

XRDUG Seminar IV

*Screen Shots of  
Profile Fitting  
Using the  
DMSNT Software*

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2/1/2007

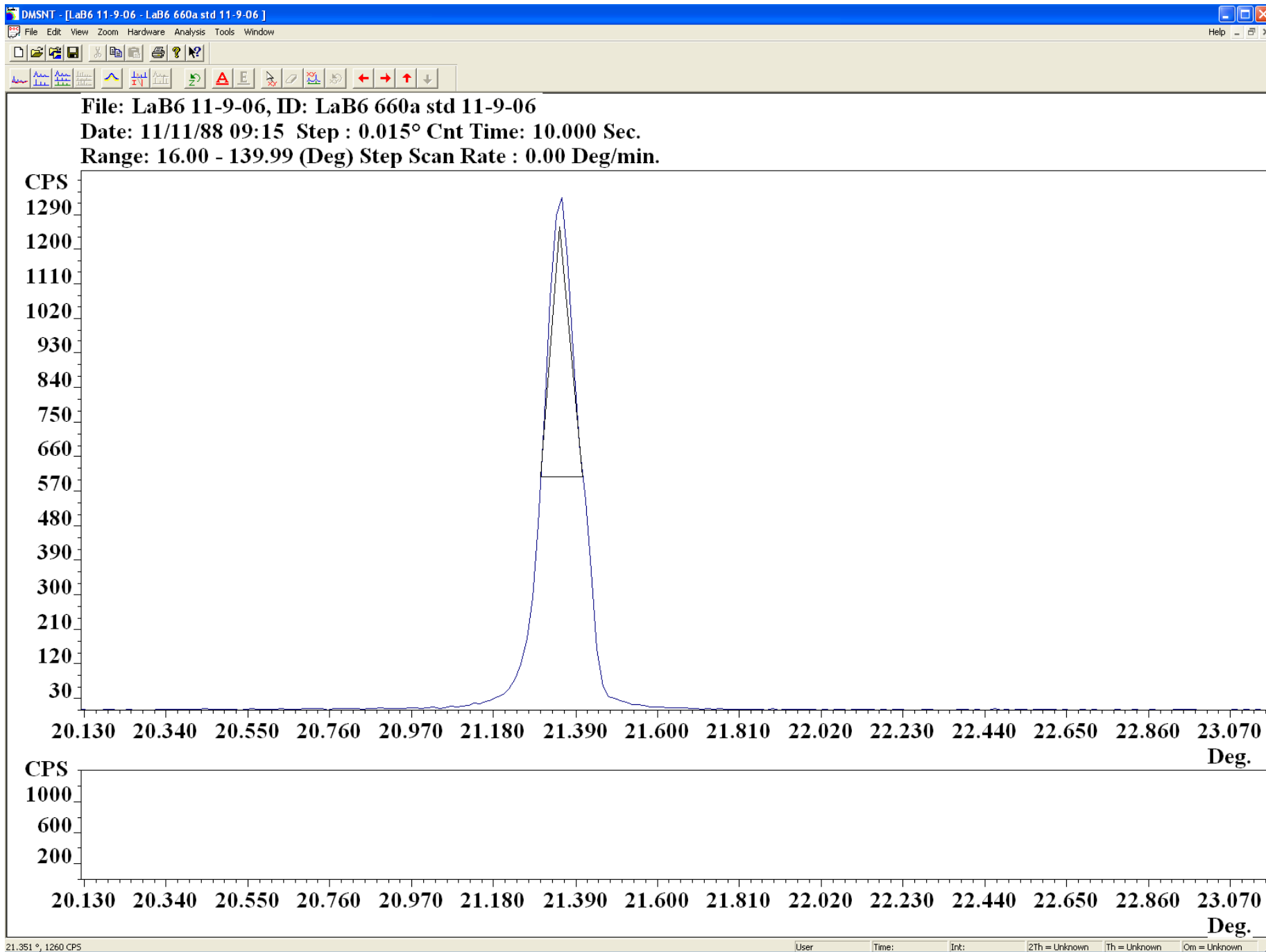


Figure 1 Inserting a Peak Manually



File: LaB6 11-9-06, ID: LaB6 660a std 11-9-06  
Date: 11/11/88 09:15 Step : 0.015° Cnt Time: 10.000 Sec.  
Range: 16.00 - 139.99 (Deg) Step Scan Rate : 0.00 Deg/min.

