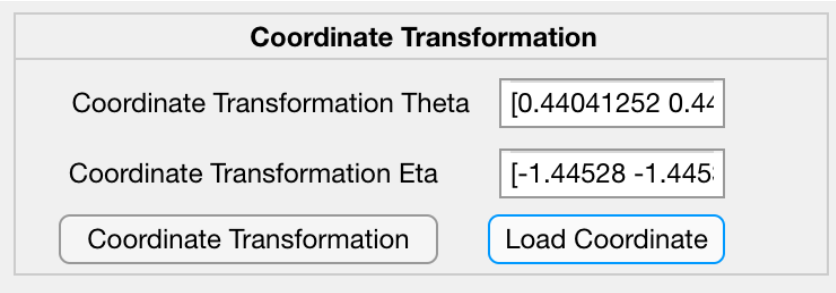

Figure 3. Coordinate transformation

3.1.3 2D data reduction

To facilitate subsequent data analysis, it is necessary to compress the two-dimensional raw data into one-dimensional diffraction peaks and rocking curves, which are performed in the 2D Reduction Scan panel. 3DSOC has provided initial values for Theta Scan Step Size and Eta Scan Step Size in advance, which represent the scanning step size when compressing into one-dimensional diffraction peaks and rocking curves, respectively. Users can adjust them according to actual situations. Click the SCAN button to obtain one-dimensional diffraction peaks and rocking curves in Overall Diffraction and Rocking Curve according to the set step size. The operation is shown in Figure 4.

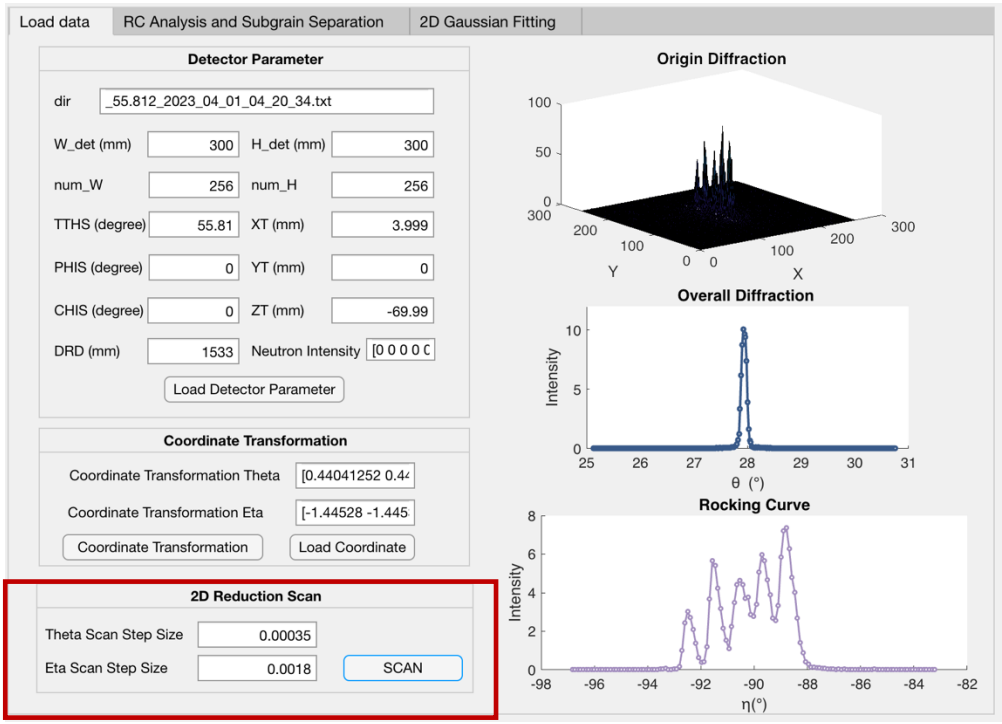

Figure 4. 2D data reduction

3.2 RC Analysis and Subgrain Separation

3.2.1 RC fitting analysis

For subsequent separation of subgrain diffraction peaks, it is necessary to first fit and analyze the rocking curve obtained, which is mainly performed in the Rocking Curve Fitting Parameter panel.

