
# The Slope Background for the near-peak regimen of photoemission spectra

**Alberto Herrera-Gomez**

CINVESTAV-Unidad Queretaro

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# Content

## The Slope Background for the near-peak regimen of photoemission spectra

- The various regions of the background: Si 2*p* example
- The total background as the sum of various terms
- The Slope Background
- The Slope Background in the Tougaard formalism
  - The near-peak regimen
  - The universal Tougaard cross sections
- Other examples:
  - Cr 2*p*
  - Comparison with Cr 2p simulated data from ***SESSA***
  - Au 4*f*
  - Sr 3*d*
- Application of the Slope Background to decaying intensities
  - C 1*s*
  - Au 4*d*
- Conclusions

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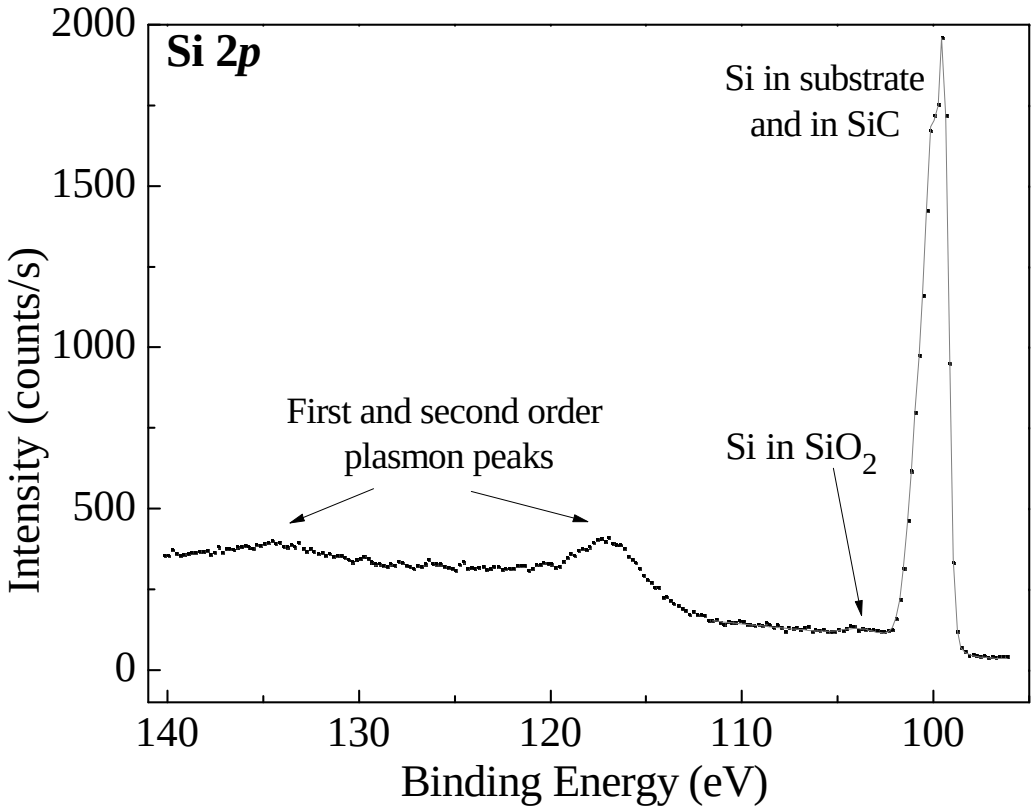
# The Si 2*p* example

The various regions of the background



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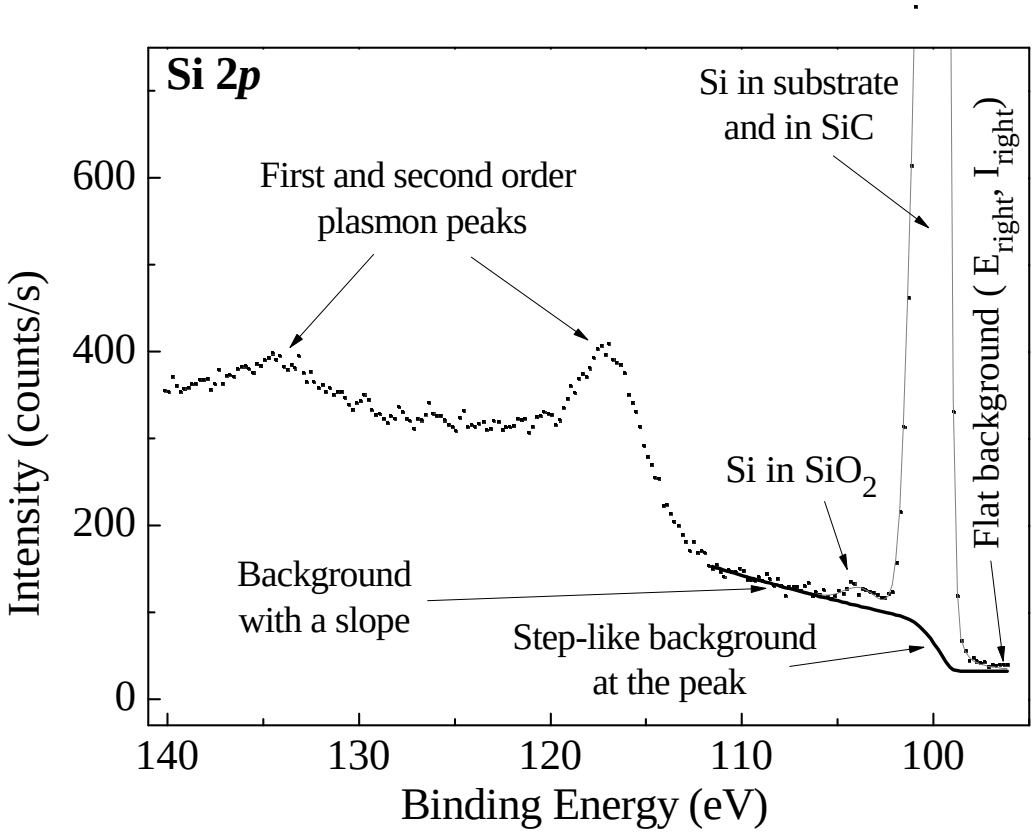
The various regions of the background



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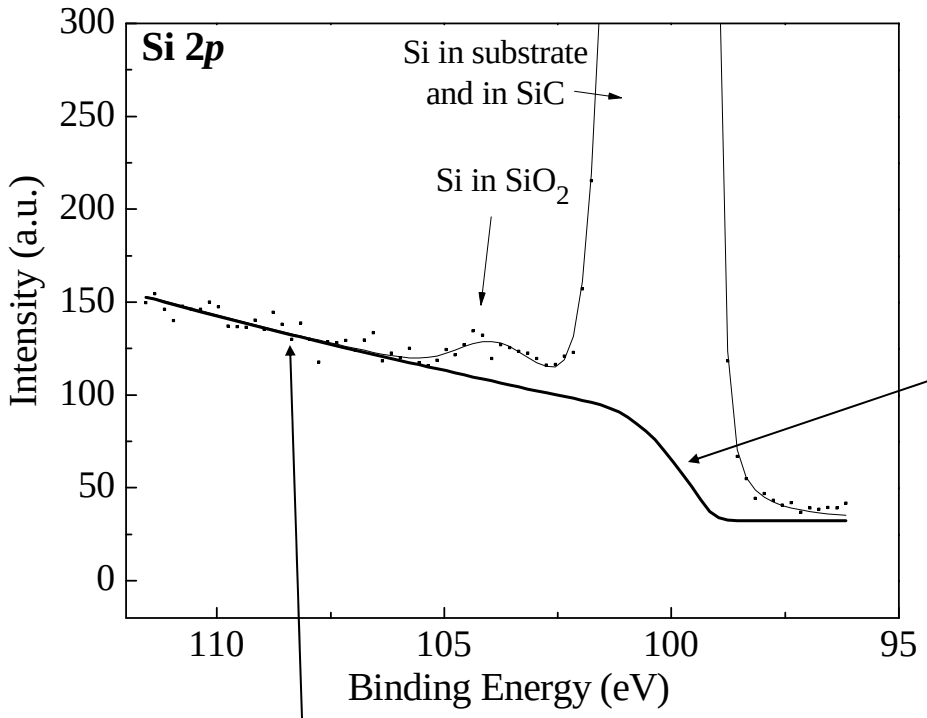


"Step" Background (Iterative Shirley-Sherwood)

"Slope" Background

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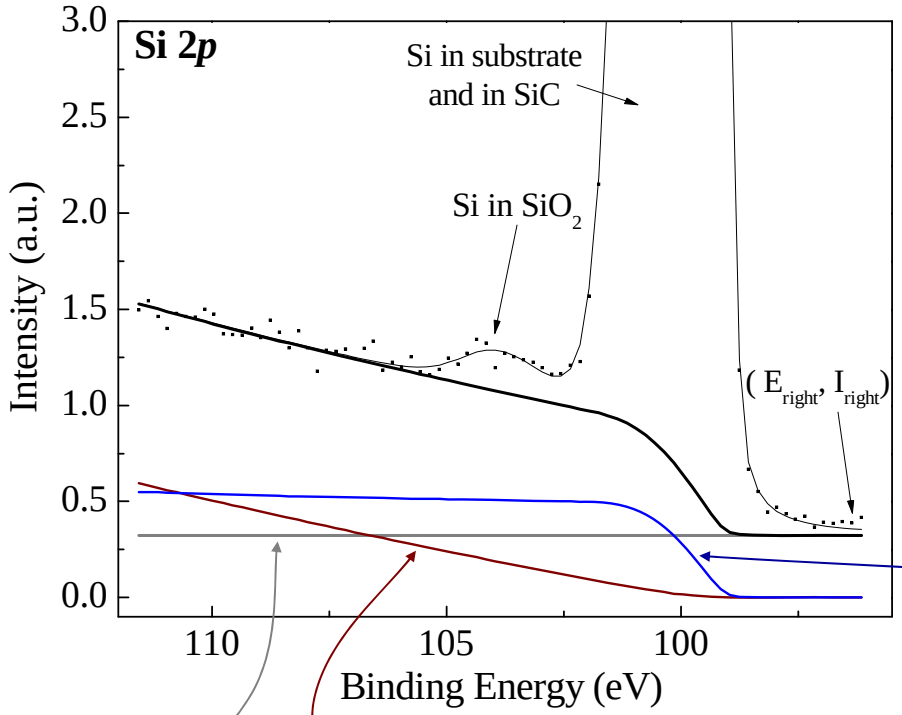
# The Si 2*p* example

The total background as a sum of various terms




Shirley-Sherwood Background

Baseline

Slope Background

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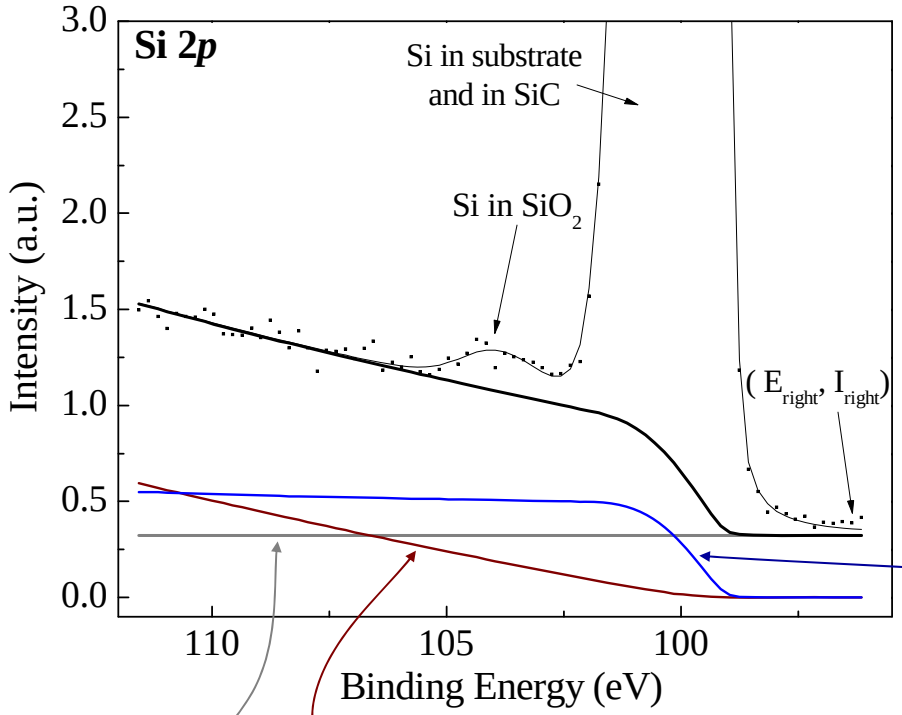
# The Si 2*p* example