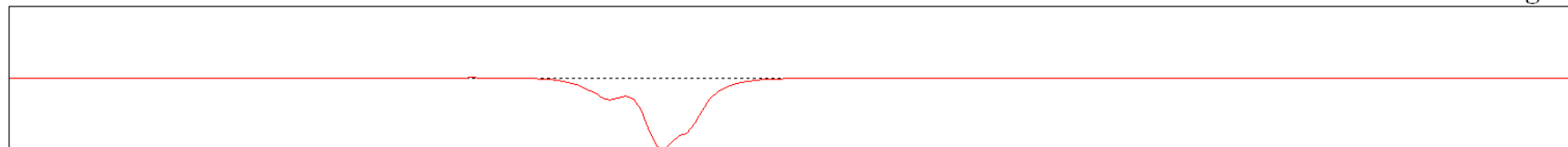
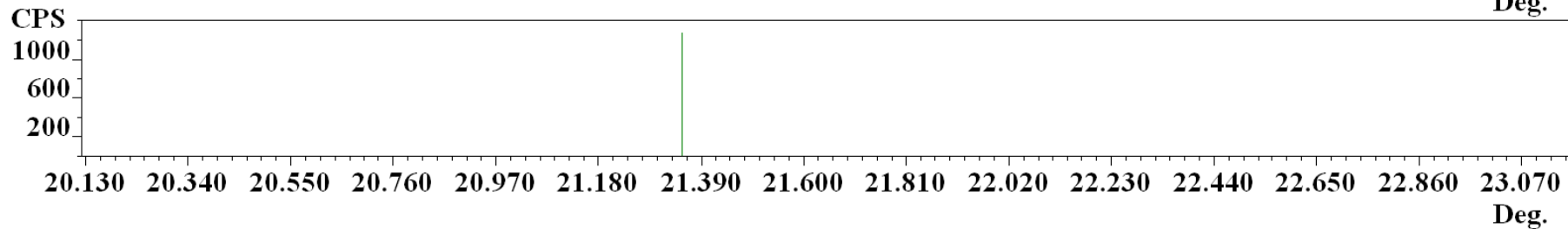
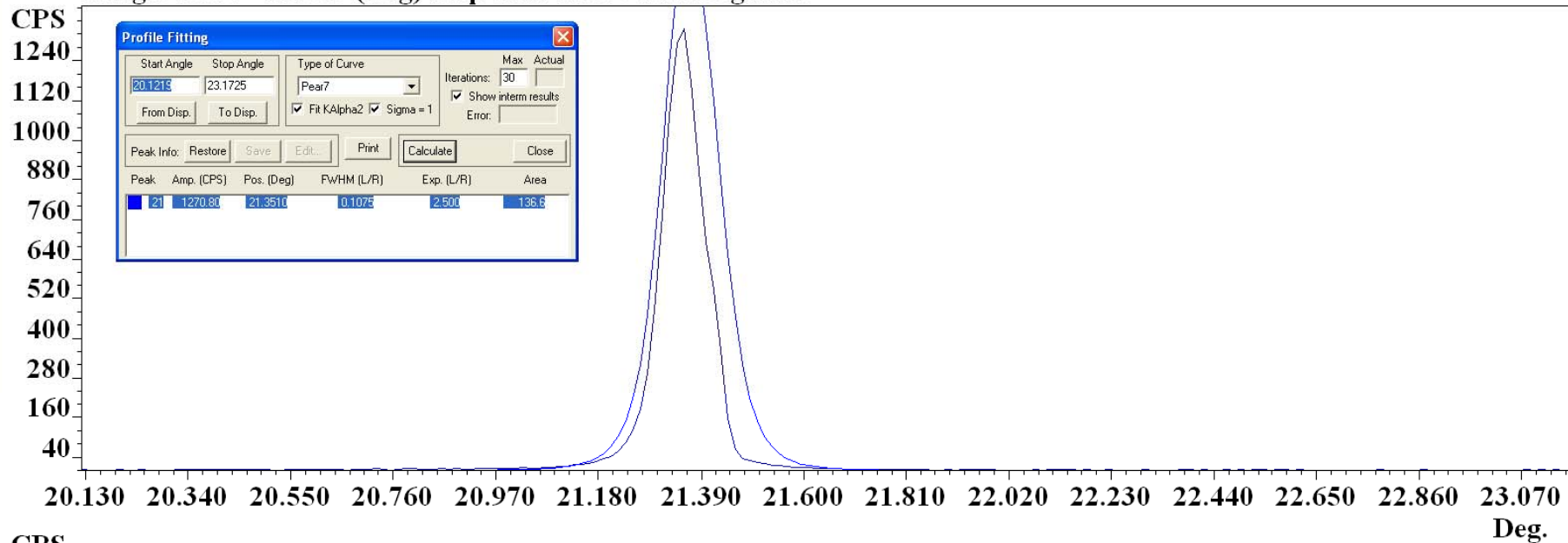
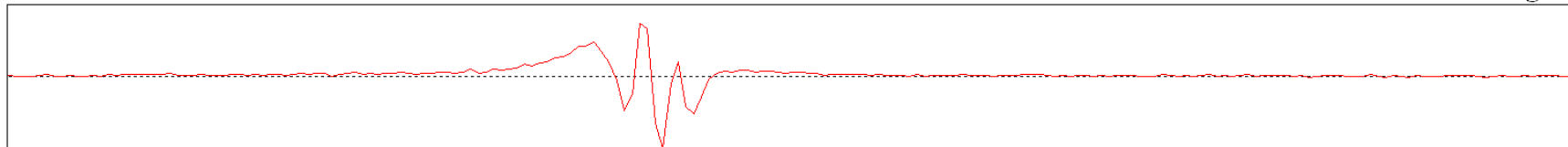
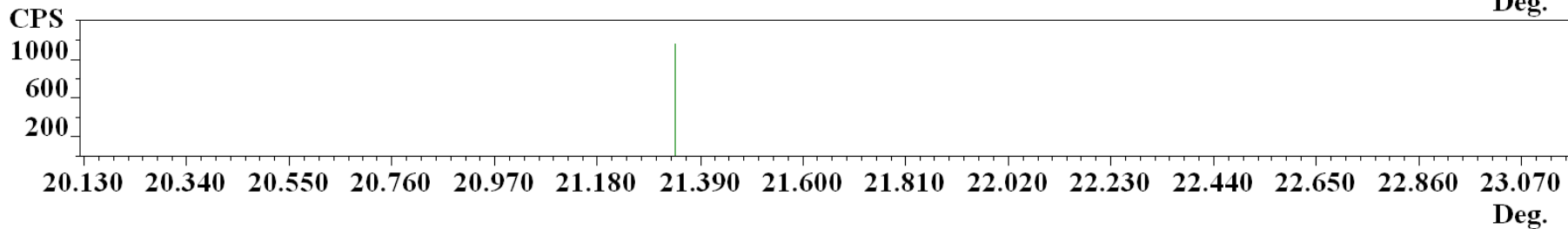
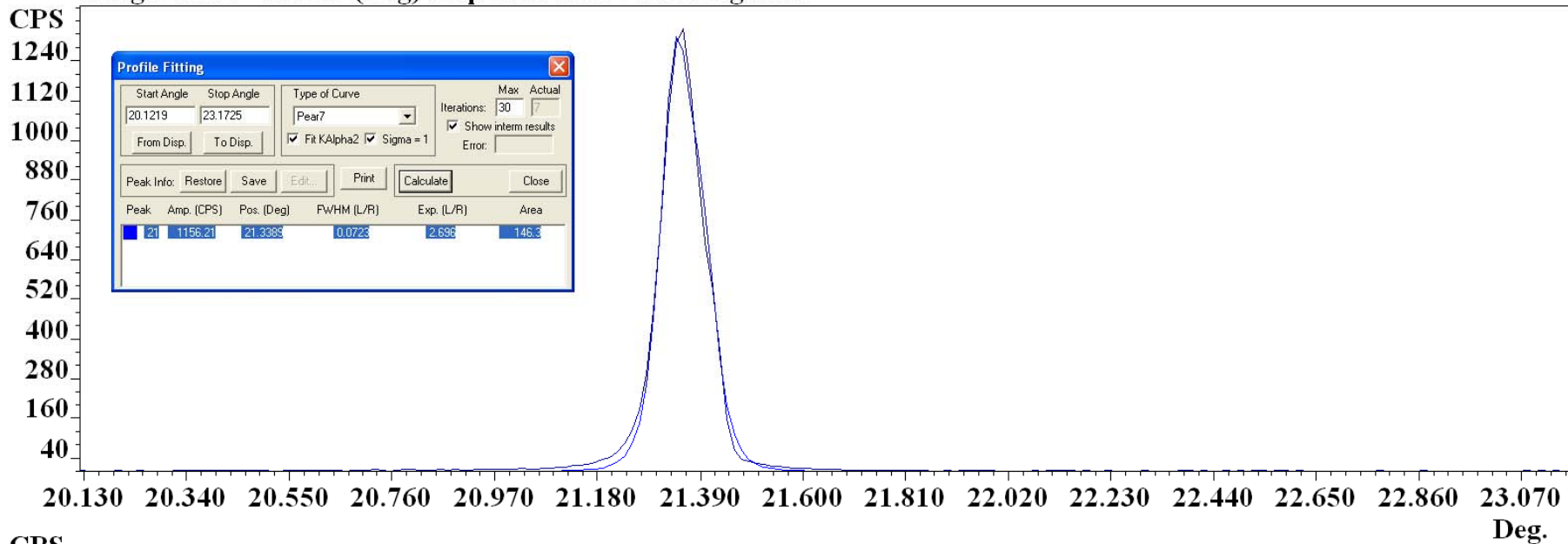


Figure 2 Profile Function from Manual Peak Insertion



File: LaB6 11-9-06, ID: LaB6 660a std 11-9-06  
Date: 11/11/88 09:15 Step : 0.015° Cnt Time: 10.000 Sec.  
Range: 16.00 - 139.99 (Deg) Step Scan Rate : 0.00 Deg/min.