User needs to first determine the number of subgrains to determine the number of Gaussian peaks in the fitting analysis. Secondly, it is necessary to determine the Left Interception and Right Interception values, which represent the number of scattered points intercepted on the left and right sides of the RC obtained, thereby limiting the fitting range. Then, the value of Peak position (relative to highest) needs to be determined, and the input format can refer to the system preset value. It is mainly used to determine the initial peak position of the diffraction peak during the rocking curve fitting process. The setting method is to set the maximum value of the rocking curve as origin 0, then the distance between the maximum values of the other diffraction peaks and the origin are calculated based on the number of scattered points. The setting result of Peak Position is represented by the green scattered points in the subsequent RC Fitting curve graph and can be continuously adjusted according to the results. Finally, Eta_std_RC needs to be determined, which represents the initial peak width of the diffraction peak during the rocking curve fitting process. The system has pre-set this parameter to 0.01, which can meet most situations.

After completing the above parameter settings, click the Fitting curve button to start fitting. Fitting results are presented in table and the plot is shown in RC Fitting. The table is divided into two columns, the first column is the parameters of RC, the second column is the 95% confidence interval corresponding to each row of parameters. Every three rows of table are a group result of one subgrain, representing the peak height, peak position, and standard deviation. The total number of parameters should be 3 * Peak number+1, with the last parameter being the noise.

If the fitting results under the current parameter conditions do not meet

expectations, parameters can be adjusted and re-fitted. The operation is shown in Figure 5.

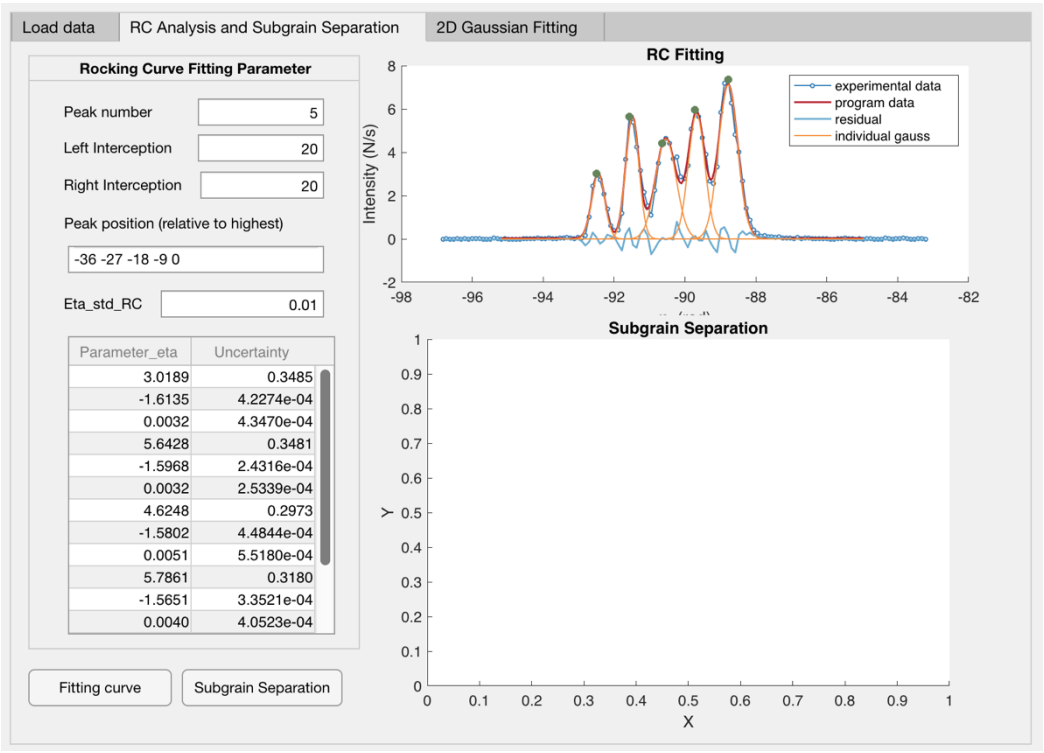

Figure 5. RC fitting and analysis

3.2.2 Subgrain Separation

After fitting and analyzing the RC, click on Subgrain Separation to separate the diffraction peaks, as shown in Figure 7. It can be found that the original two-dimensional diffraction peak is replaced by several diffraction peaks of different colors. By analyzing the diffraction peaks of a single color, the diffraction parameters of the subgrain can be obtained.