The total background as a sum of various terms




Shirley-Sherwood Background

$$B_n(E) = k_n \int_E^{E_{\text{right}}} dE' \left[ I(E') - I_{\text{right}} - B_{n-1}(E') \right]$$

Baseline

Slope Background

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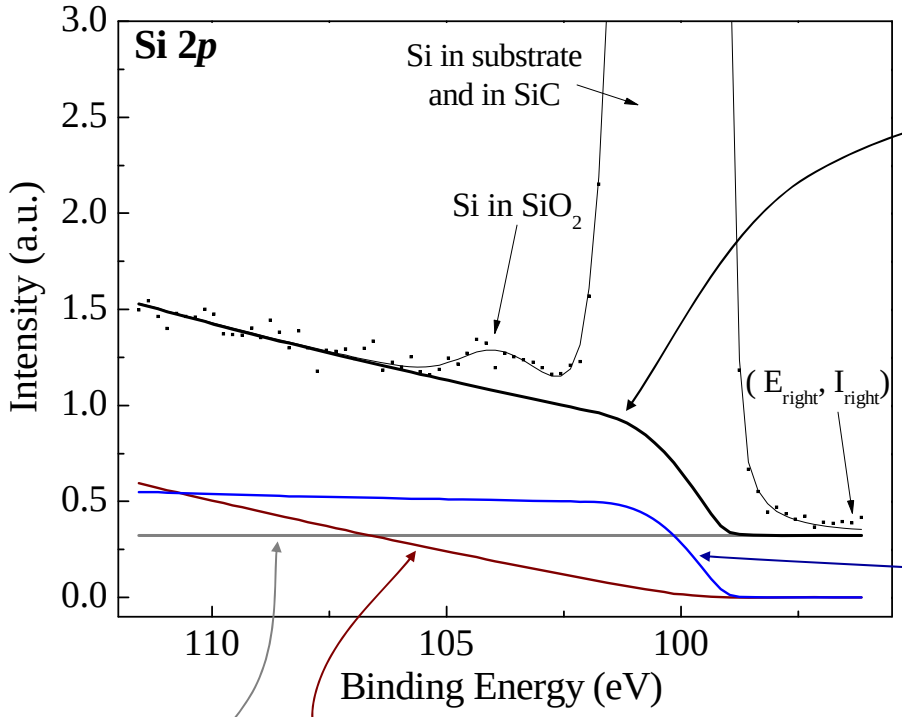
# The Si 2*p* example

The total background as a sum of various terms




Total Background =

- Baseline +
- Iterative Shirley +
- Slope

Shirley-Sherwood Background

$$B_n(E) = k_n \int_E^{E_{\text{right}}} dE' \left[ I(E') - I_{\text{right}} - B_{n-1}(E') \right]$$

Baseline

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# The Si 2*p* example

The Slope Background

Slope Background

$$\frac{dB_S(E)}{dE} = -k_S \int_{E+\Delta}^{E_{\text{right}}} dE' \left[ I(E') - I_{\text{right}} \right]$$

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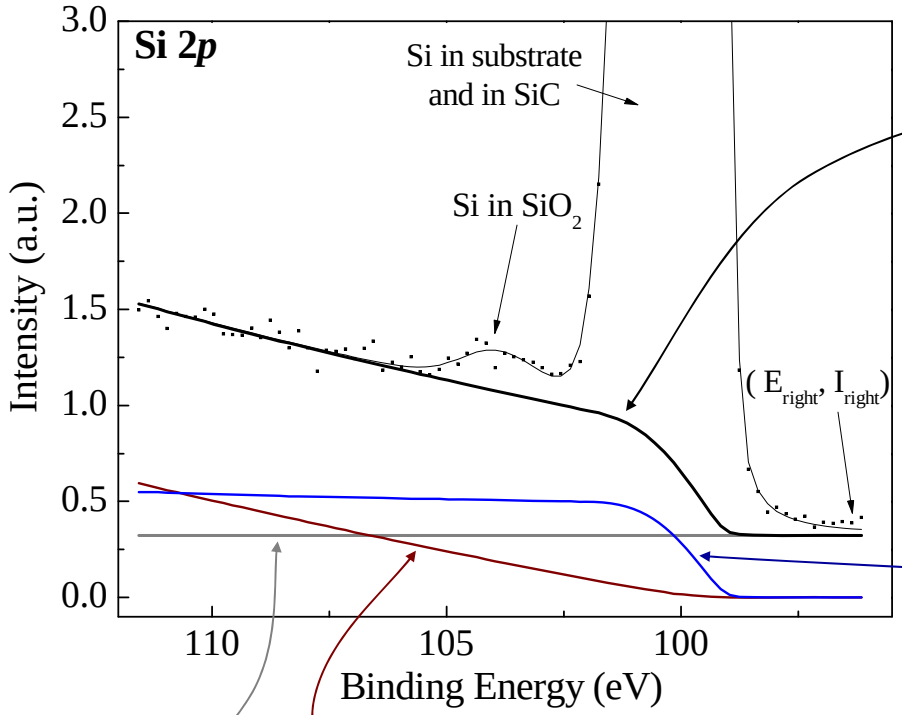
The Slope Background

# The Si 2*p* example




Total Background =

- Baseline +
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Shirley-Sherwood Background

$$B_n(E) = k_n \int_{E}^{E_{\text{right}}} dE' \left[ I(E') - I_{\text{right}} - B_{n-1}(E') \right]$$

Baseline

Slope Background

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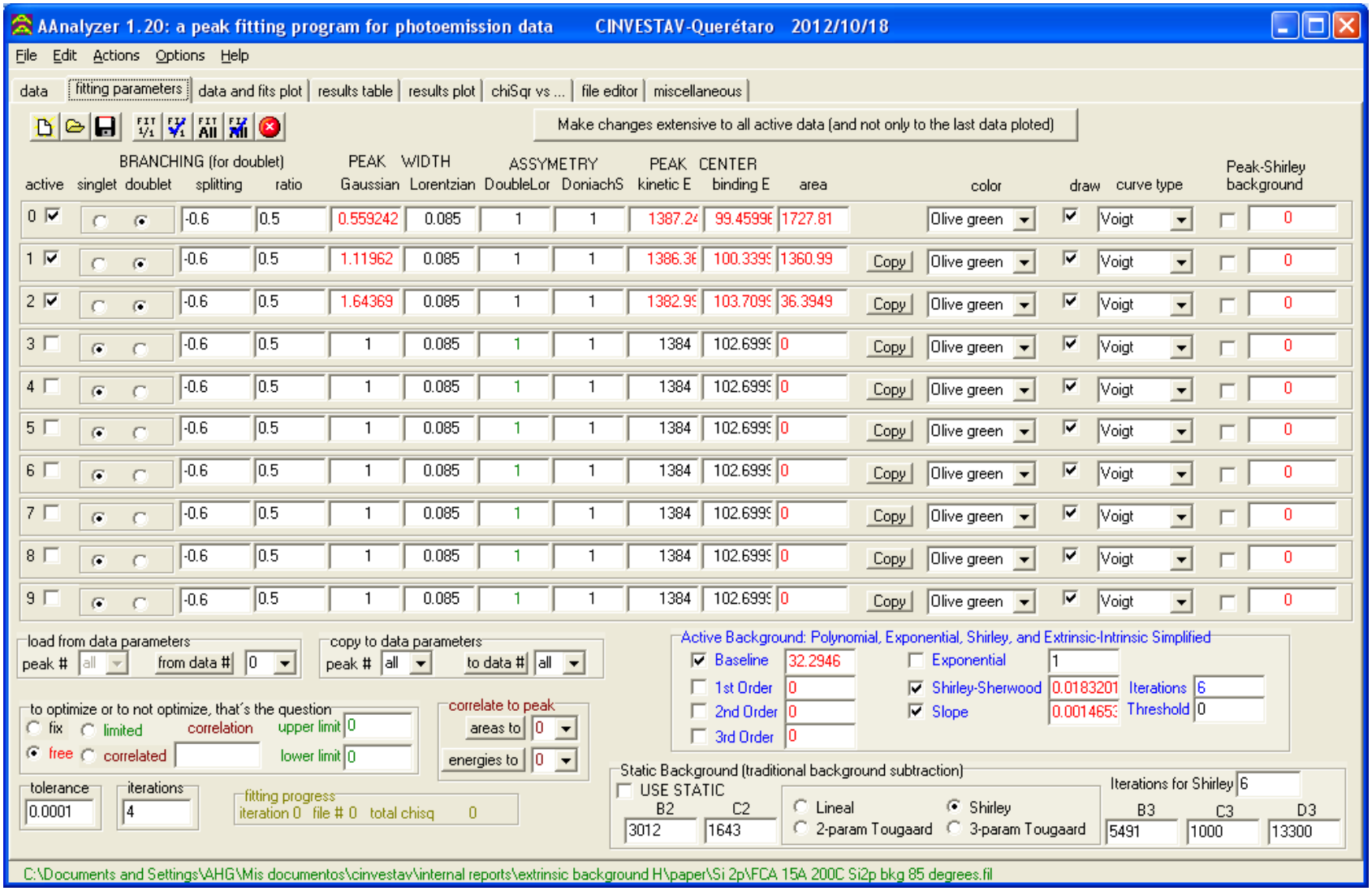

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The Slope Background

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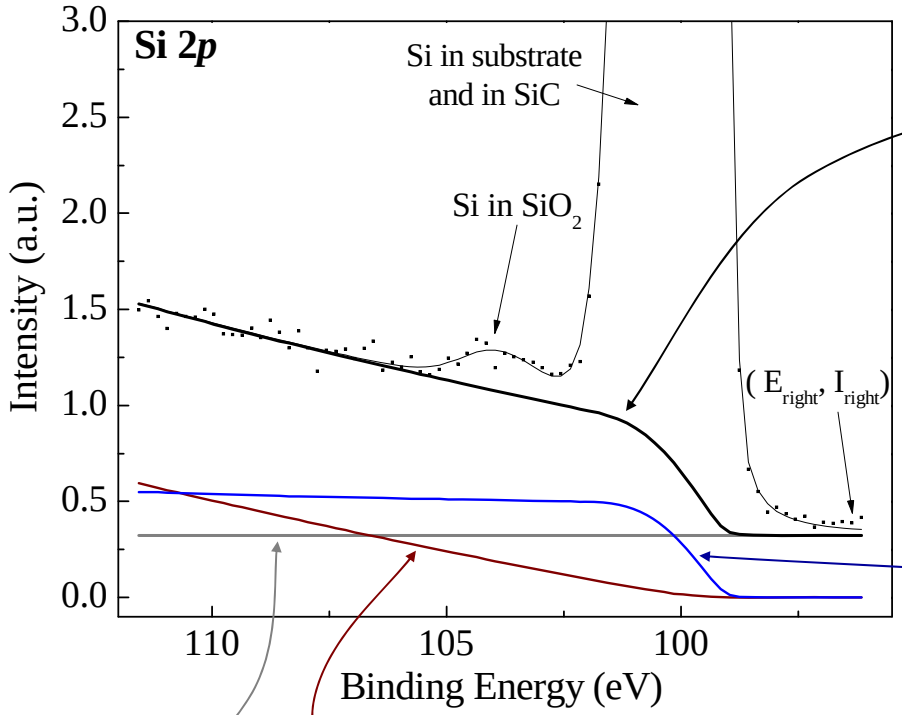


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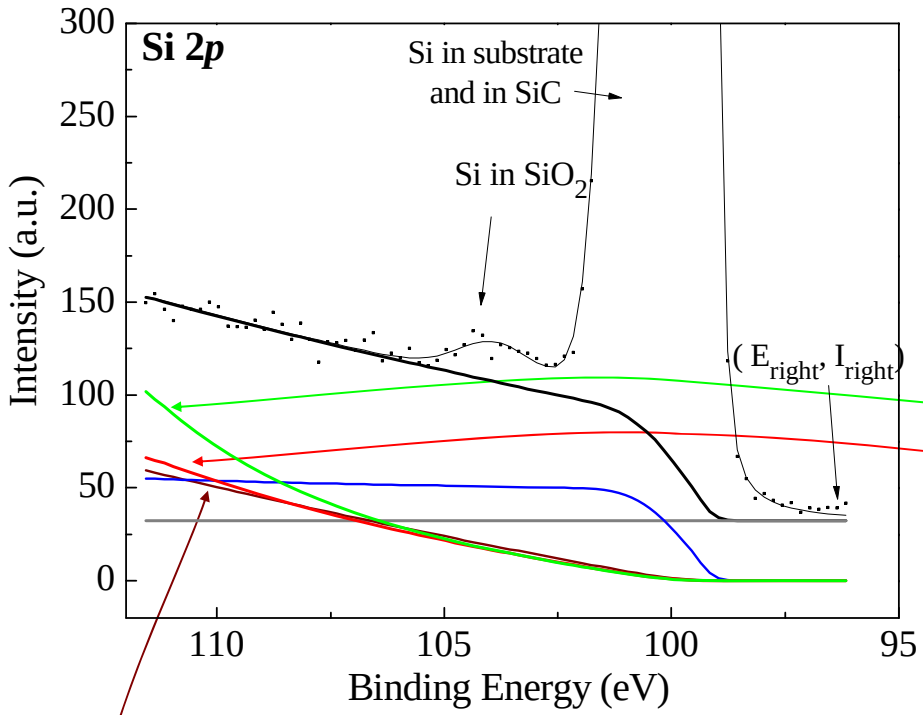
The Slope Background in the Tougaard formalism