For Help, press F1 User Time: Int: 2Th = Unknown 1Th = Unknown Om = Unknown

Figure 3 Profile Function After Convergence

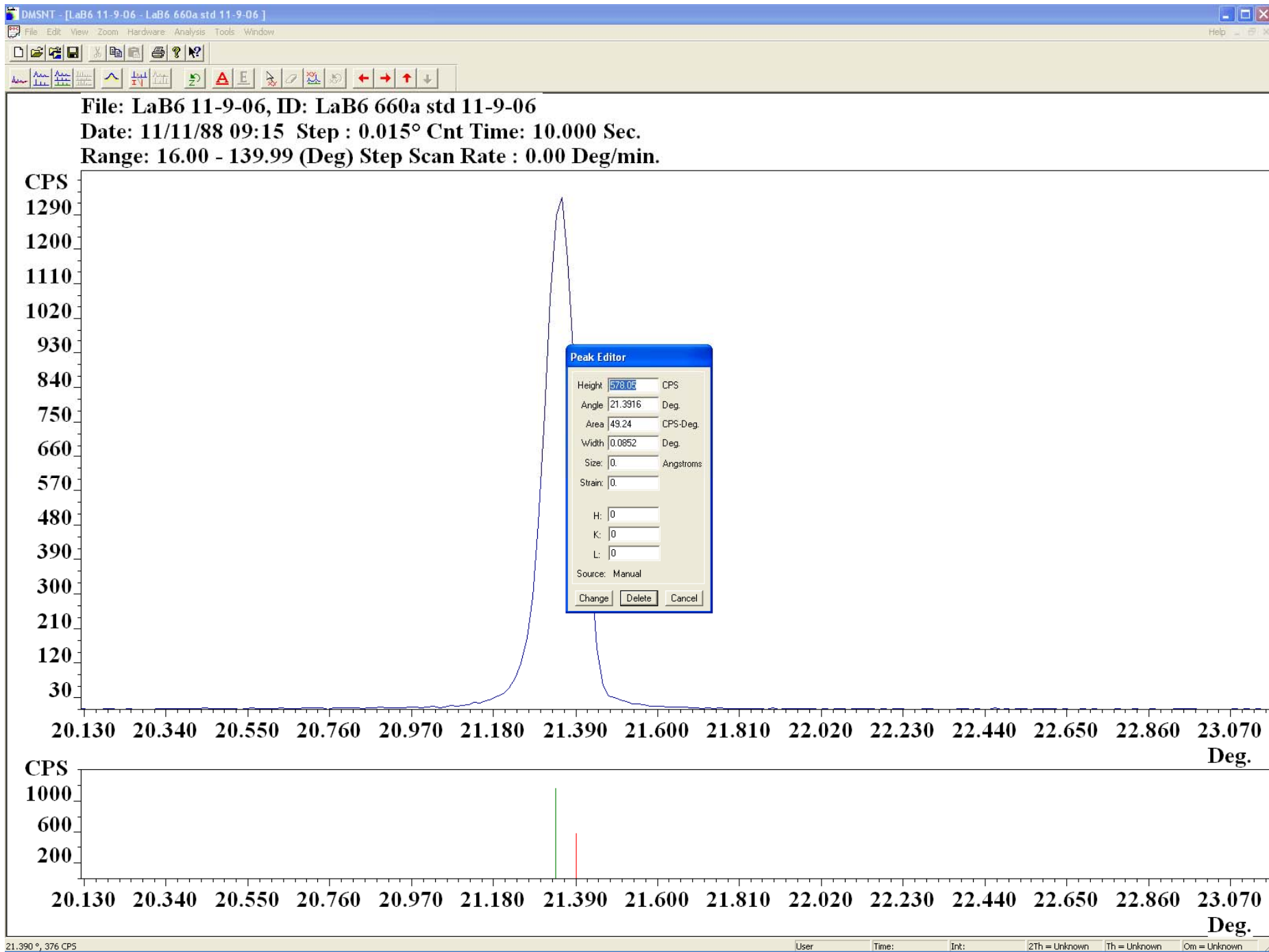
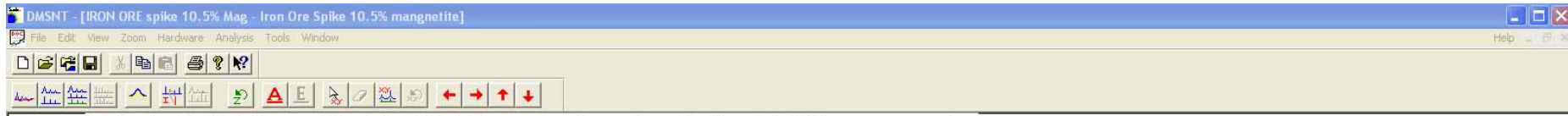


Figure 4 Deleting Peaks



File: IRON ORE spike 10.5% Mag, ID: Iron Ore Spike 10.5% magnetite  
 Date: 06/24/05 06:40 Step : 0.020° Cnt Time: 5.000 Sec.  
 Range: 26.20 - 36.30 (Deg) Step Scan Rate : 0.00 Deg/min.

