

XRDUG Seminar III

Screen Shots of DMSNT Software for XRD Data Smoothing, Background Corrections, and Generating Peak Files

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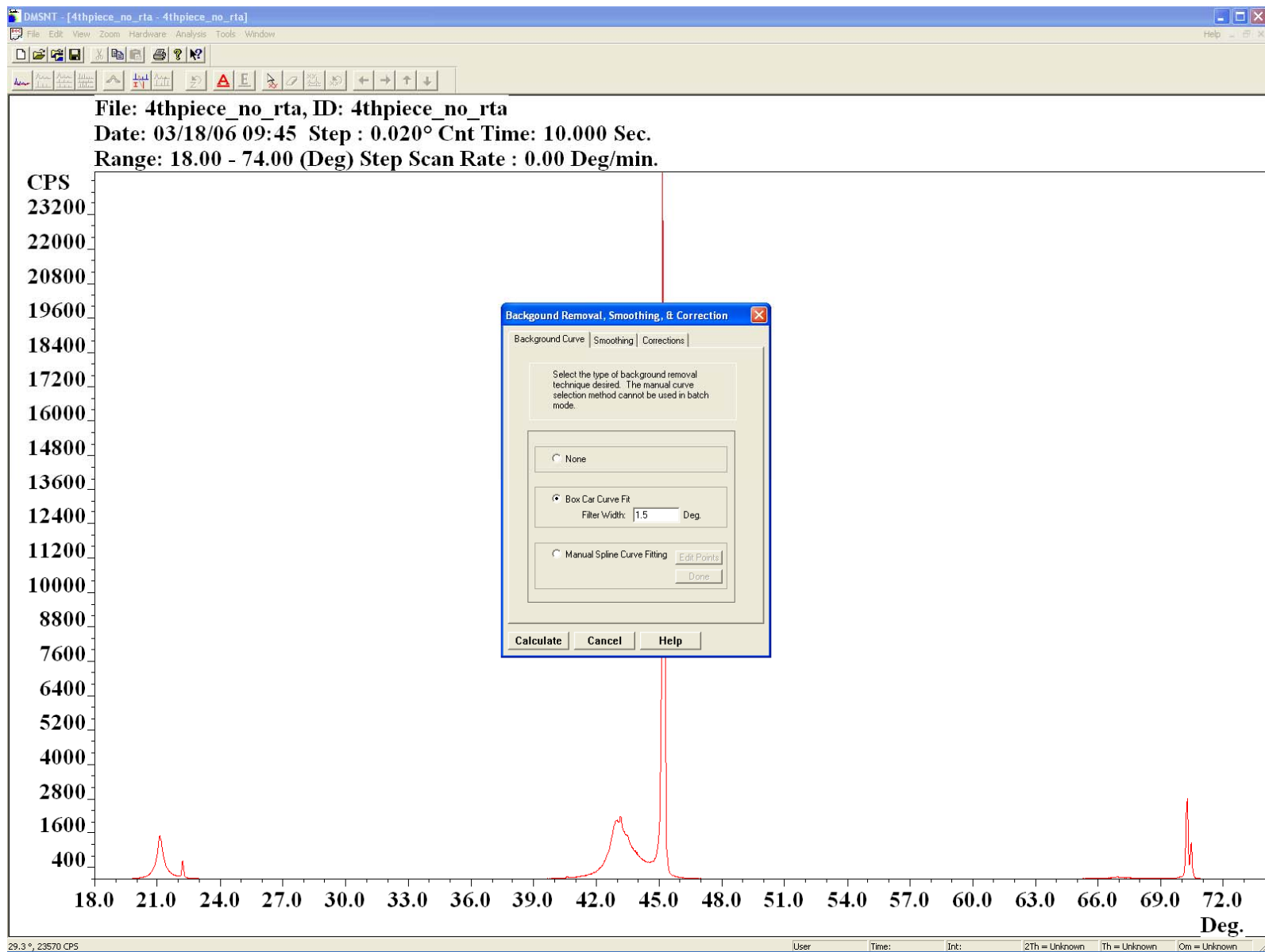