## The near-peak regimen




Tougaard: 3 param Si

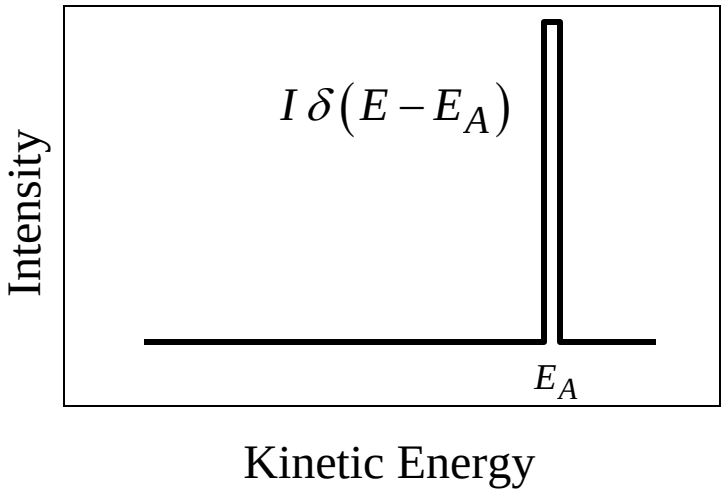
Tougaard: 3 param Polymer

Slope Background

$$\frac{dB_S(E)}{dE} = -k_S \int_{E+\Delta}^{E_{\text{right}}} dE' \left[ I(E') - I_{\text{right}} \right]$$

## The near-peak regimen

Tougaard Formalism for the electron flux in the near-peak regimen




* S. Tougaard and P. Sigmund. Phys. Rev. B 25, 4452 (1982).

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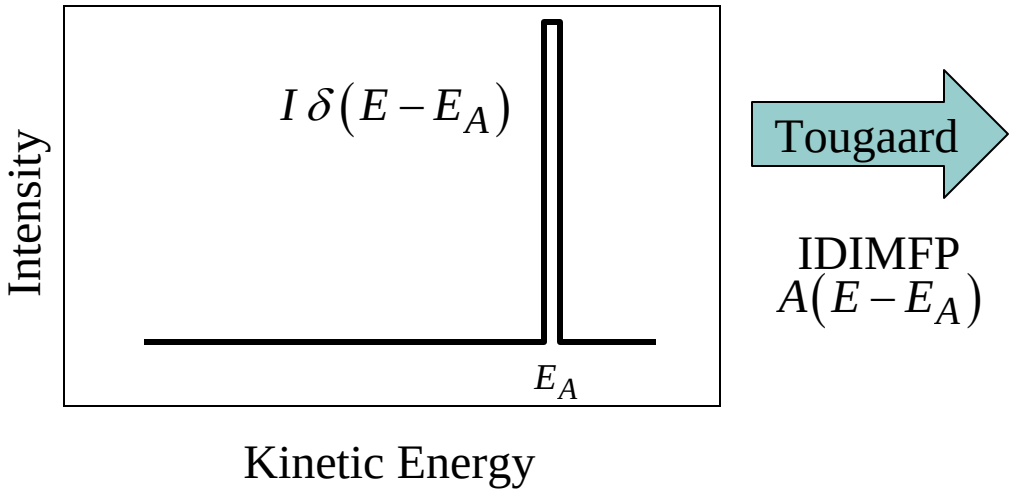


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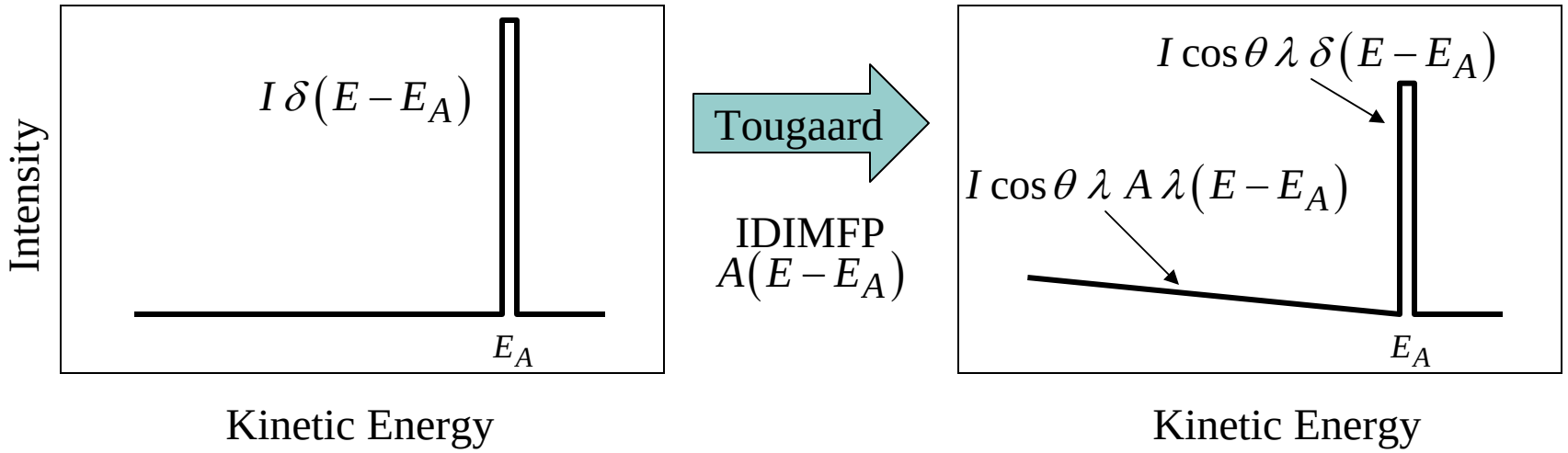


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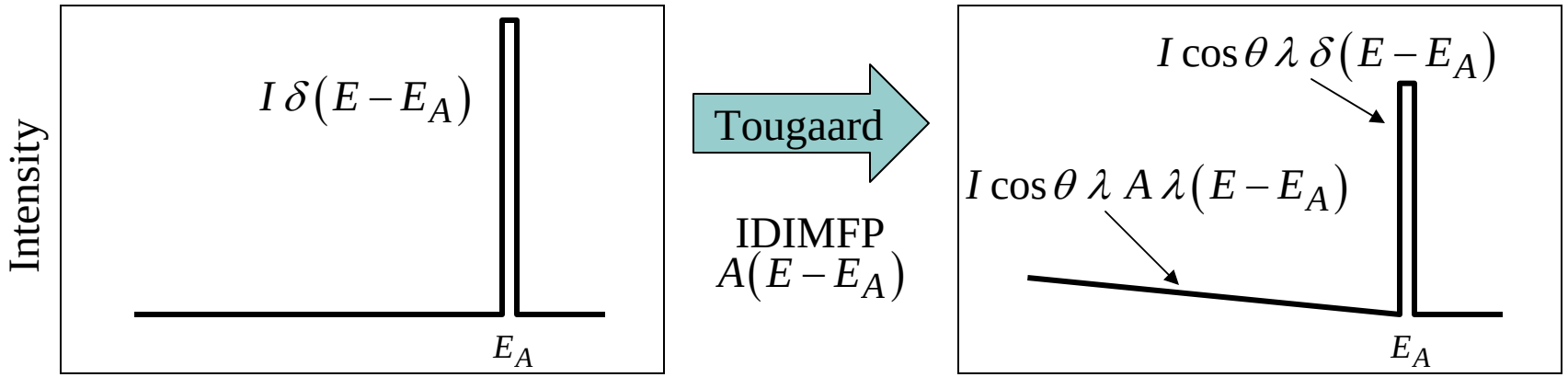


$$J(E,\Omega) \simeq I\cos\theta\,\lambda\left[\delta(E-E_A)+A\,\lambda(E-E_A)+\ldots\right]$$

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## The near-peak regimen

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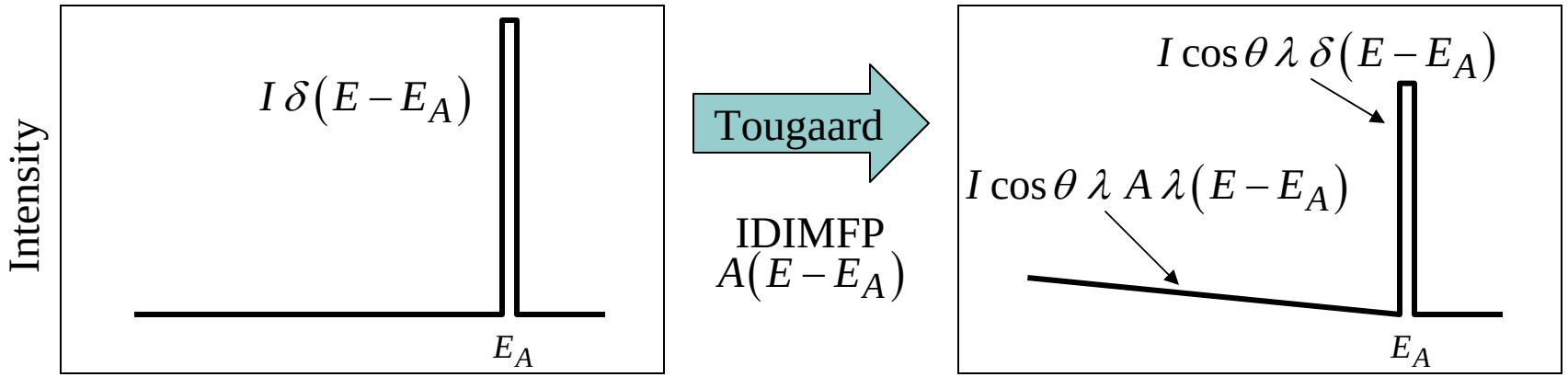


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$$\frac{dB_{NP}(E,\Omega)}{dE} = -\lambda\,A\int_{E}^{\infty} dE_A\, I_P(E_A,\Omega)$$

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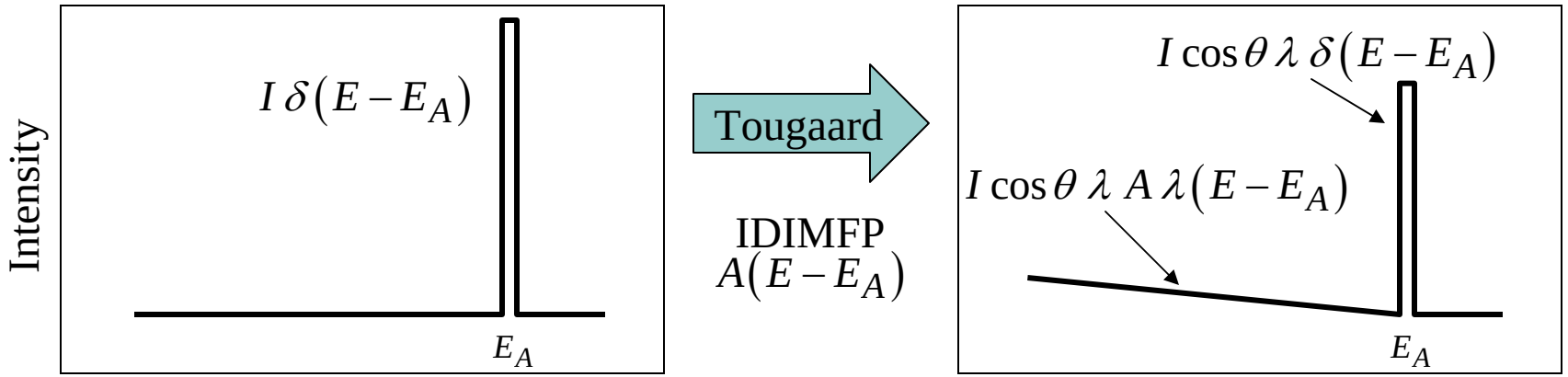