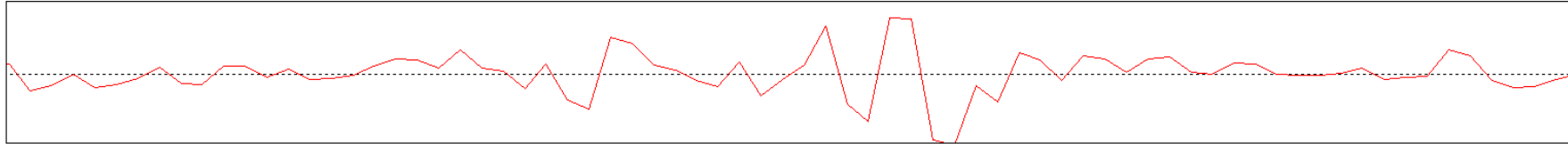
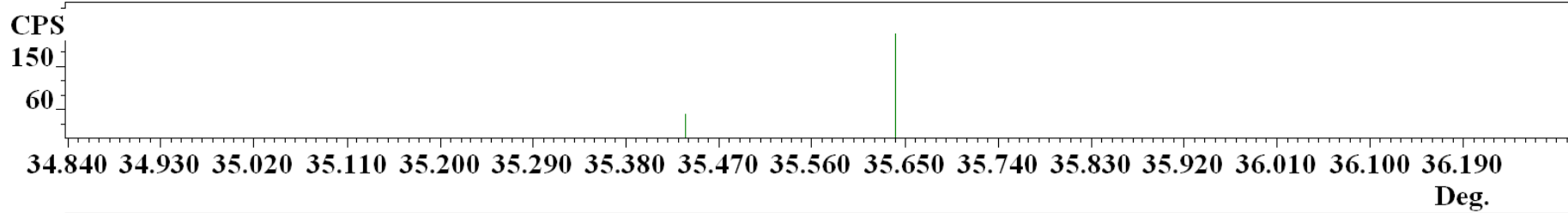
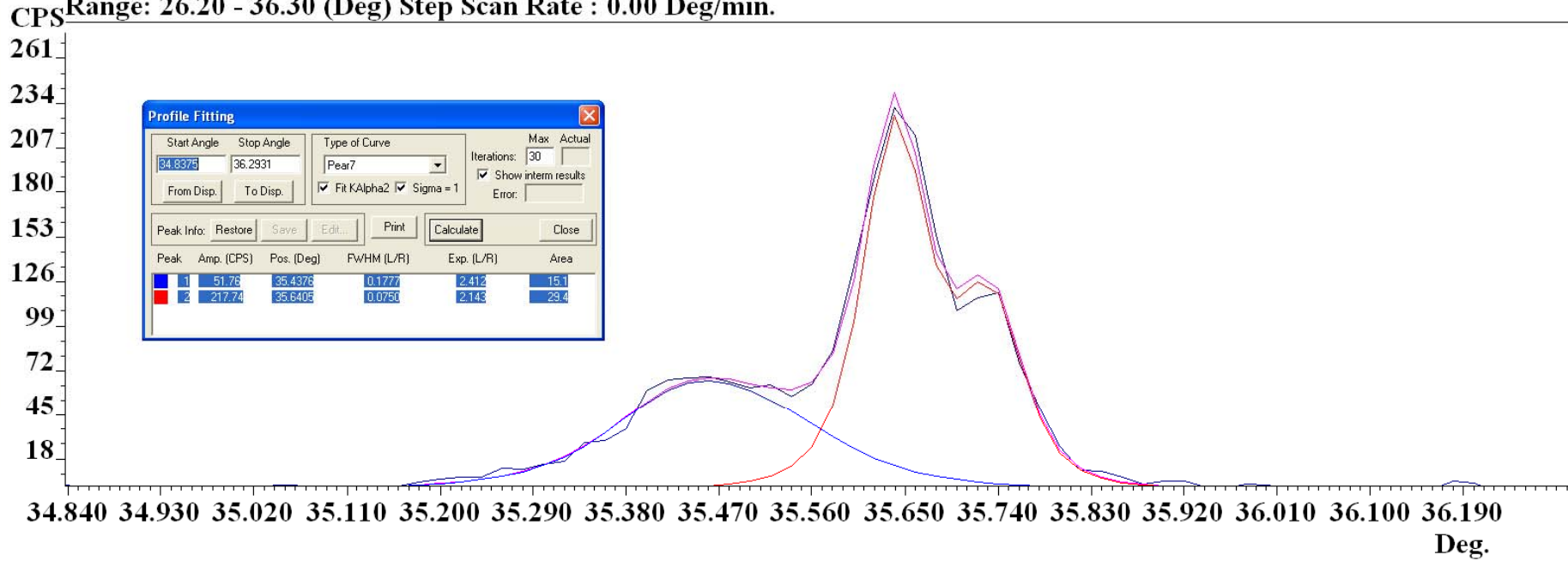
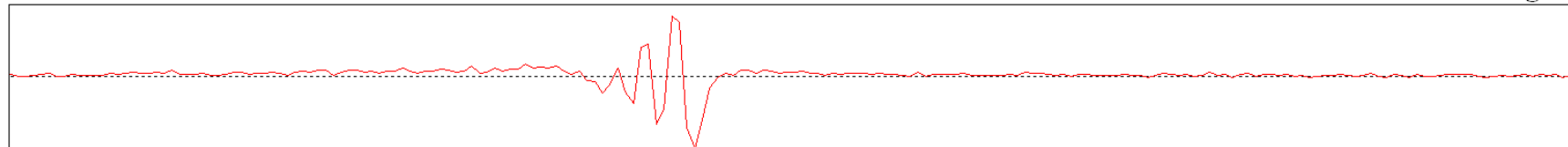
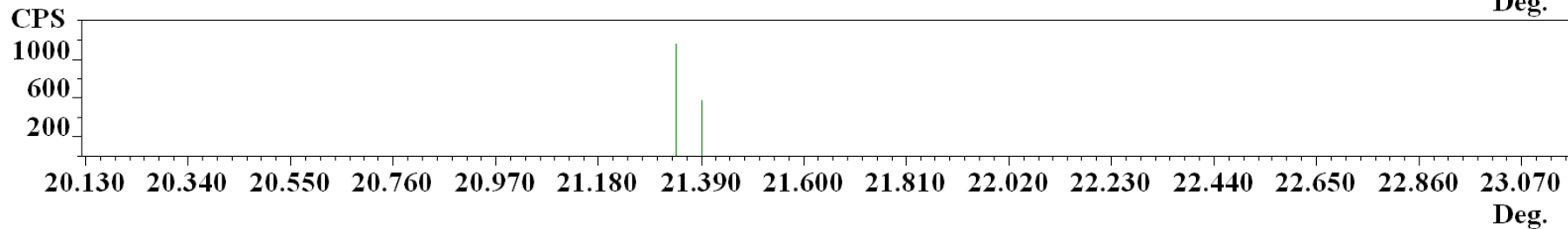
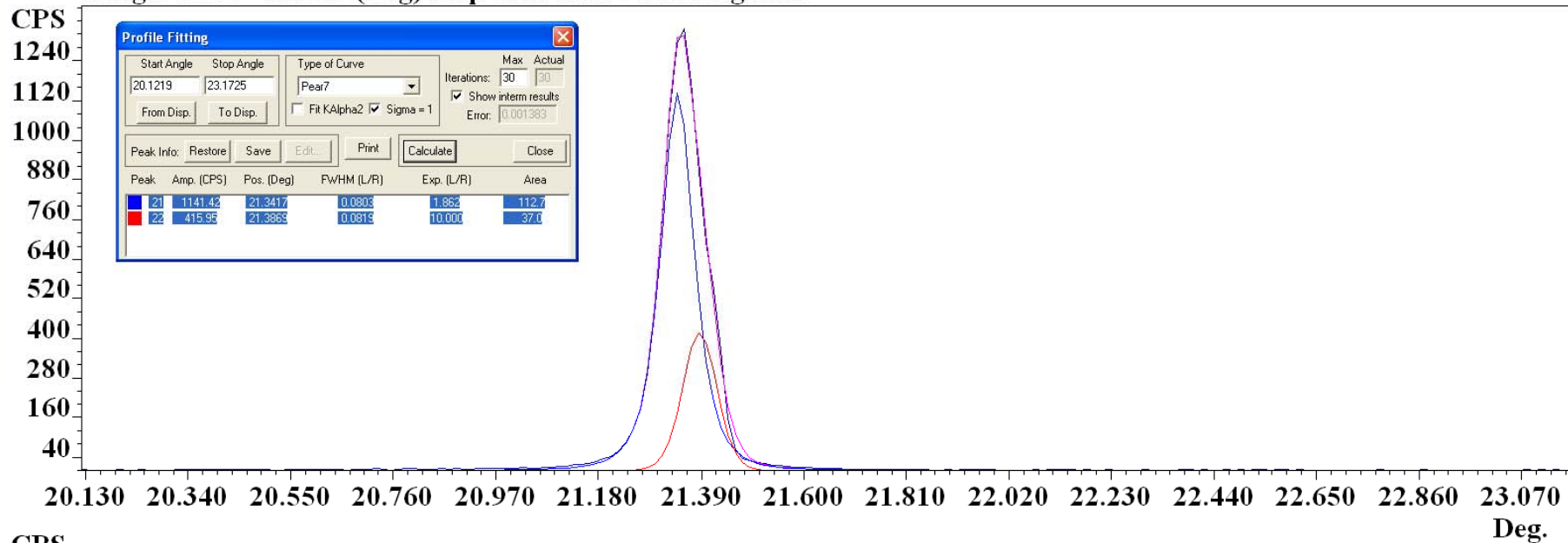


Figure 5 Inserting Peaks with Minimal Features

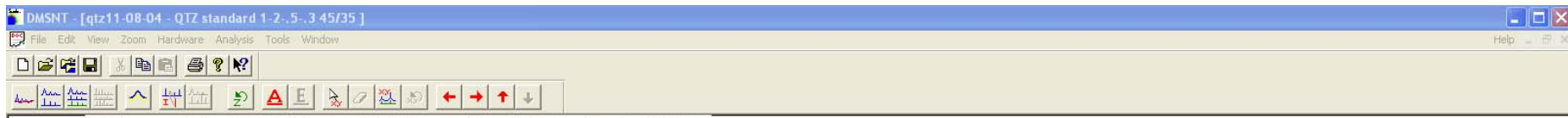


File: LaB6 11-9-06, ID: LaB6 660a std 11-9-06  
Date: 11/11/88 09:15 Step : 0.015° Cnt Time: 10.000 Sec.  
Range: 16.00 - 139.99 (Deg) Step Scan Rate : 0.00 Deg/min.



21.179 °, 895 CPS User Time: Int: 2Th = Unknown 1Th = Unknown Om = Unknown

Figure 6 Profile Functions Manually Fitting  $K_{\alpha 2}$



File: qtz11-08-04, ID: QTZ standard 1-2-.5-.3 45/35  
 Date: 11/08/04 09:01 Step : 0.010° Cnt Time: 5.000 Sec.  
 Range: 24.00 - 69.50 (Deg) Step Scan Rate : 0.00 Deg/min.