Figure 1 Background Correction - Box Car Fit

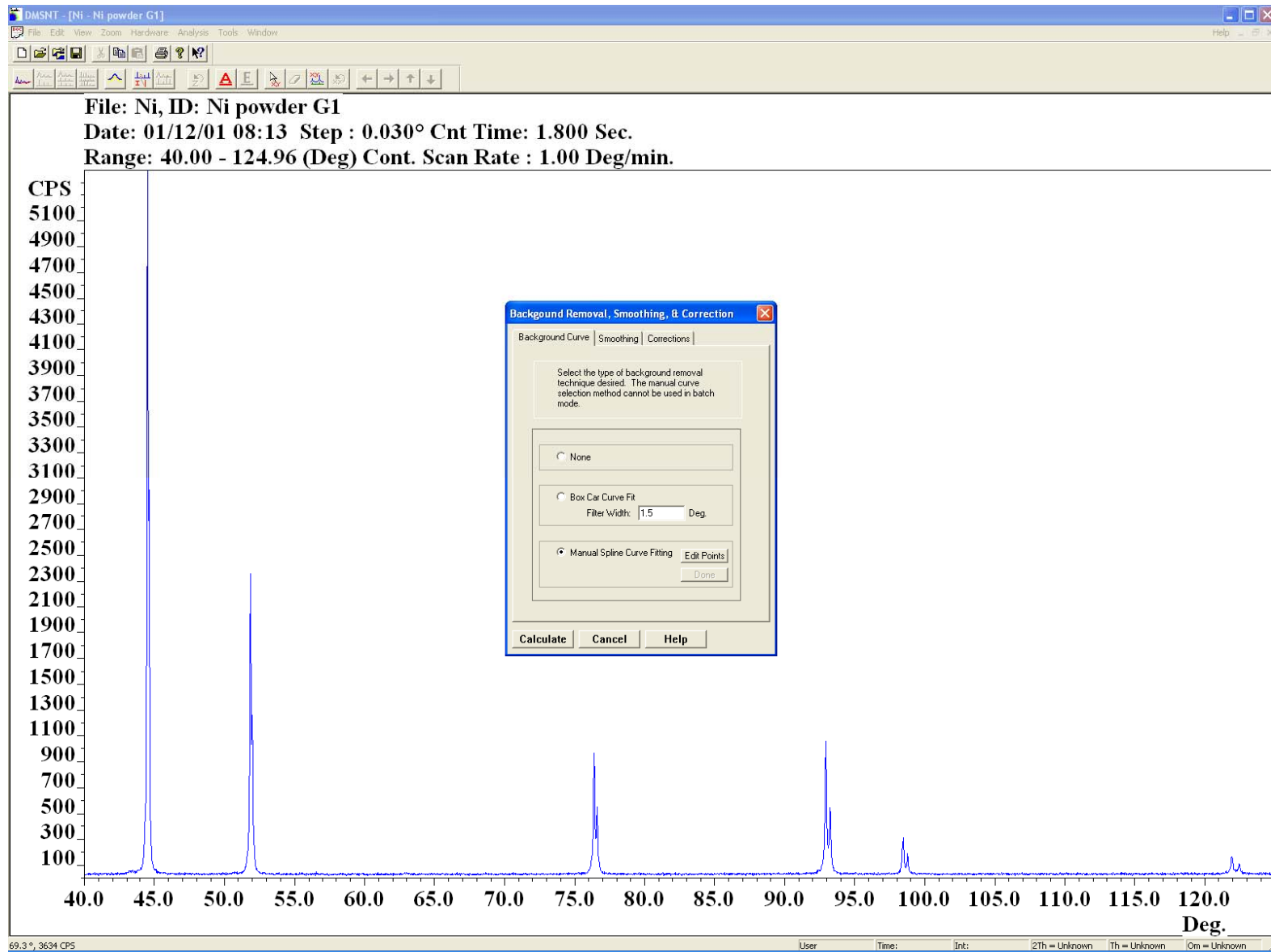


Figure 2 Background Correction - Cubic Spline Option

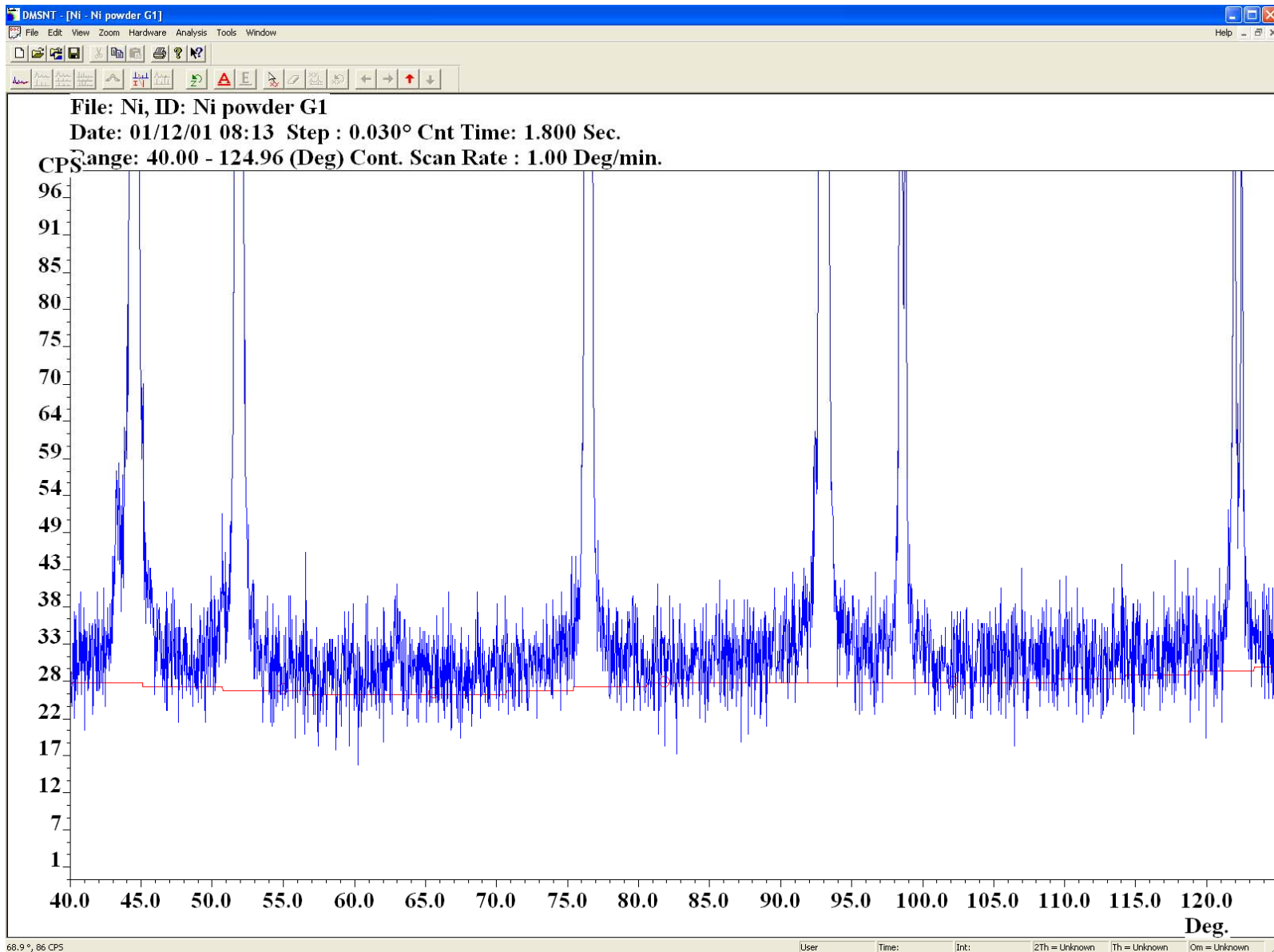


Figure 3 Background Correction - Cubic Spline Data Point Entry

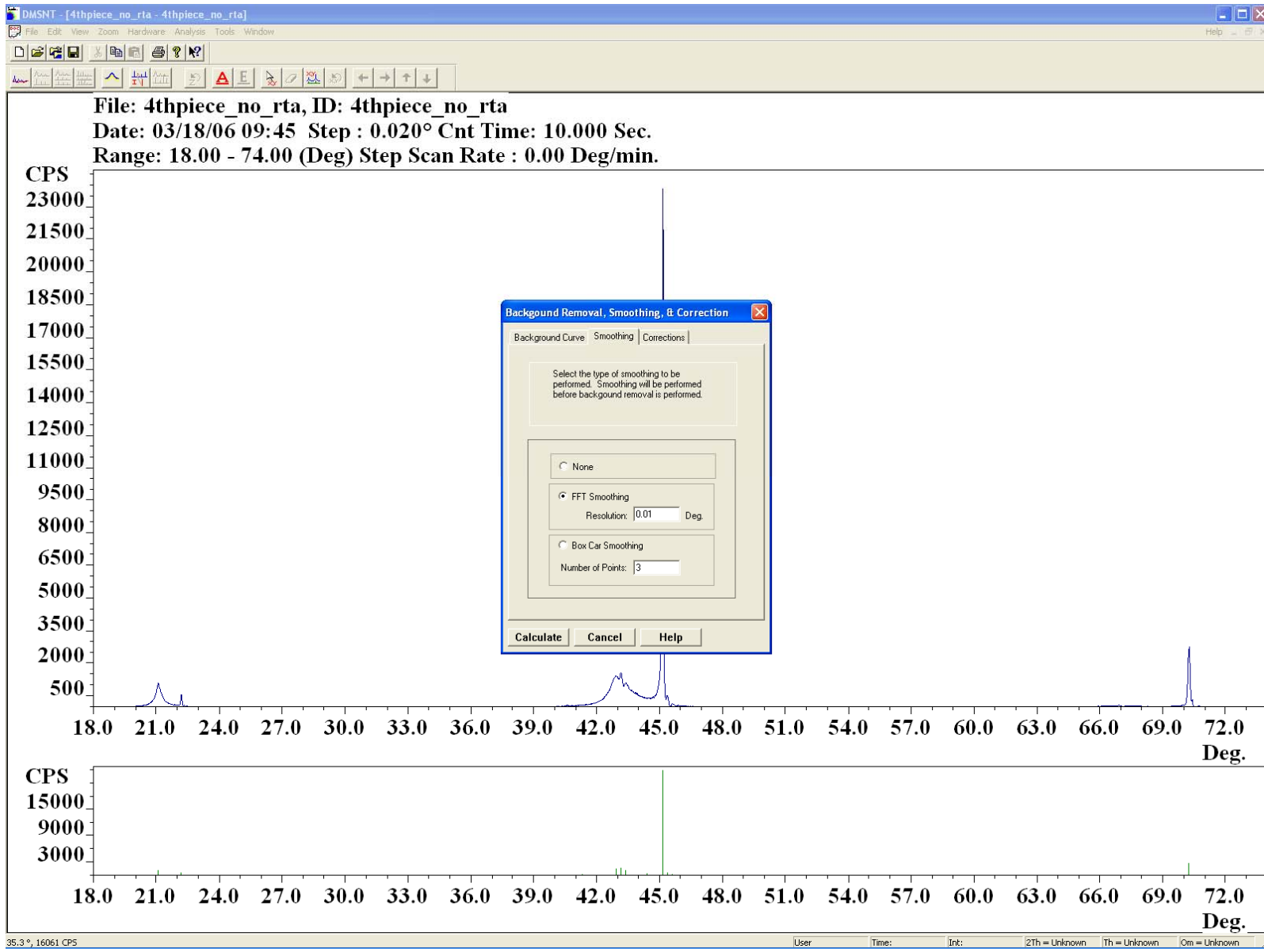


Figure 4 Background Correction - Smoothing Tab