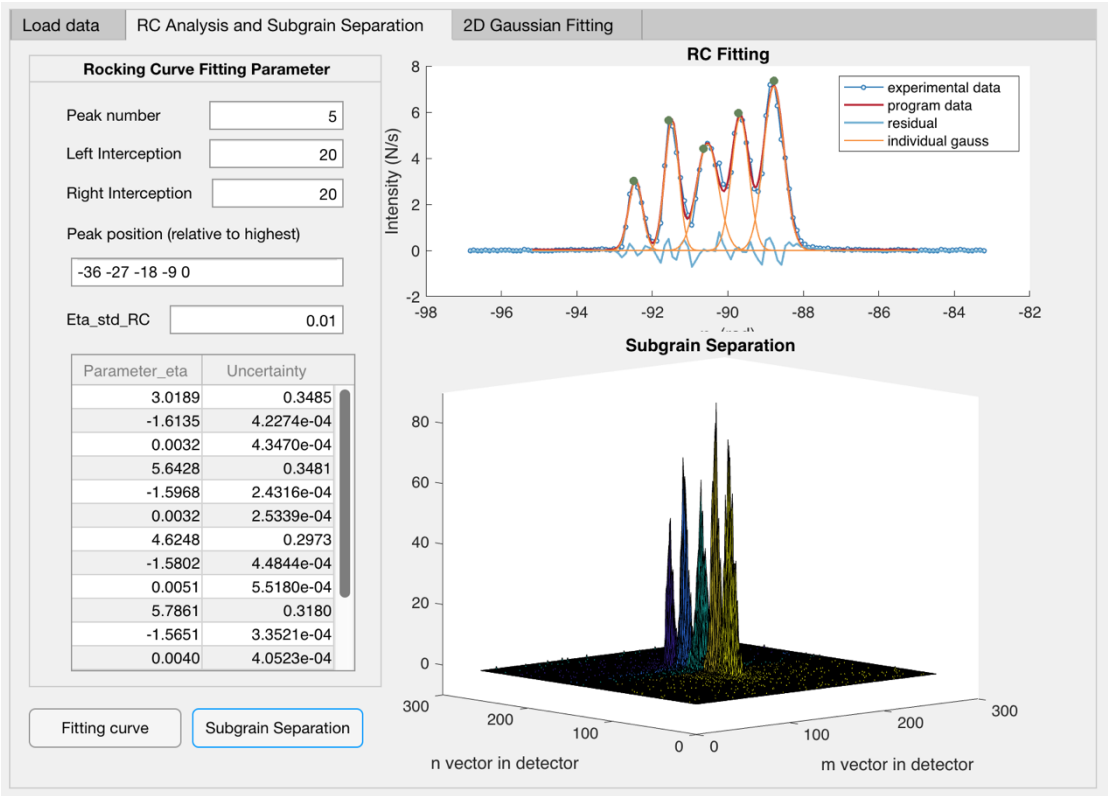

Figure 7. Subgrain Separation

3.3 2D Gaussian Fitting

3.3.1 2D Gaussian Fitting

After subgrain diffraction separation, it is necessary to perform two-dimensional Gaussian function fitting analysis, which is mainly distributed in the Fitting Range and Initial Parameter panels.

User needs to first set the Fitting Range, m_ Width and n_ Width, which represents the extraction size along the m and n directions of detector. Then, a rectangle containing (2 * m_width+1) * (2 * n_width+1) pixels is regarded as the fitting data source. Secondly, it is necessary to set theta _ 0, theta_ std, eta_std and noise, which represent the initial fitting values of subgrain theta position and standard deviation, eta standard deviation, and noise, respectively. Above values have been pre-provided by 3DSOC and can adapt to most fitting situations. Secondly, the eta position does not need to be

provided by the user, 3DSOC has extracted settings from the analysis and fitting of RC.。

After setting above fitting parameters, click 2D Gaussian Fitting button to visualize results in Overall 2D Gaussian Fitting. If the fitting is not satisfactory, initial parameters can be continuously modified and re-fit. Figure 7 shows the fitting results of two-dimensional Gaussian function.