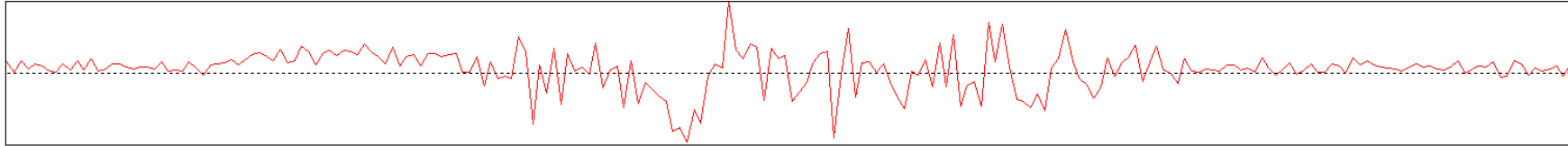
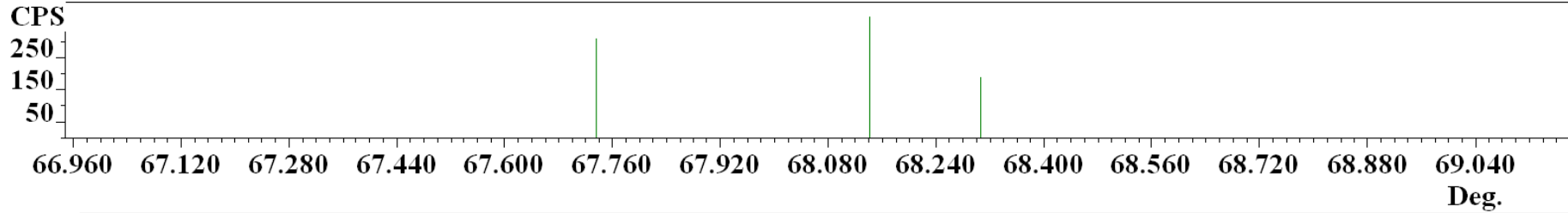
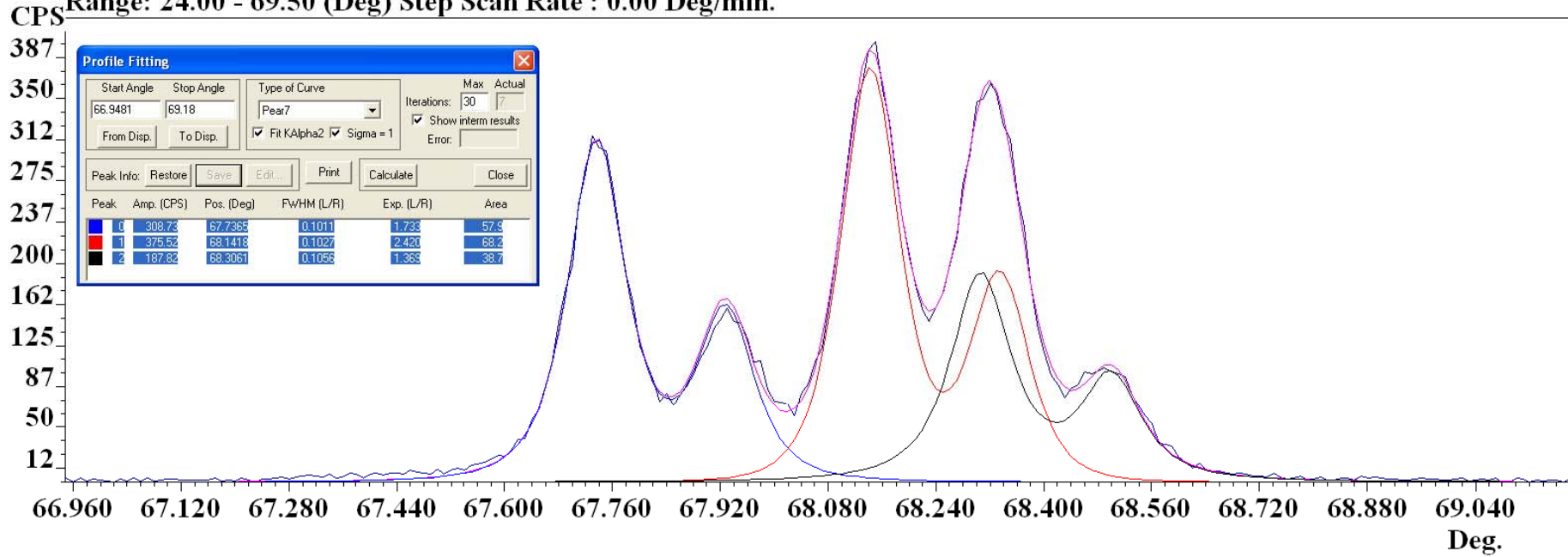
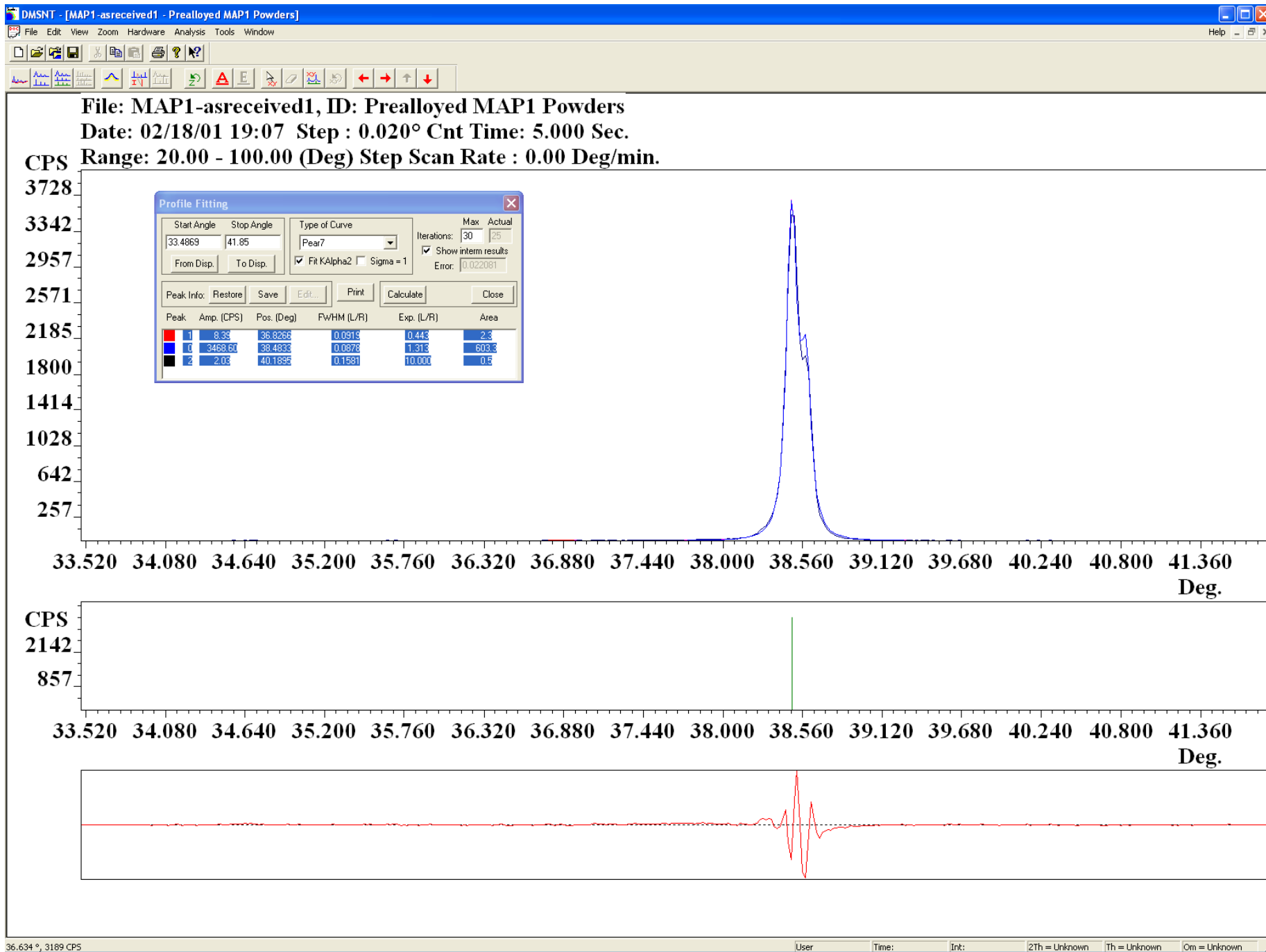
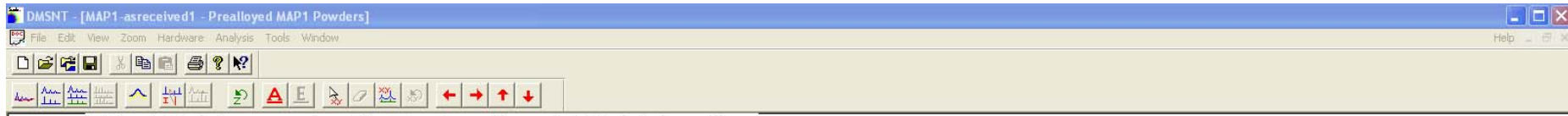


Figure 7 Five Fingers of Quartz





**Figure 8 Example of Low Intensity Peak Near a High Intensity Peak**



File: MAP1-asreceived1, ID: Prealloyed MAP1 Powders  
Date: 02/18/01 19:07 Step : 0.020° Cnt Time: 5.000 Sec.  
Range: 20.00 - 100.00 (Deg) Step Scan Rate : 0.00 Deg/min.