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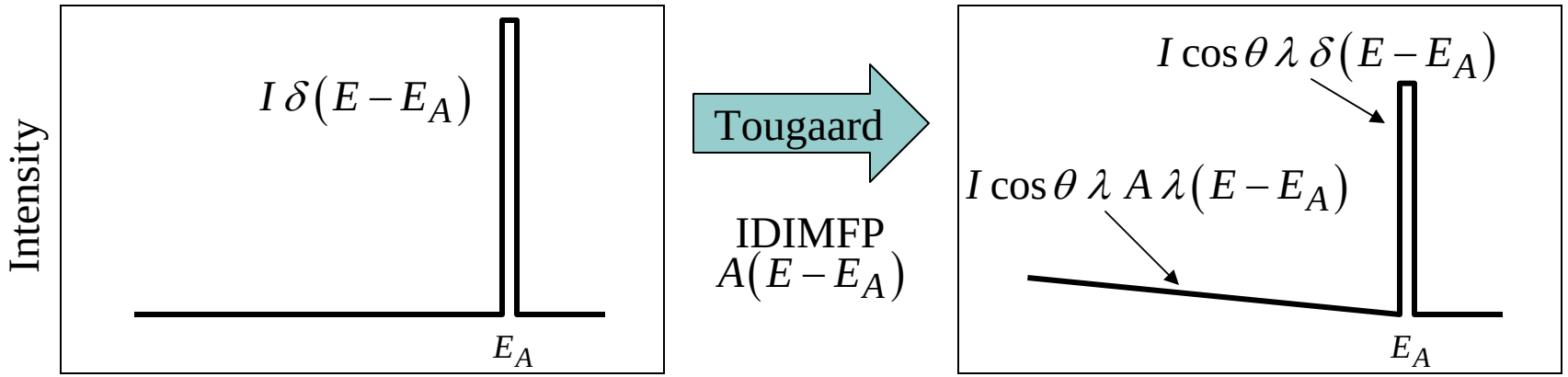


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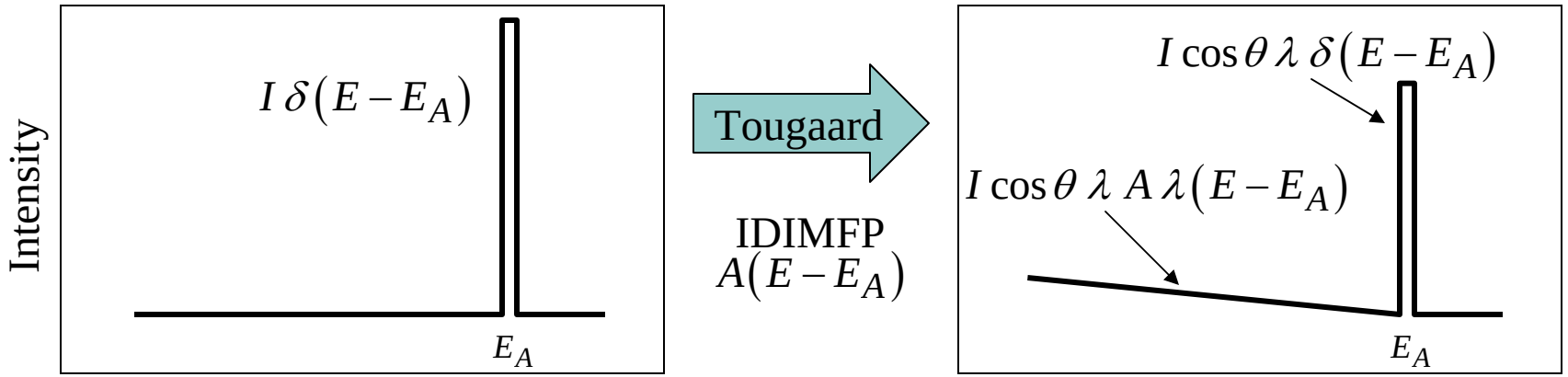


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$$\frac{dB_S(E)}{dE} = -k_S\int_{E+\Delta}^{E_{\text{right}}} dE'\left[I(E')-I_{\text{right}}\right],$$

The Slope Background is identical to the near-peak regimen of the Tougaard Background

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The Slope Background in the Tougaard formalism

## Comparison with the practical Universal Tougaard Backgrounds

$$B_{\text{2P-T}}(E) = \int_{E}^{E_{\text{right}}} dE' \frac{B(E'-E)}{\left[(E'-E)^2 + C\right]^2}\left[I(E') - I_{\text{right}}\right]$$

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The Slope Background in the Tougaard formalism

## Comparison with the practical Universal Tougaard Backgrounds

$$B_{\text{2P-T}}(E) = \int_{E}^{E_{\text{right}}} dE' \frac{B(E'-E)}{\left[(E'-E)^2 + C\right]^2}\left[I(E') - I_{\text{right}}\right]$$

$$\frac{dB_{\text{2P-T}}(E)}{dE} \sim -\frac{B}{C^2}\int_{E}^{E_{\text{right}}} dE'\left[I(E') - I_{\text{right}}\right]$$

## Comparison with the practical Universal Tougaard Backgrounds

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## Comparison with the practical Universal Tougaard Backgrounds

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$$\frac{dB_S(E)}{dE} = -k_S \int_{E+\Delta}^{E_{\text{right}}} dE'\left[I(E') - I_{\text{right}}\right],$$

$k_S \sim \frac{B}{C^2}$ for ***both*** the two- and the three-parameters Tougaard Background

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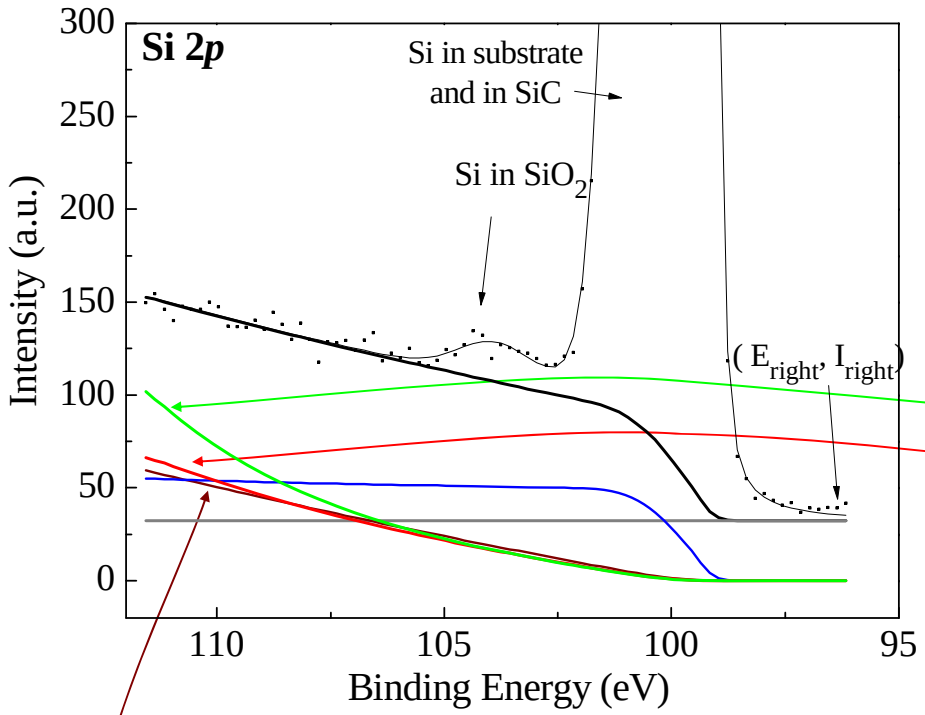
The Slope Background in the Tougaard formalism

## Comparison with the practical Universal Tougaard Backgrounds




Tougaard: 3 param Si

Tougaard: 3 param Polymer

Slope Background

$0.0014 / eV^2$

$$\frac{dB_S(E)}{dE} = -k_S \int_{E+\Delta}^{E_{\text{right}}} dE' \left[ I(E') - I_{\text{right}} \right],$$

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The Slope Background in the Tougaard formalism

# Comparison with the practical Universal Tougaard Backgrounds

AAnalyzer 1.20: a peak fitting program for photoemission data  CINVESTAV-Querétaro  2012/10/18

File  Edit  Actions  Options  Help

data | fitting parameters | data and fits plot | results table | results plot | chiSqr vs ... | file editor | miscellaneous

Make changes extensive to all active data (and not only to the last data ploted)

| active | singlet | doublet | BRANCHING (for doublet) splitting | ratio | PEAK Gaussian | WIDTH Lorentzian | ASSYMETRY DoubleLor | DoniachS | PEAK CENTER kinetic E | binding E | area | | color | draw | curve type | Peak-Shirley background |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | | | -0.6 | 0.5 | 0.559242 | 0.085 | 1 | 1 | 1387.24 | 99.4599 | 1727.81 | | Olive green | | Voigt | 0 |
| 1 | | | -0.6 | 0.5 | 1.11962 | 0.085 | 1 | 1 | 1386.36 | 100.339 | 1360.99 | Copy | Olive green | | Voigt | 0 |
| 2 | | | -0.6 | 0.5 | 1.64369 | 0.085 | 1 | 1 | 1382.99 | 103.709 | 36.3949 | Copy | Olive green | | Voigt | 0 |
| 3 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |
| 4 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |
| 5 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |
| 6 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |
| 7 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |
| 8 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |
| 9 | | | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.699 | 0 | Copy | Olive green | | Voigt | 0 |

load from data parameters: peak # all  from data # 0

copy to data parameters: peak # all  to data # all

Active Background: Polynomial, Exponential, Shirley, and Extrinsic-Intrinsic Simplified

Baseline 32.2946 | Exponential 1

1st Order 0 | Shirley-Sherwood 0.0183201 | Iterations 6

2nd Order 0 | Slope 0.0014653 | Threshold 0

3rd Order 0

to optimize or to not optimize, that´s the question: fix / free; limited / correlated; correlation; upper limit 0; lower limit 0

correlate to peak: areas to 0; energies to 0

tolerance 0.0001  iterations 4

fitting progress: iteration 0  file # 0  total chisq 0

Static Background (traditional background subtraction)

USE STATIC

B2 3012  C2 1643

Lineal / Shirley-Sherwood / 2-param Tougaard / 3-param Tougaard

Iterations for Shirley-Sherwood 6

B3 5491  C3 1000  D3 13300

C:\Documents and Settings\AHG\Mis documentos\cinvestav\internal reports\extrinsic background H\paper\Si 2p\FCA 15A 200C Si2p bkg 85 degrees.fil

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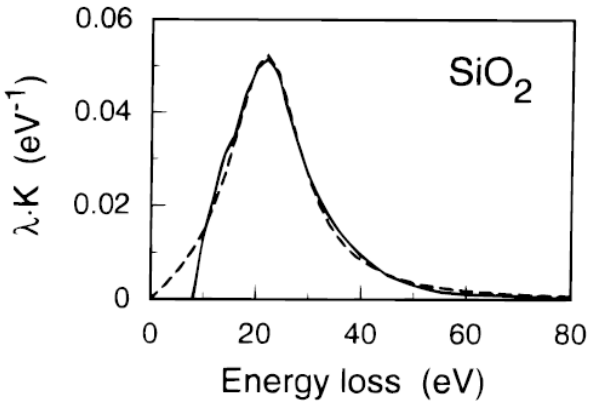
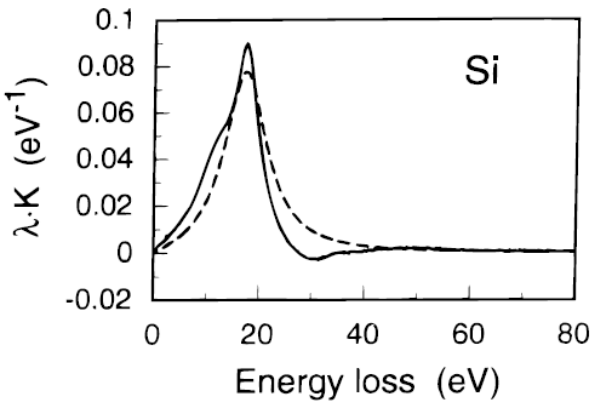
# Comparison with the practical Universal Tougaard Backgrounds

$$k_S = 0.0014$$



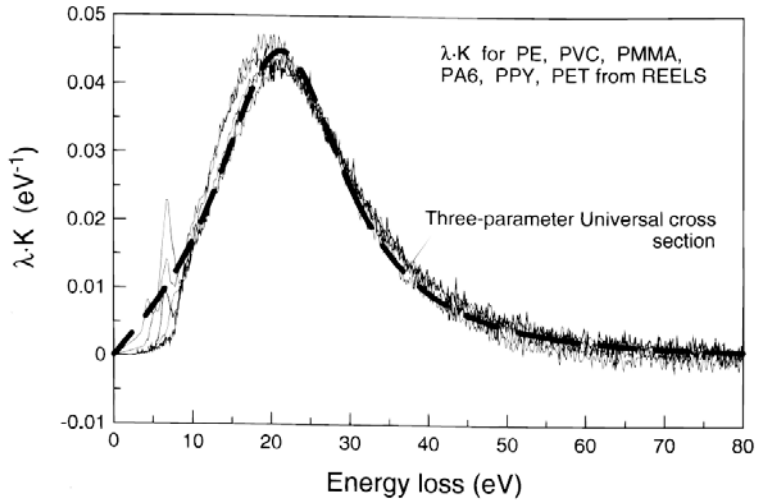




**Table 1. Parameters for the Universal cross-sections in Eqns (5) and (6)[a]**

| Class of materials | $B$ (eV²) | $B^N$ (eV²) | $C$ (eV²) | $D$ (eV²) |
|---|---|---|---|---|
| *Universal cross-section* [*Eqn* (*5*)] | | | | |
| Metals and their oxides | 2866 | 3286 | 1643 | — |
| *Three-parameter Universal cross-section* [*Eqn* (*6*)] | | | | |
| Polymers | 434 | 396 | 551 | 436 |
| Silicon dioxide | 325 | 299 | 542 | 275 |
| Silicon | 132 | 131 | 325 | 96 |
| Germanium | 73 | 93 | 260 | 62 |
| Aluminum | 16.5 | 21.4 | 230 | 4.5 |

[a] $B^N$ is the value of $B$ for which the cross-section is normalized. Some of the cross-sections are plotted in Fig. 16.