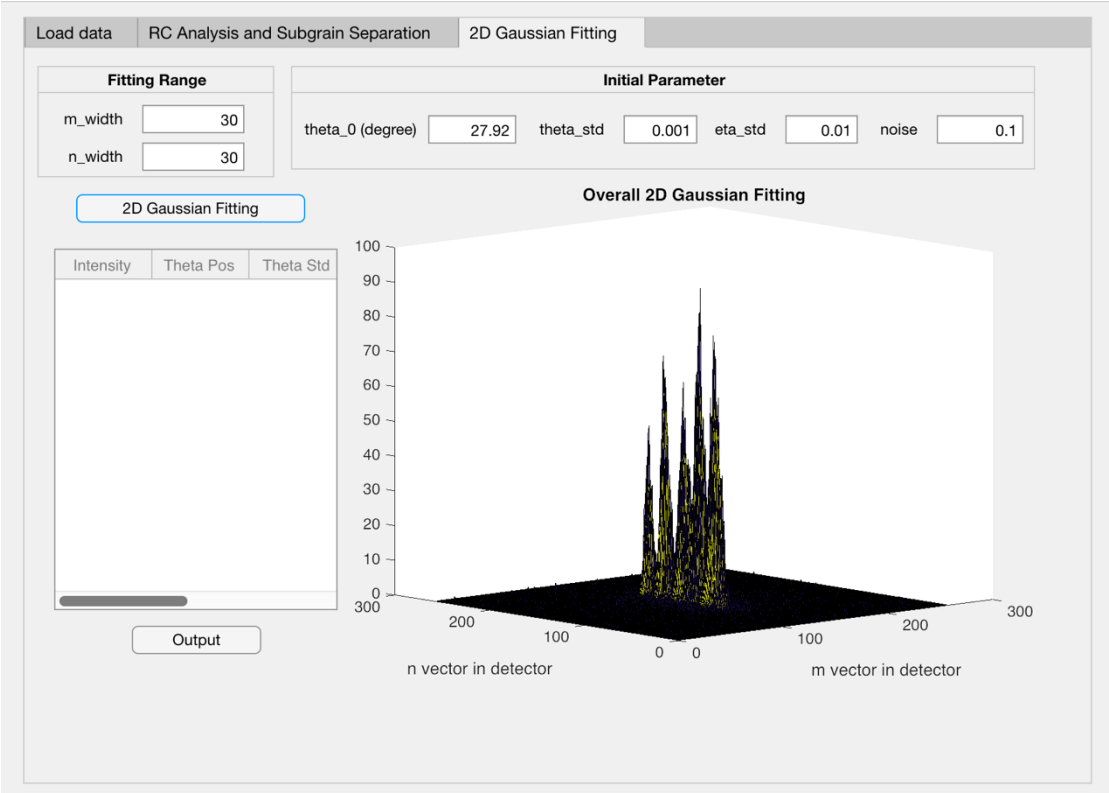

Figure 7. 2D Gaussian Fitting

3.3.2 Output

Click Output button to output fitting data. Final data will be displayed in the table in Figure 8, and a result file *datafile.txt* will be output under the current file path in MATLAB, as shown in Figure 9. The output file should contain 2 * Peak_ Number rows and 6 columns. The first 2*Peak_ Number rows are the fitting parameter of each subgrain, arranged according to diffraction intensity, theta direction position, theta standard deviation, eta direction position, eta standard deviation and bottom noise, the followed rows represent the 95% confidence interval corresponding to the first part of the data.