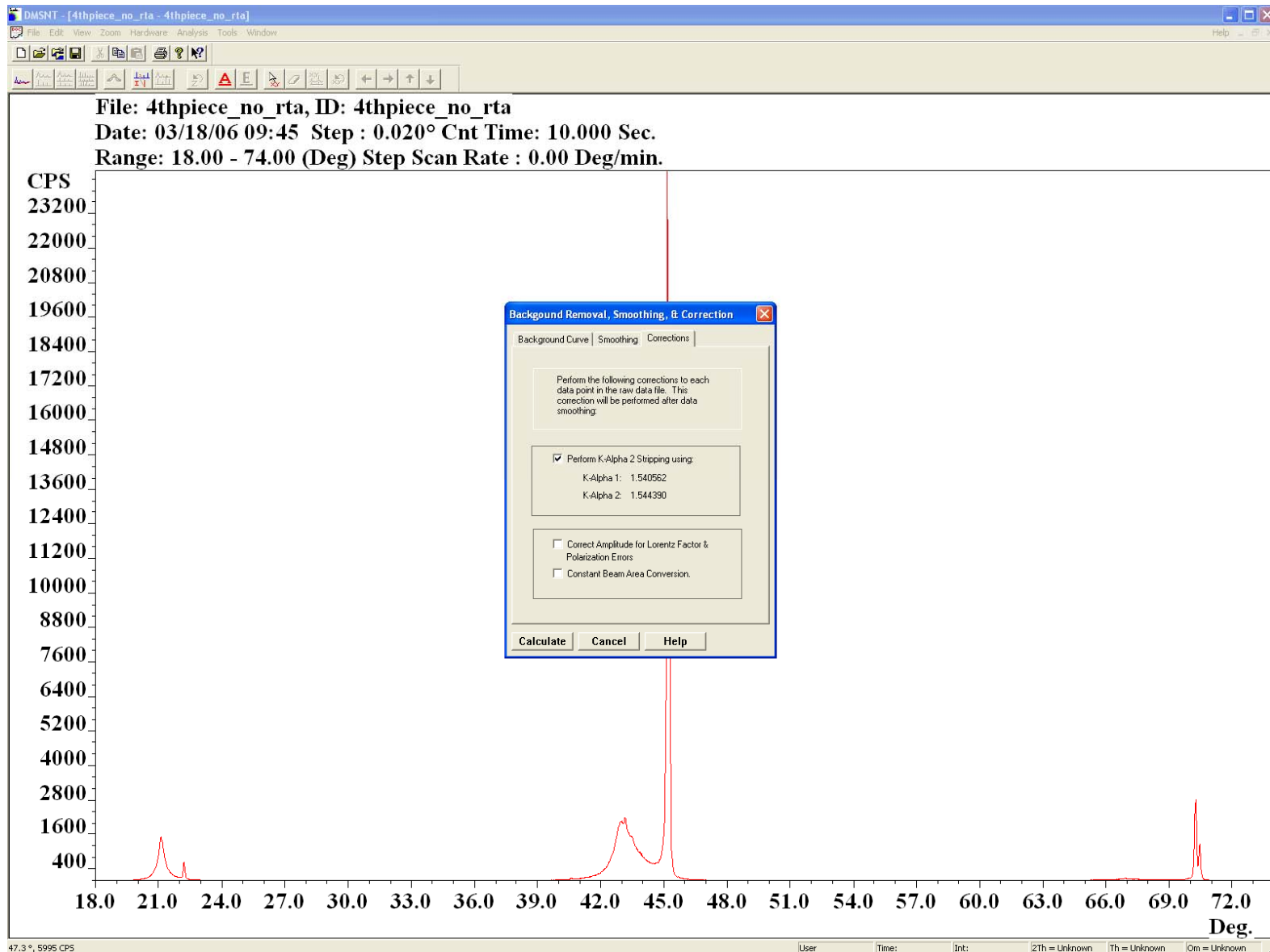


Figure 5 Background Correction - Corrections Tab

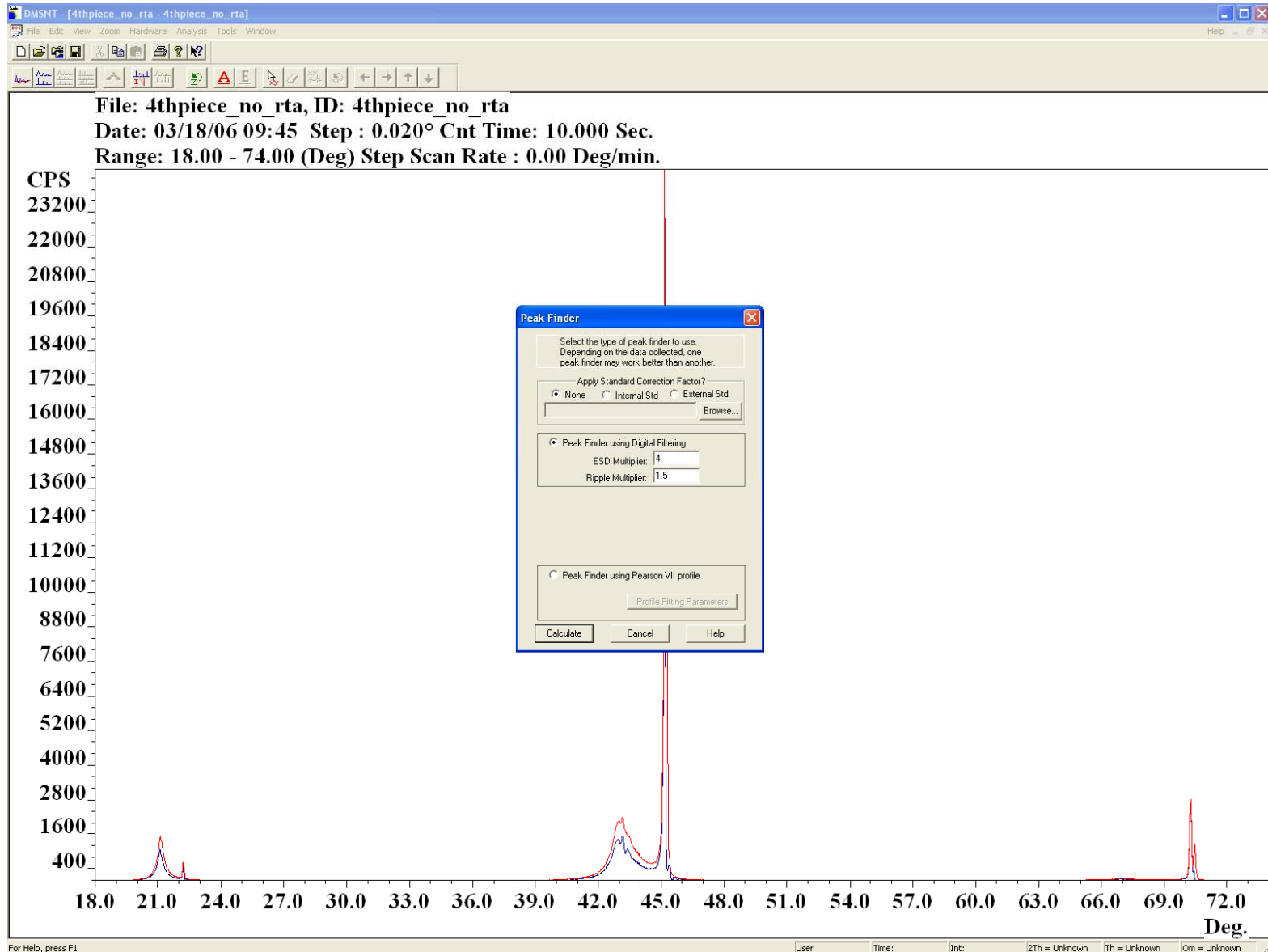


Figure 6 Peak Finder using Digital Filtering

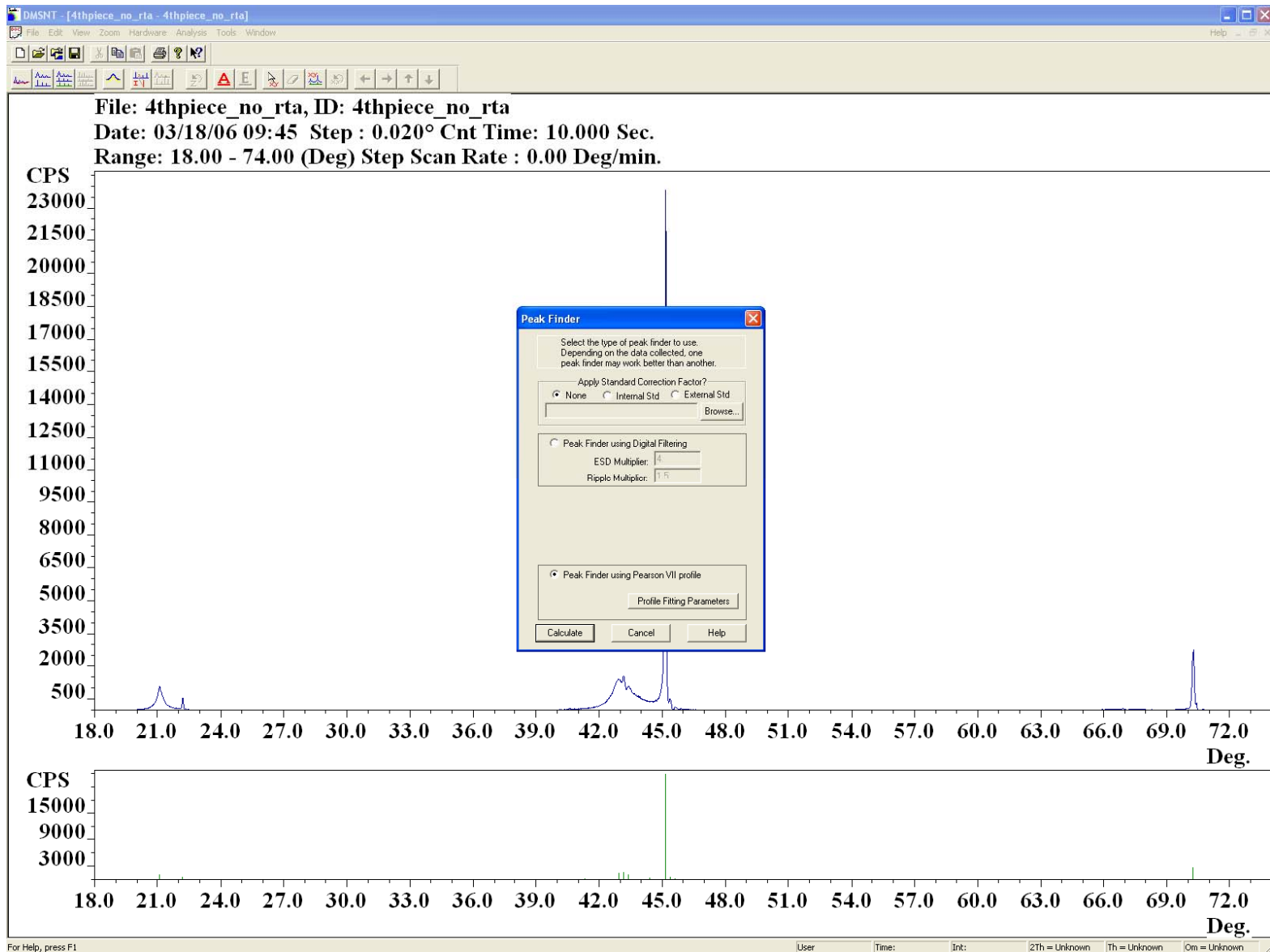


Figure 7 Peak Finder - Profile Fitting

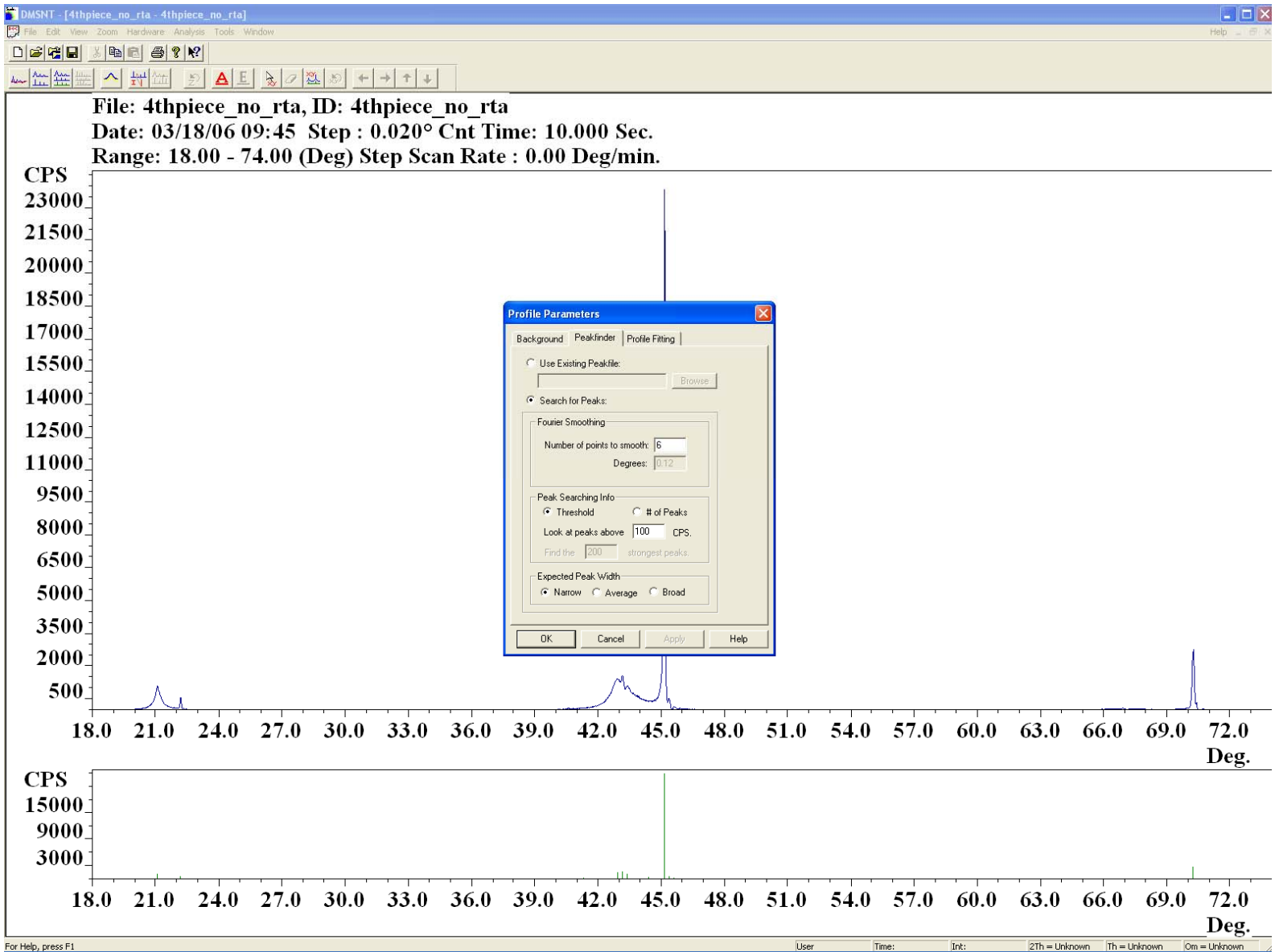


Figure 8 Peak Finder - Profile Fitting Parameters