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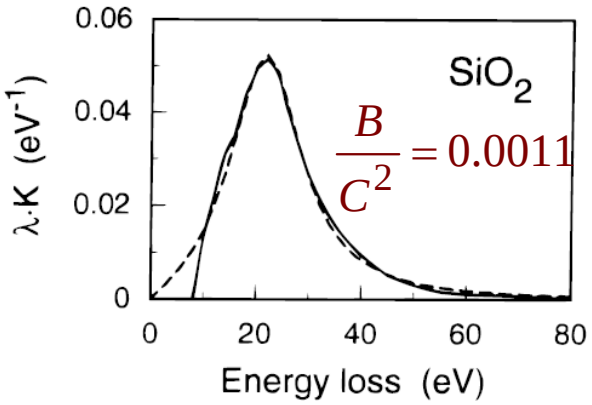
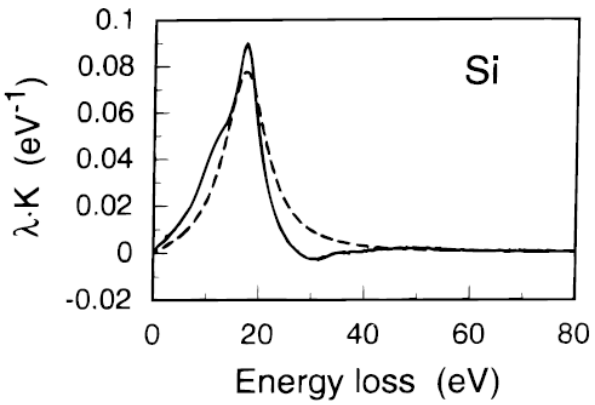
# Comparison with the practical Universal Tougaard Backgrounds

$$k_S = 0.0014$$



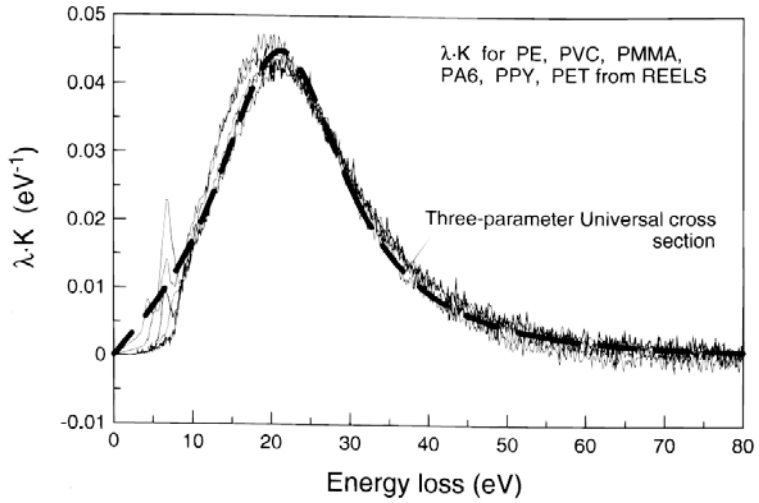




**Table 1. Parameters for the Universal cross-sections in Eqns (5) and (6)[a]**

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| Silicon dioxide | 325 | 299 | 542 | 275 |
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[a] $B^N$ is the value of $B$ for which the cross-section is normalized. Some of the cross-sections are plotted in Fig. 16.

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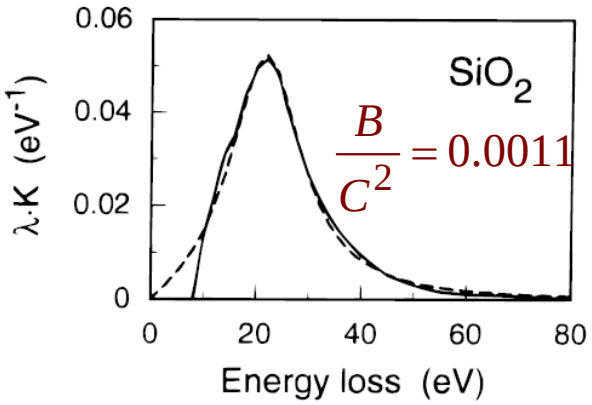
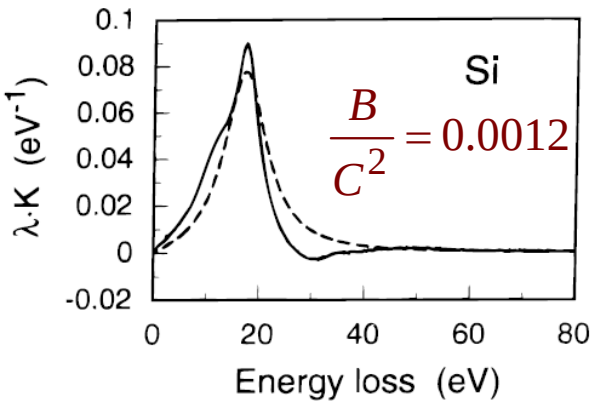
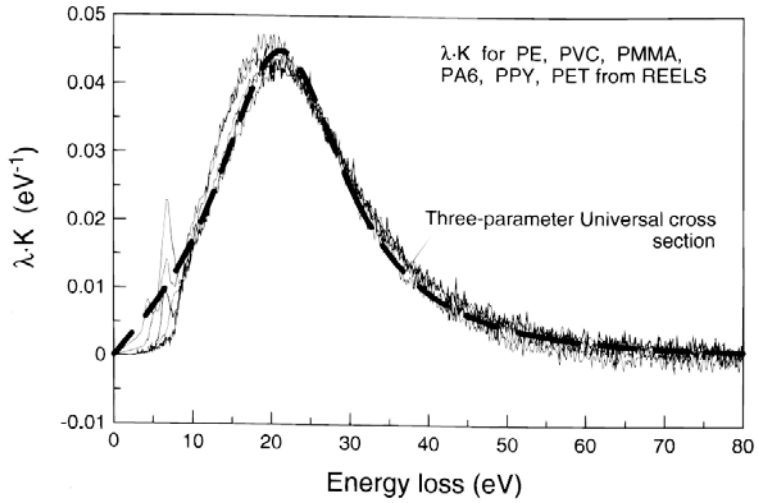
The Slope Background in the Tougaard formalism

# Comparison with the practical Universal Tougaard Backgrounds

$$k_S = 0.0014$$

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# Comparison with the practical Universal Tougaard Backgrounds

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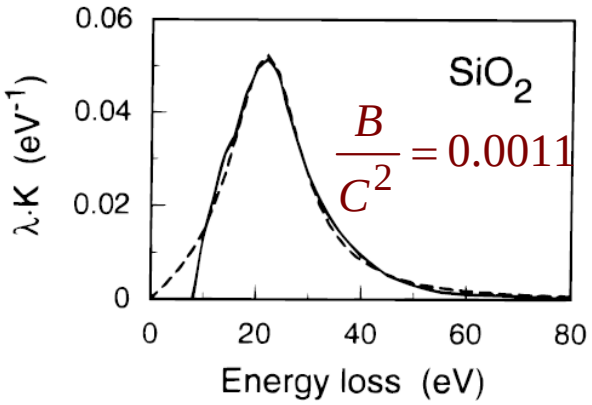


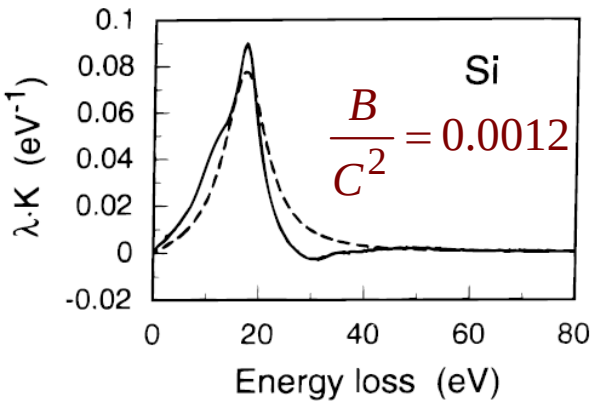


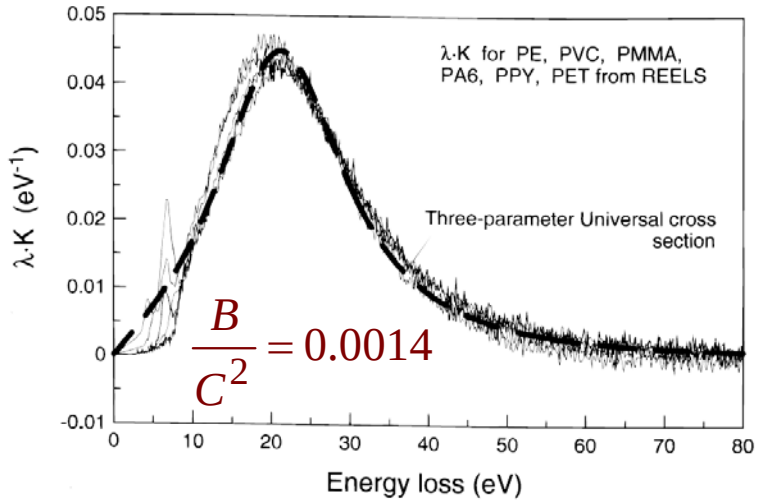


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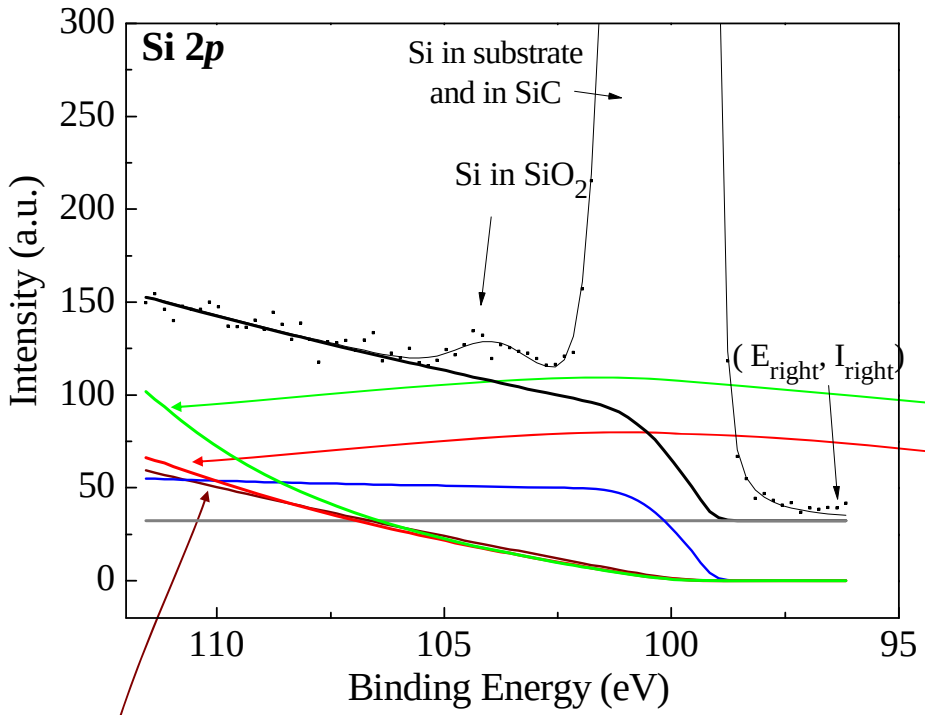
The Slope Background in the Tougaard formalism