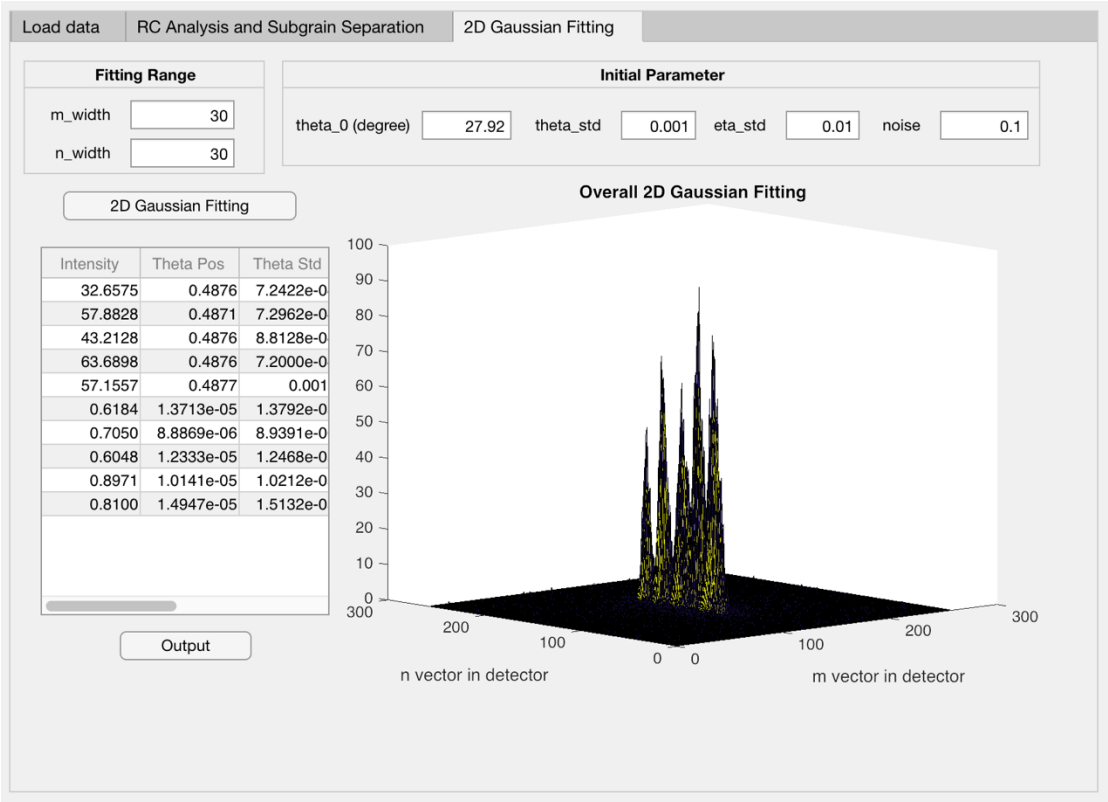

Figure 8 Data Output in 3DSOC

datafile.txt

```
3.2657475e+01   4.8755678e-01   7.2421652e-04   -1.6131690e+00   3.1698908e-03   2.3015622e-03
5.7882755e+01   4.8714414e-01   7.2961814e-04   -1.5971240e+00   3.2211190e-03   4.7064192e-02
4.3212805e+01   4.8757695e-01   8.8127544e-04   -1.5794775e+00   4.7839584e-03   4.1592033e-02
6.3689762e+01   4.8758764e-01   7.2000299e-04   -1.5649863e+00   3.8170025e-03   6.3036648e-02
5.7155700e+01   4.8774416e-01   1.0546900e-03   -1.5497884e+00   4.4744623e-03   5.6460301e-02
6.1837699e-01   1.3713268e-05   1.3791936e-05    6.0022606e-05   6.0366670e-05   3.3170122e-02
7.0502662e-01   8.8869427e-06   8.9391128e-06    3.9233896e-05   3.9464035e-05   3.8251225e-02
6.0476266e-01   1.2333473e-05   1.2468032e-05    6.6950839e-05   6.7680691e-05   4.4790946e-02
8.9708191e-01   1.0141433e-05   1.0211555e-05    5.3763118e-05   5.4134554e-05   5.2841392e-02
8.1001832e-01   1.4947250e-05   1.5131696e-05    6.3412233e-05   6.4194321e-05   6.3828432e-02
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Figure 9 Data Output in datafile.txt

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