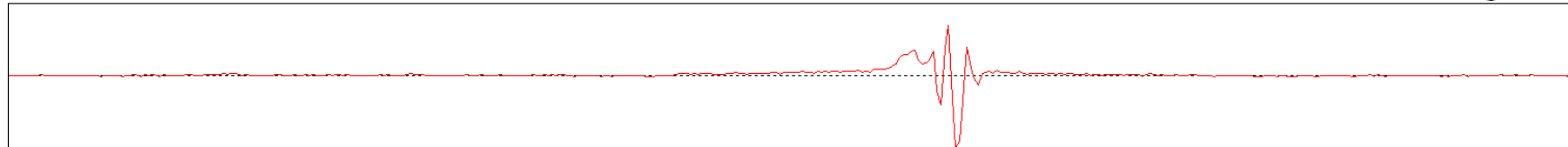
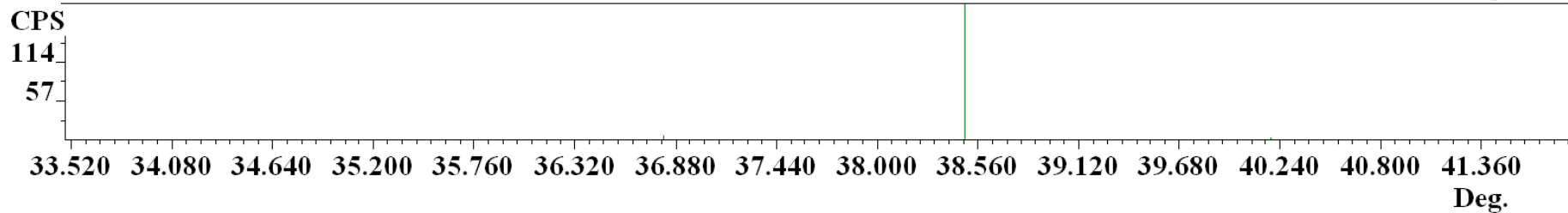
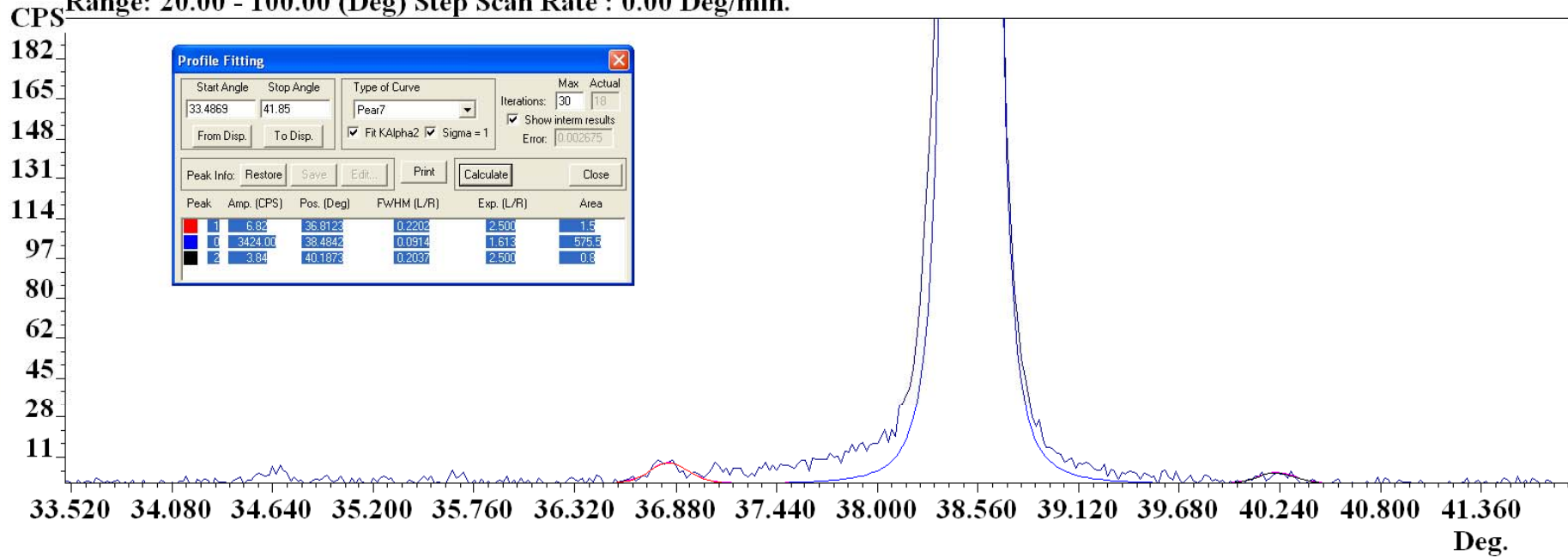
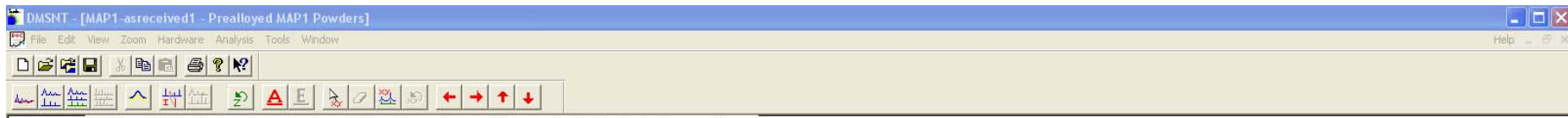


Figure 9 Figure 8 Zoomed To Observe Low Intensity Peaks - Initial Peak Insertions



File: MAP1-asreceived1, ID: Prealloyed MAP1 Powders  
 Date: 02/18/01 19:07 Step : 0.020° Cnt Time: 5.000 Sec.  
 Range: 20.00 - 100.00 (Deg) Step Scan Rate : 0.00 Deg/min.