## Comparison with the practical Universal Tougaard Backgrounds




Tougaard: 3 param Si

Tougaard: 3 param Polymer

$$\frac{B}{C^2} = 0.0014 / \mathrm{eV}^2$$

$0.0014 / \mathrm{eV}^2$

Slope Background

$$\frac{dB_S(E)}{dE} = -k_S \int_{E+\Delta}^{E_{\mathrm{right}}} dE' \left[ I(E') - I_{\mathrm{right}} \right]$$

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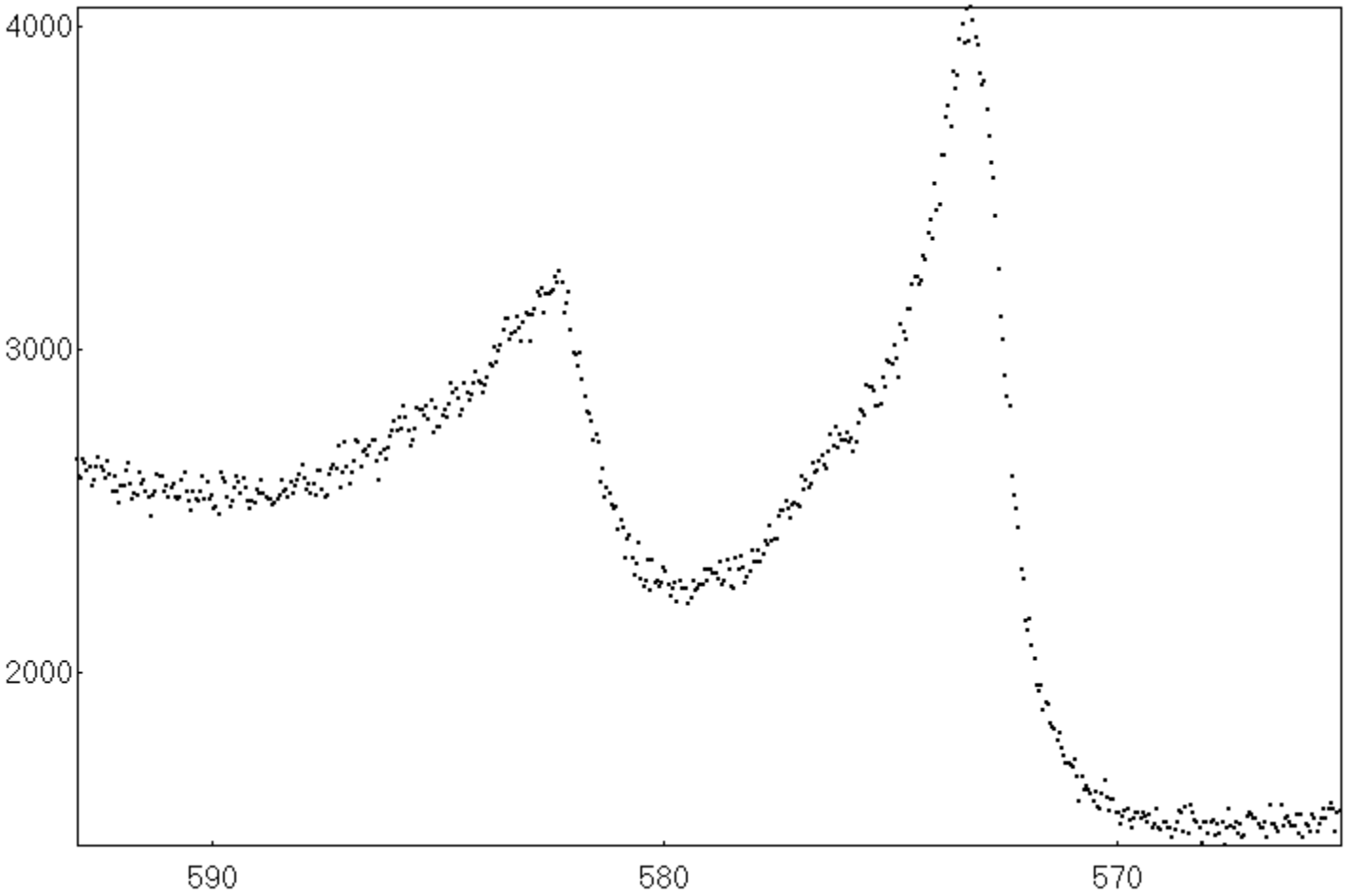
# Cr 2*p*



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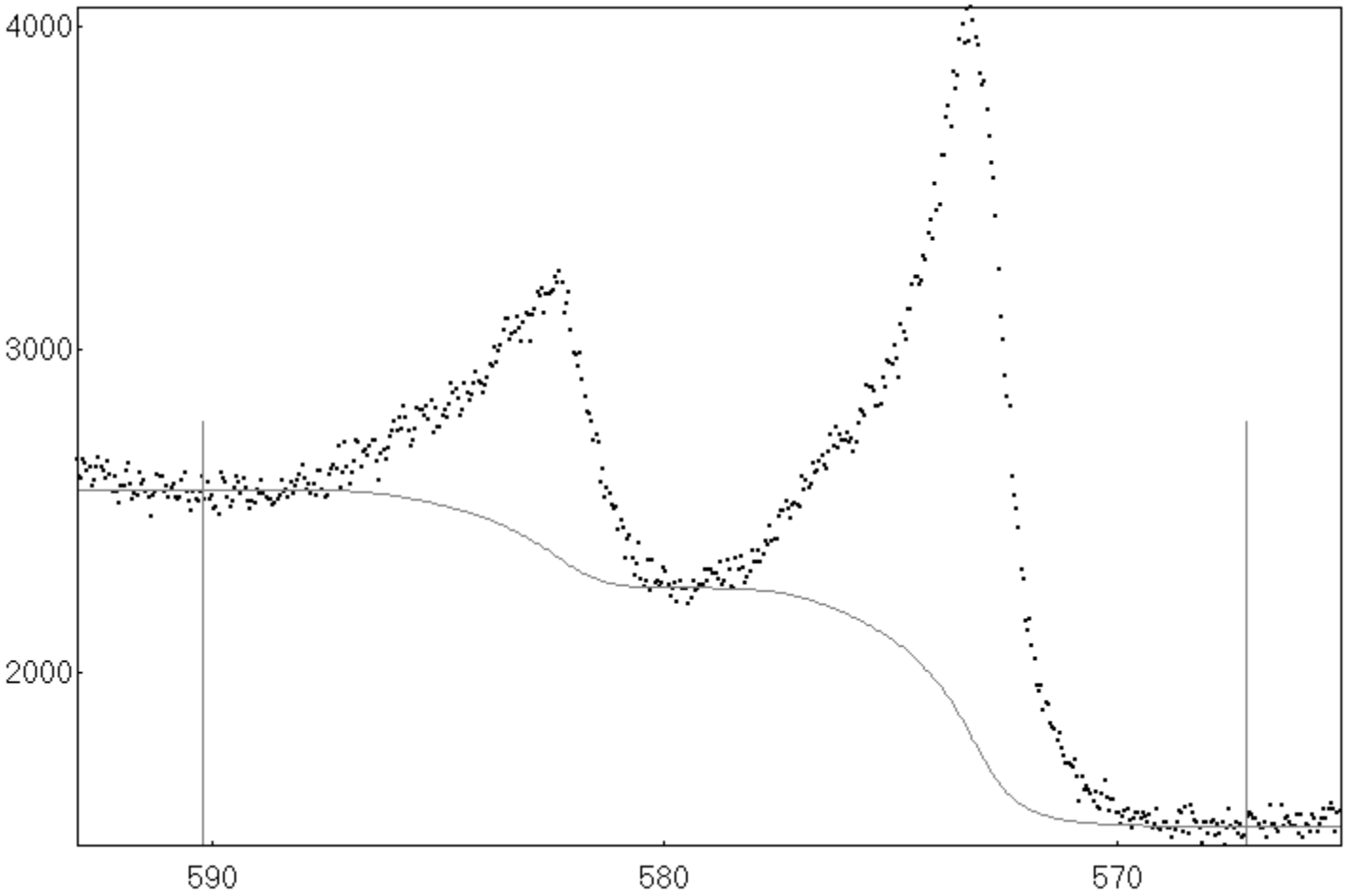
Other Examples

## Cr 2*p*

Iterative Shirley-Sherwood Background




$$B_n(E) = k_n \int_E^{E_\infty} dE' \left[ I(E') - B_{n-1}(E') \right]$$

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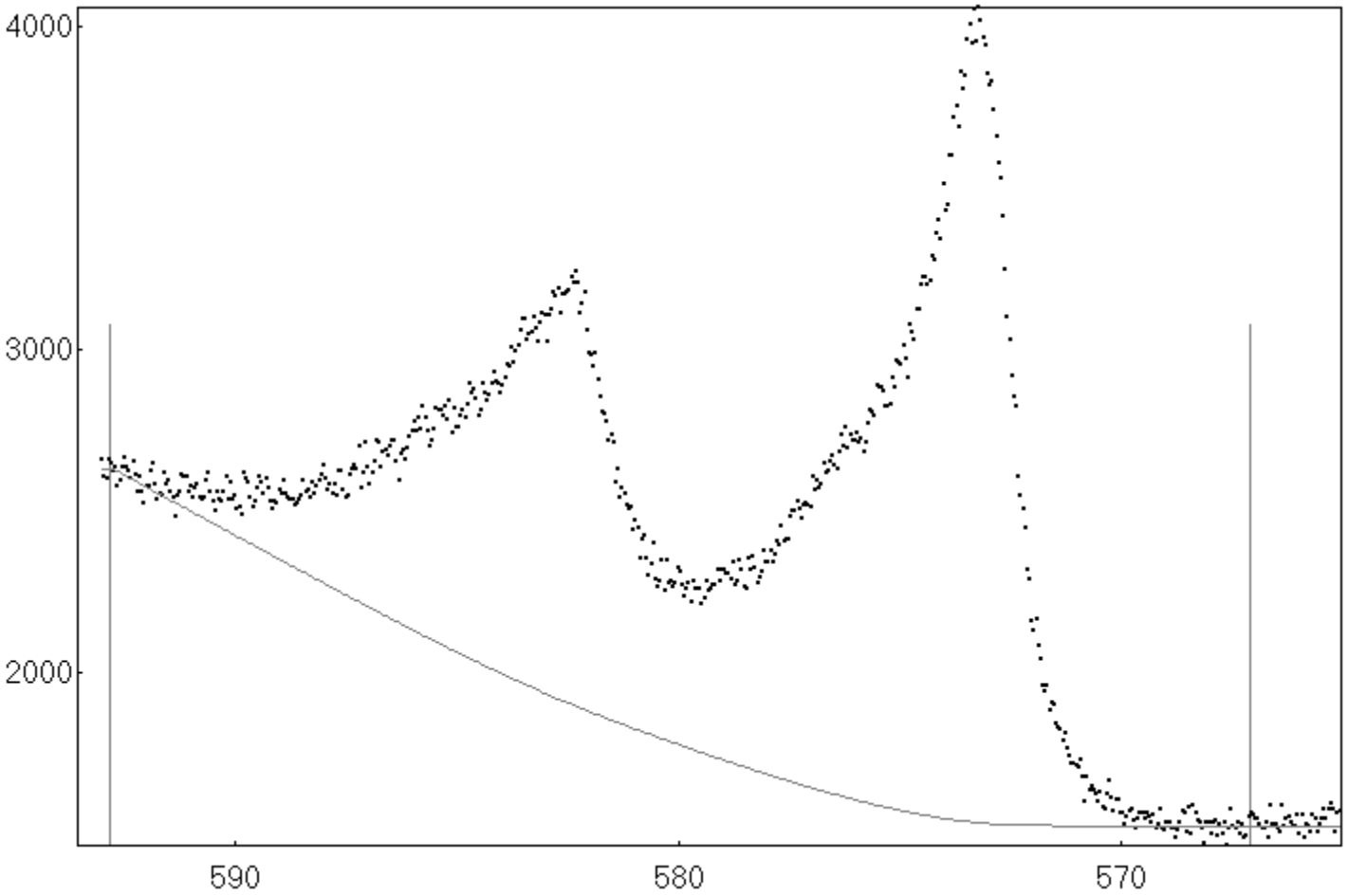
Other Examples