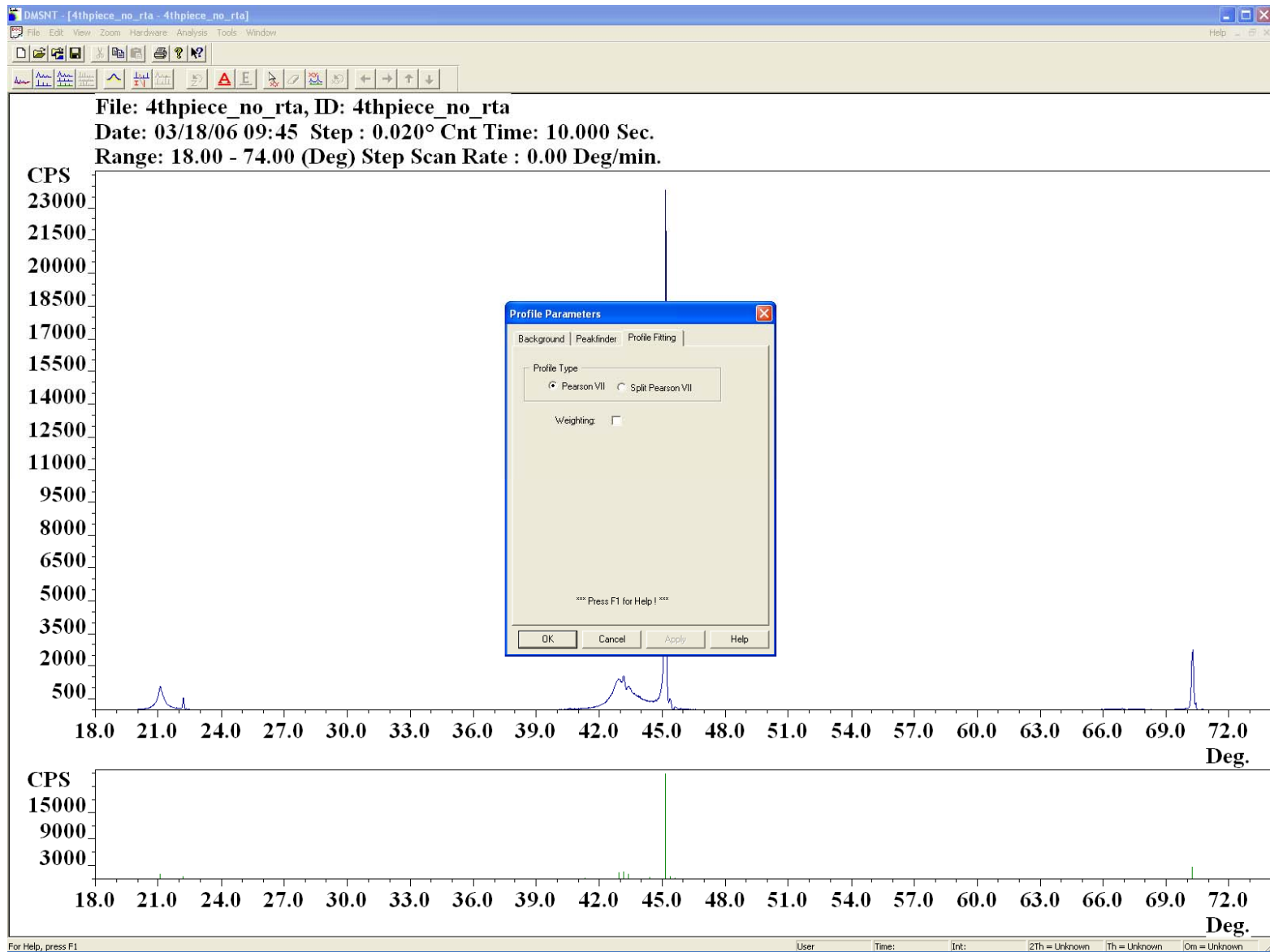


Figure 9 Peak Finder - Profile Fitting Functions



Figure 10 Exporting Peak File Information

Table 1 Peak File Text Output

ID: Ni powder G1

Comment:

Scan Type: Normal
 Start Angle: 40 deg.
 Stop Angle: 124.96 deg.
 Num Points: 2833
 Step Size: 0.03 deg.
 Datafile Res: 1600
 Scan Rate: 1.000000
 Scan Mode: Continuous