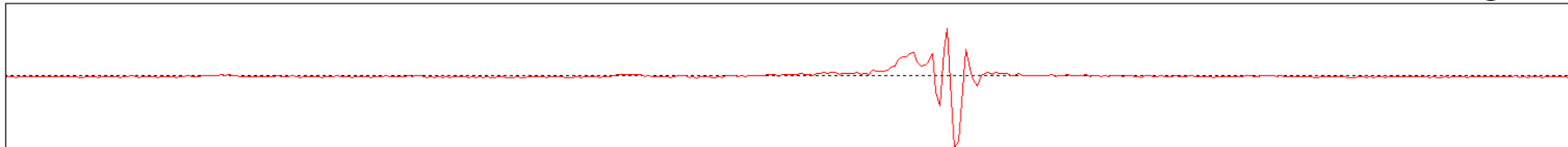
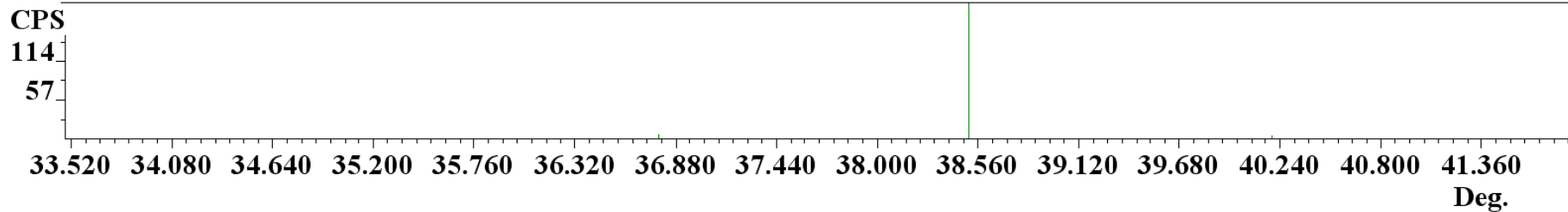
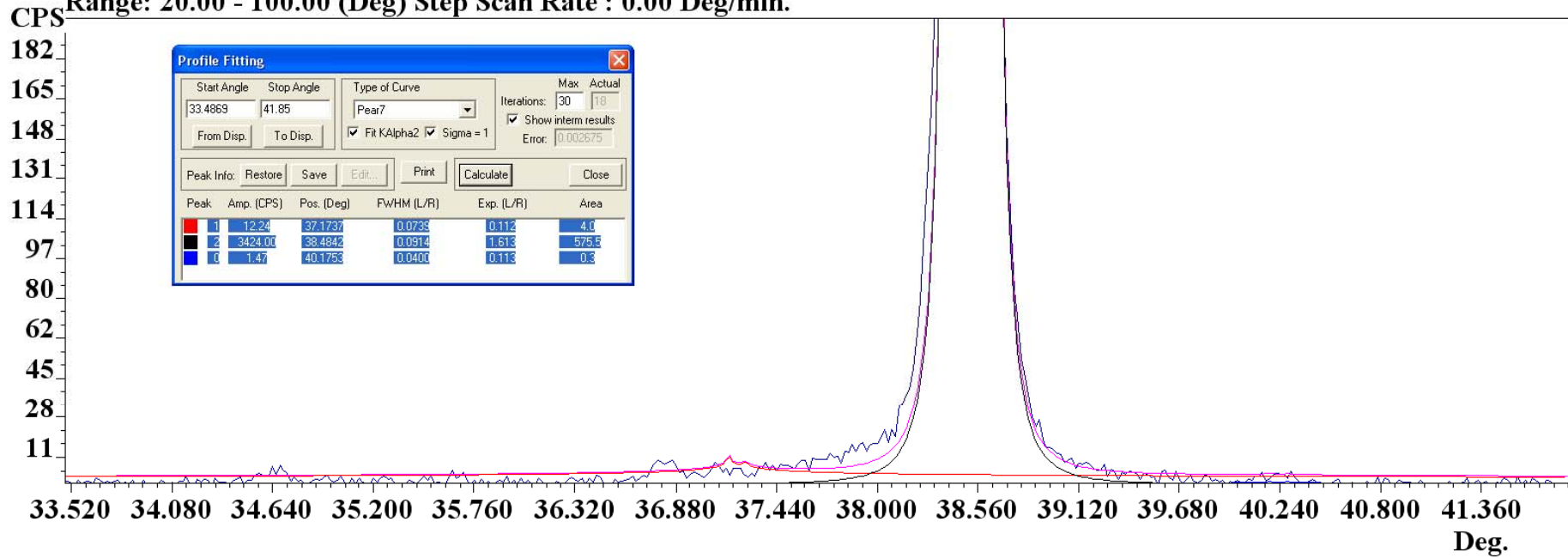


Figure 10 Curve Fit with Sigma = 1



File: MAP1-asreceived1, ID: Prealloyed MAP1 Powders  
Date: 02/18/01 19:07 Step : 0.020° Cnt Time: 5.000 Sec.  
Range: 20.00 - 100.00 (Deg) Step Scan Rate : 0.00 Deg/min.

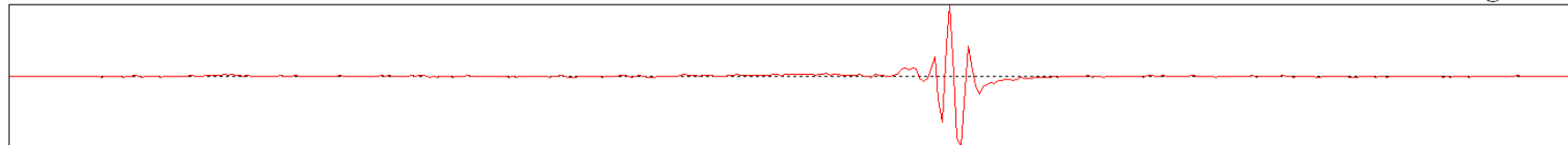
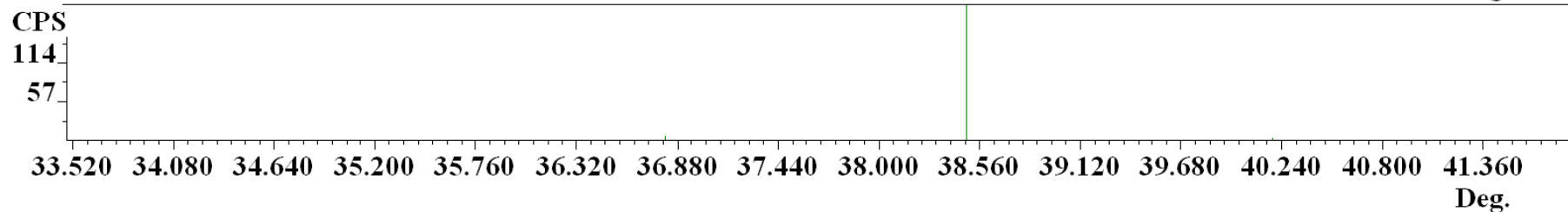
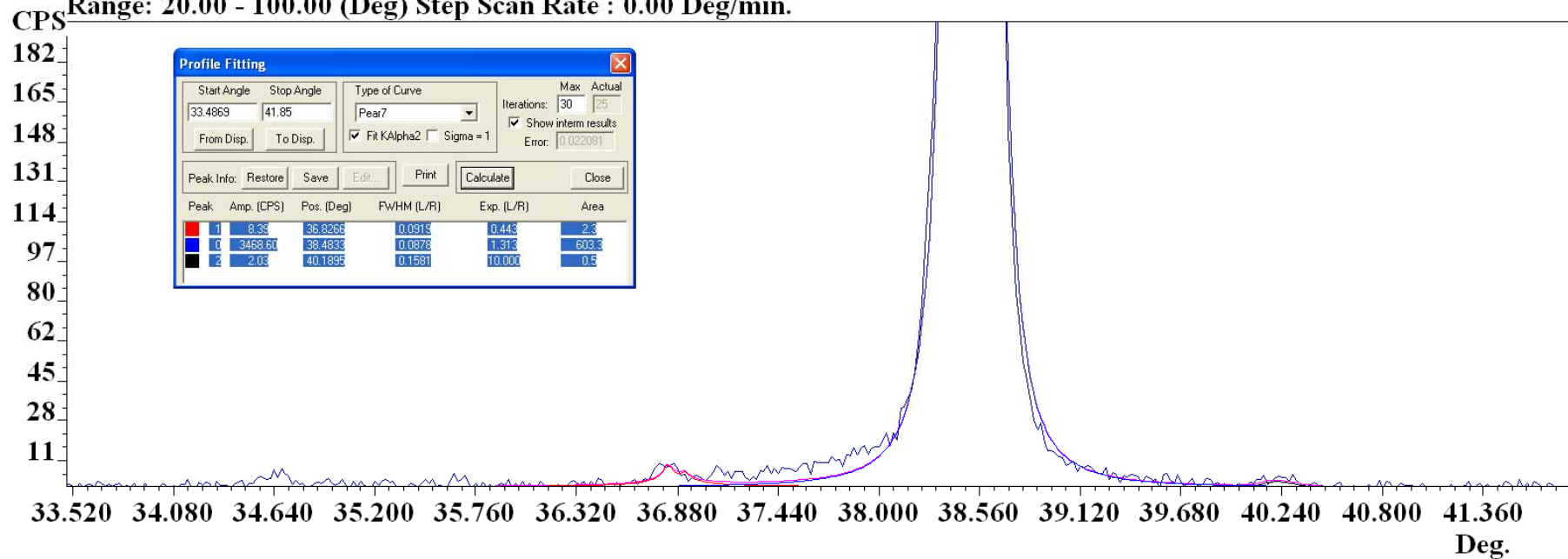