## Cr 2*p*

2-Param Tougaard but forcing to go through the chosen points




B2 = 13340 $eV^{-2}$ C2 = 1643 $eV^{-2}$

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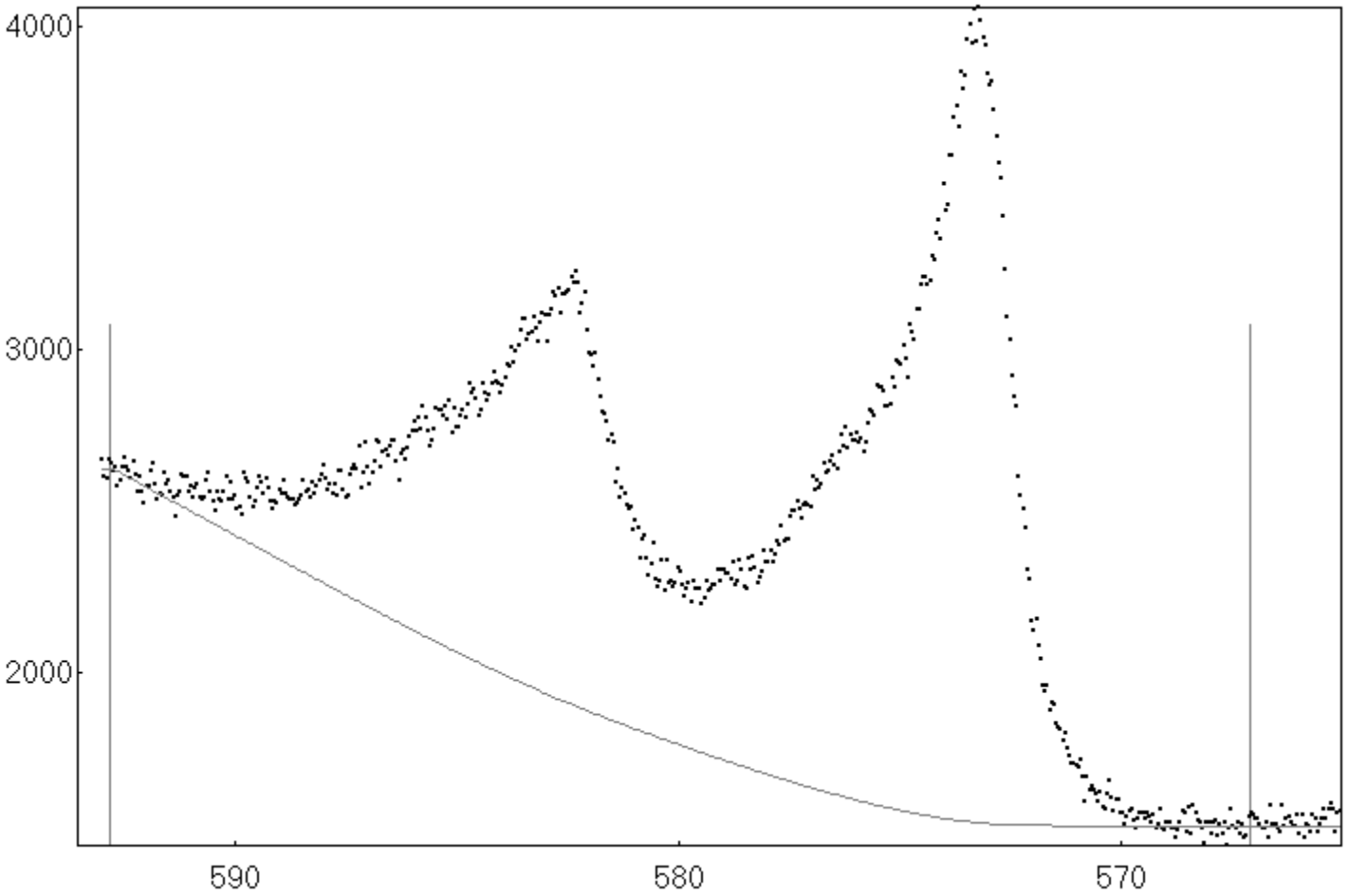
Other Examples

## Cr 2*p*

2-Param Tougaard but forcing to go through the chosen points




~~B2 = 13340 eV$^{-2}$~~

B2 = 2866 eV$^{-2}$

C2 = 1643 eV$^{-2}$

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Other Examples

# Cr 2*p*

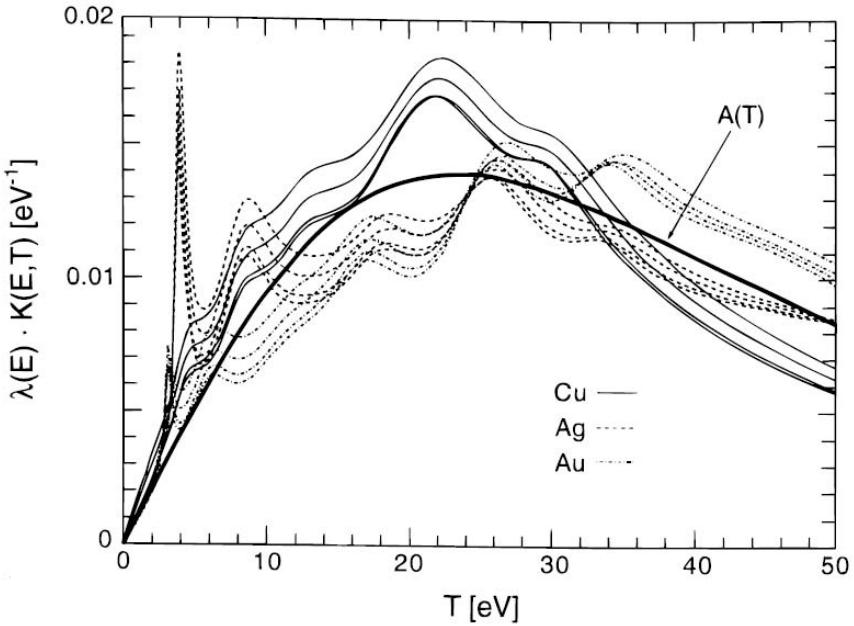


**Figure 4.** The $\lambda K$ curves evaluated by Eqn (1) for electrons of energy $E$ in Cu, Ag and Au. For each metal, four primary energy values ($E = 300$, 500, 1000 and 1500 eV) are considered. The thick solid line is the best two-parameter fit [Eqn (4) with $B = 2866$ eV$^2$].

SURFACE AND INTERFACE ANALYSIS, VOL. 25, 137–154 (1997)

$$A(T) = \frac{B\,T}{\left[T^2 + C\right]^2}$$

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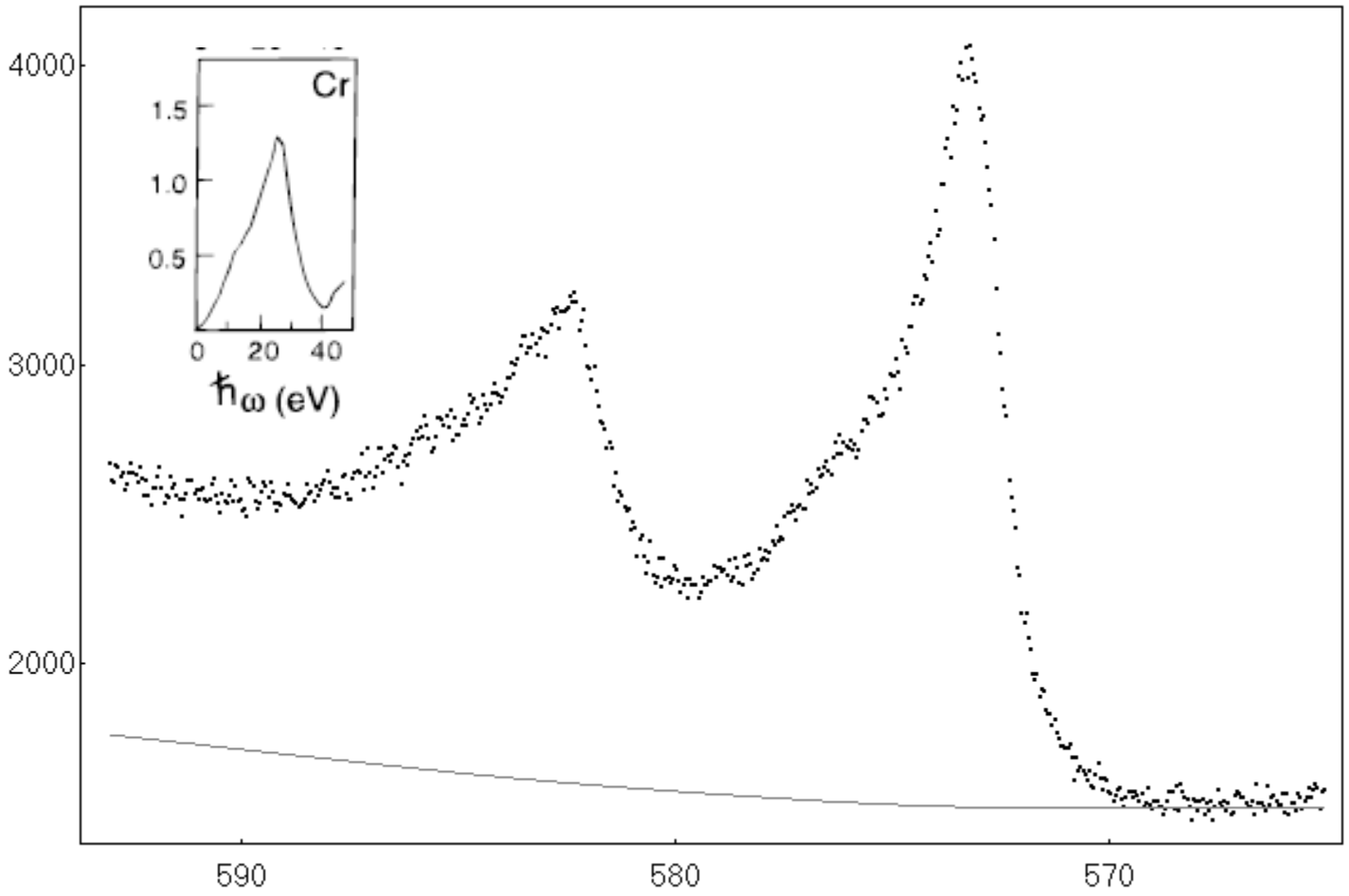
Other Examples

# Cr 2*p*

2-Param Tougaard with universal parameters




B2 = 2866 $eV^{-2}$ C2 = 1643 $eV^{-2}$

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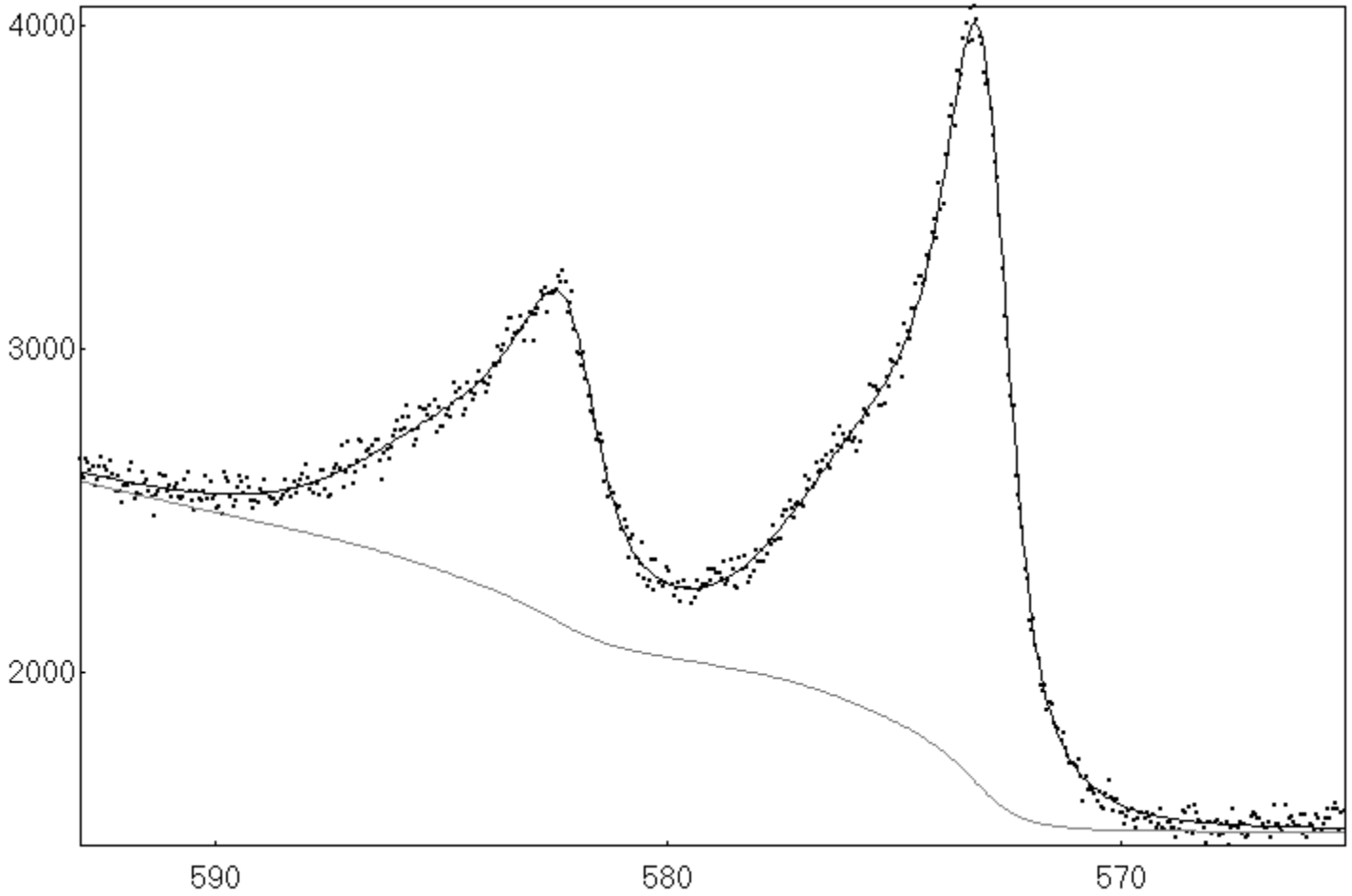
Other Examples