 Wavelength: 1.540562

Diffractometer Optics:

Tube: Type: Fixed Slits
 X2 Configuration: No
 Type: Fixed Slits
 X2 Configuration: No

Detector:

(Deg.)	Position (Deg.)	(DSp.)	ESD (Deg.)	Corr.Fact (Deg.)	Intensity (Deg.)	Rel. Int.	FWHM (L)			ESD	FWHM (R)			ESD	Area	Source	Curve
44.4995	2.0343	0.0004	0.0000	5154.24	100.00	0.0942	0.0010	0.0942	0.0000	1182.5	PFind	None	0.00	0.00	None		
51.8524	1.7618	0.0006	0.0000	2221.83	43.11	0.1017	0.0023	0.1017	0.0000	579.1	PFind	None	0.00	0.00	None		
63.0124	1.4740	0.0180	0.0000	12.79	0.25	0.0998	0.0244	0.0998	0.0000	5.6	PFind	None	0.00	0.00	None		
76.0133	1.2510	0.0182	0.0000	25.73	0.50	0.0664	1.9206	0.0000	0.0000	6.5	ProfF	Pear7	0.00	0.00	None		
76.3795	1.2459	0.0004	0.0000	968.81	18.80	0.1140	0.0014	0.0000	0.0000	220.6	ProfF	Pear7	0.00	0.00	None		
89.5389	1.0938	0.0195	0.0000	11.64	0.23	0.1003	0.0407	0.1003	0.0000	5.1	PFind	None	0.00	0.00	None		
92.9296	1.0625	0.0007	0.0000	1018.67	19.76	0.1268	0.0027	0.1268	0.0000	328.9	PFind	None	0.00	0.00	None		
98.4382	1.0173	0.0011	0.0000	266.82	5.18	0.1308	0.0041	0.1308	0.0000	90.9	PFind	None	0.00	0.00	None		
119.5950	0.8913	1.1469	0.0000	2.07	0.04	2.8910	2981032238.4899		0.0000	0.0000	31.1	ProfF	Pear7	0.00	0.00	None	None
121.9207	0.8810	0.0022	0.0000	137.36	2.67	0.1768	0.0082	0.0000	0.0000	50.6	ProfF	Pear7	0.00	0.00	None		

Strain CSize CSize Source (this is added to the headers moved here to save space).