Figure 11 Curve Fit with Sigma Deselected

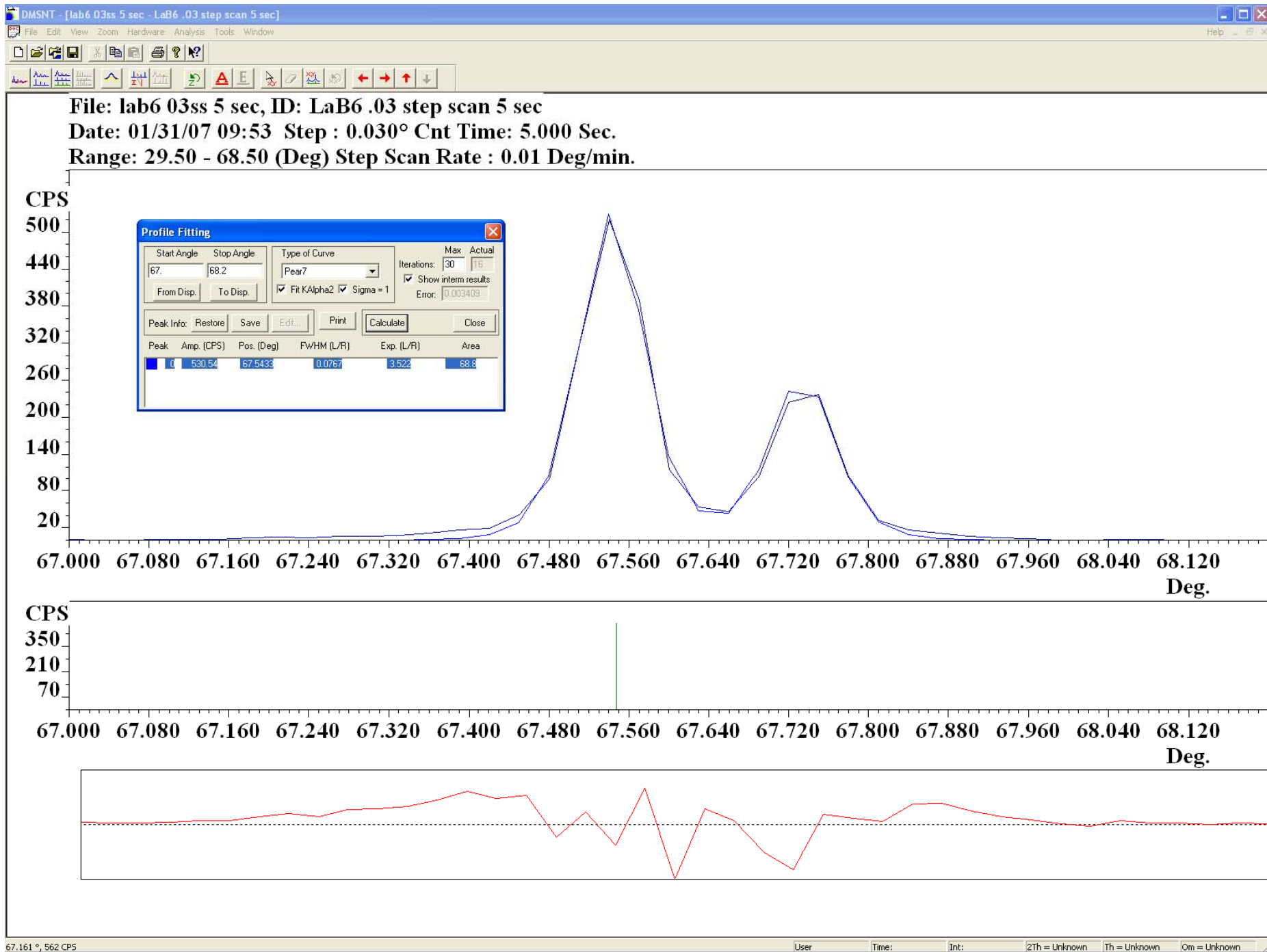
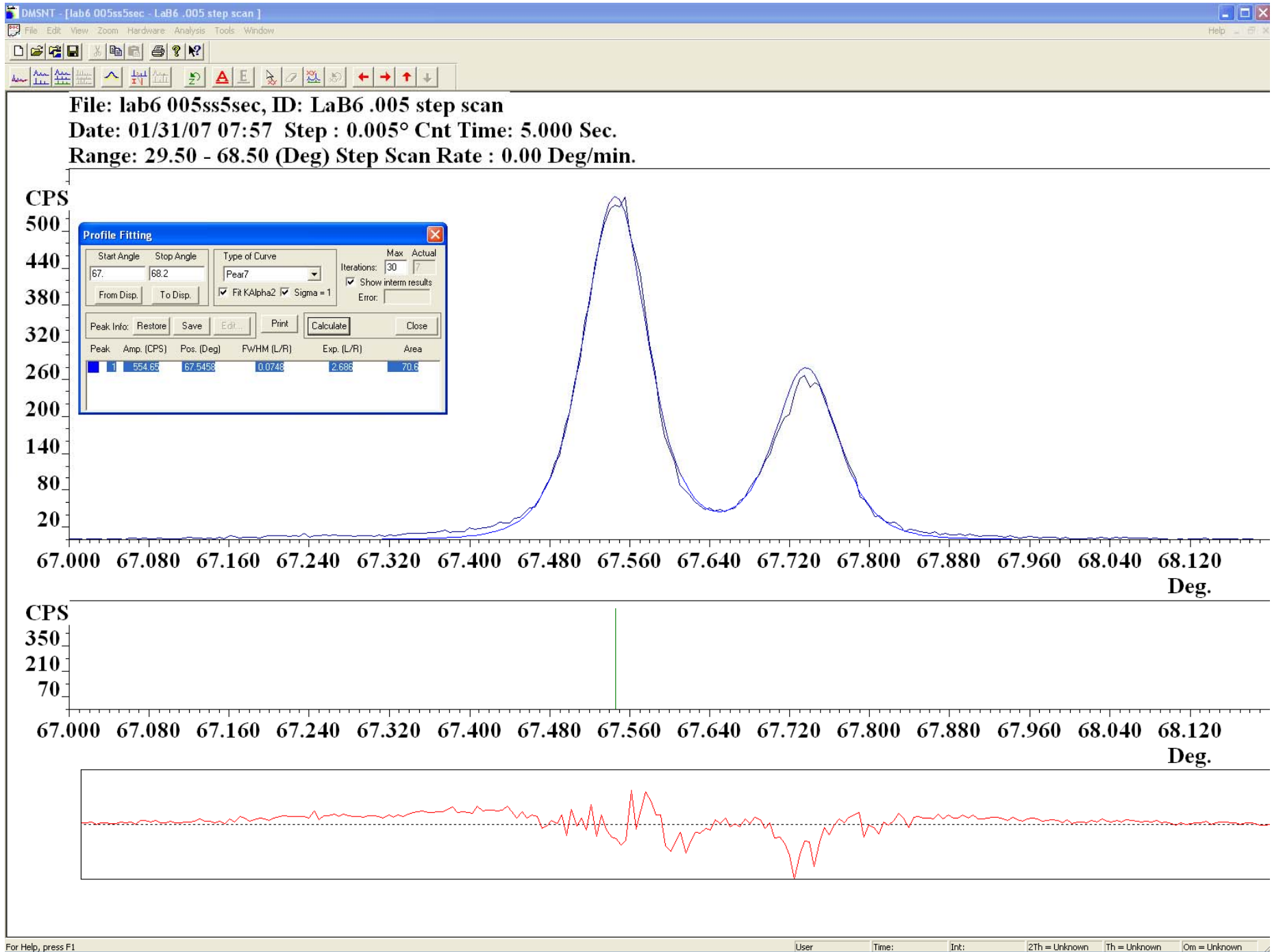


Figure 12 Effects of Step Size on Profile Function SS = 0.03° 2θ



**Figure 13 Effects of Step Size on Profile Function SS= 0.005° 2θ**