## Cr 2*p*

Iterative Shirley + Slope



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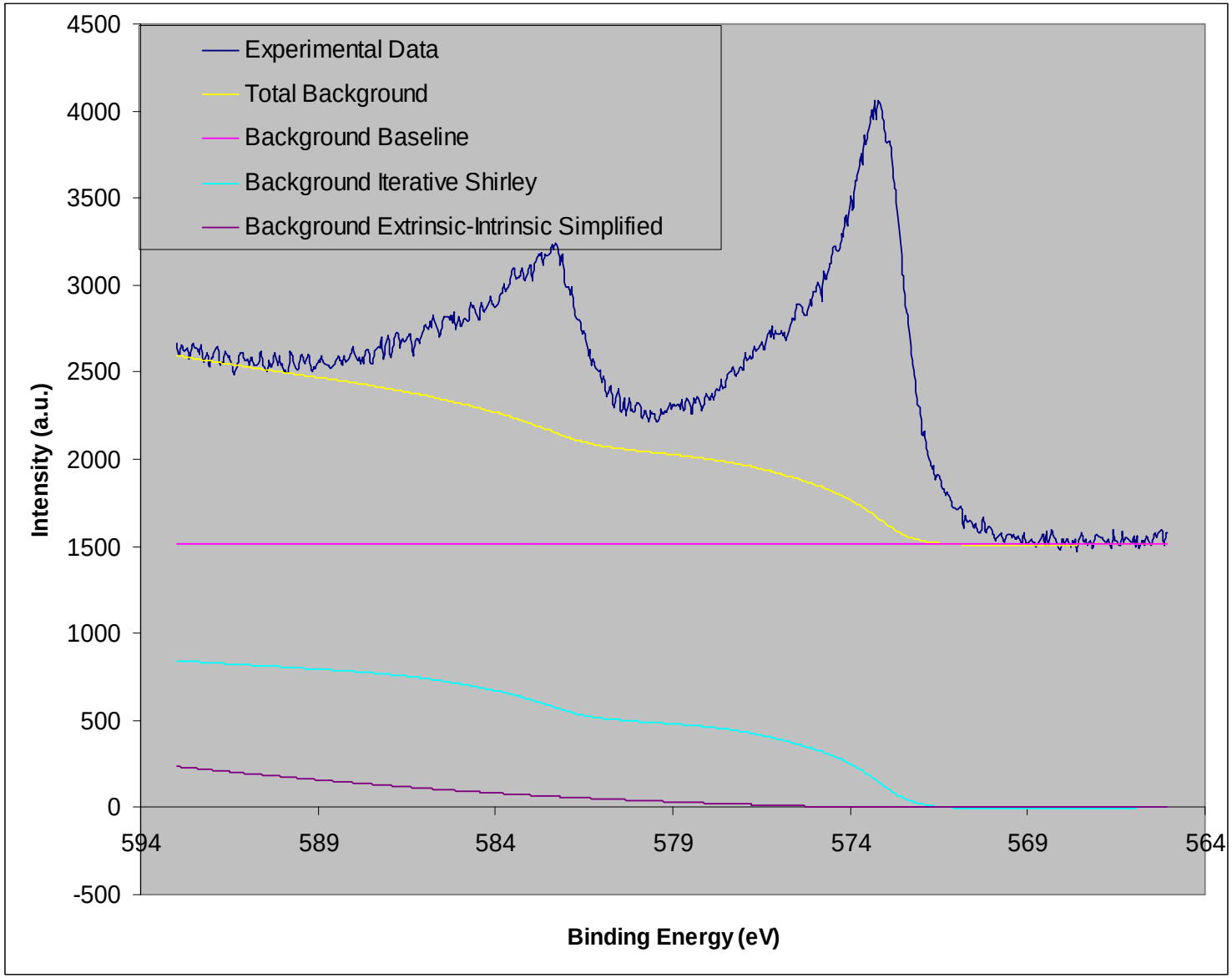
# Cr 2*p*

Other Examples



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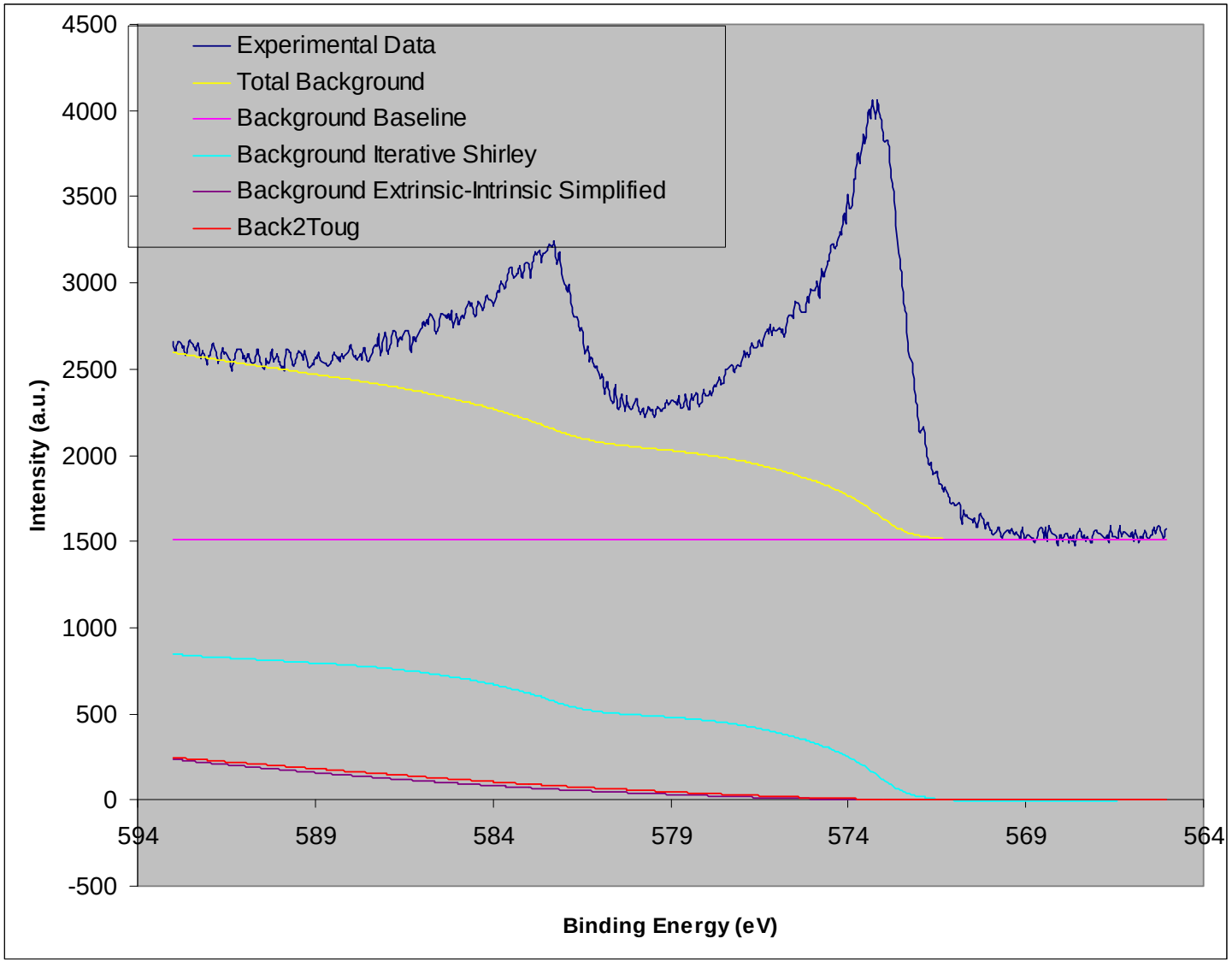
Other Examples

# Cr 2*p*



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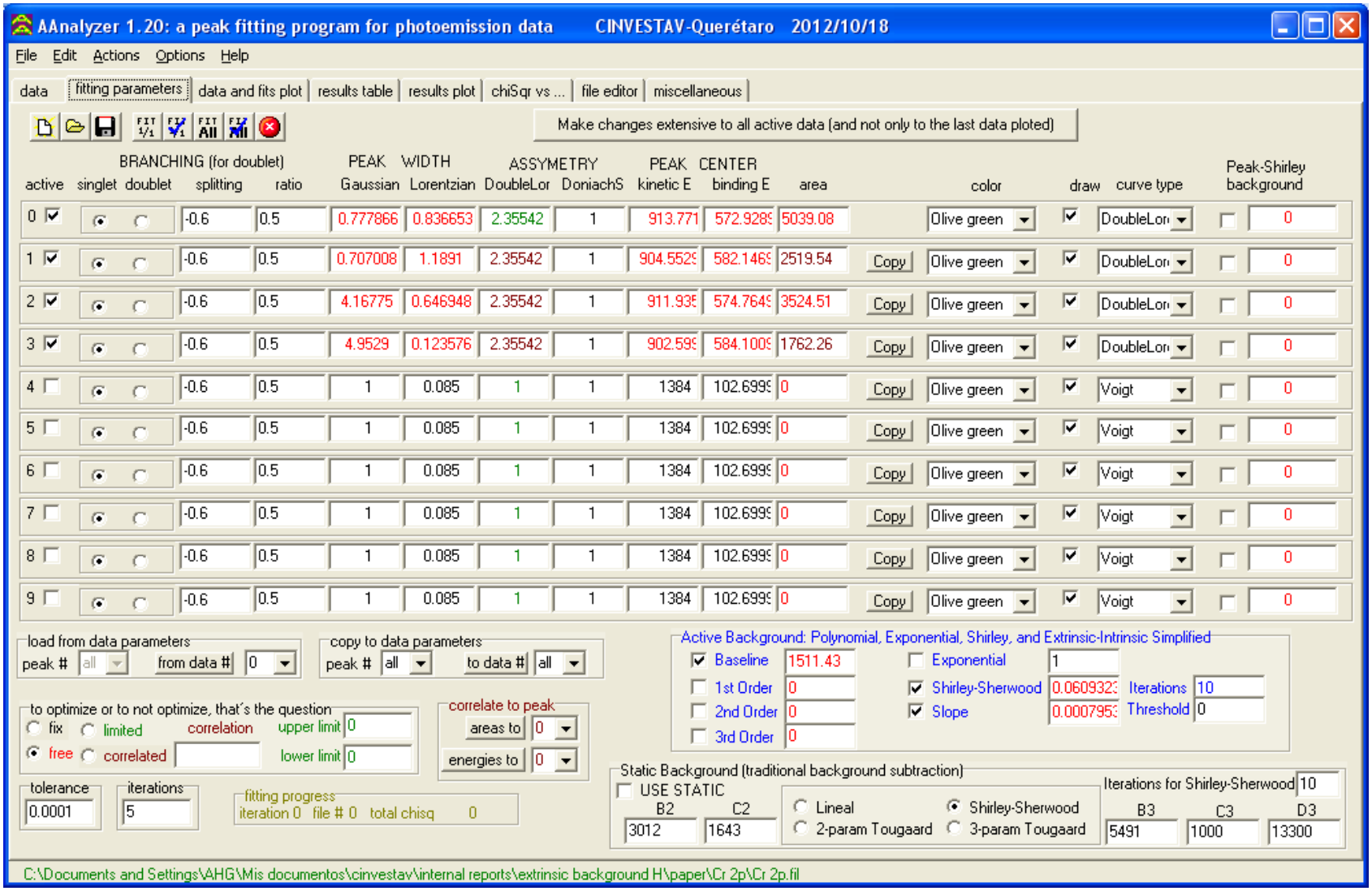
# Cr 2*p*

Other Examples



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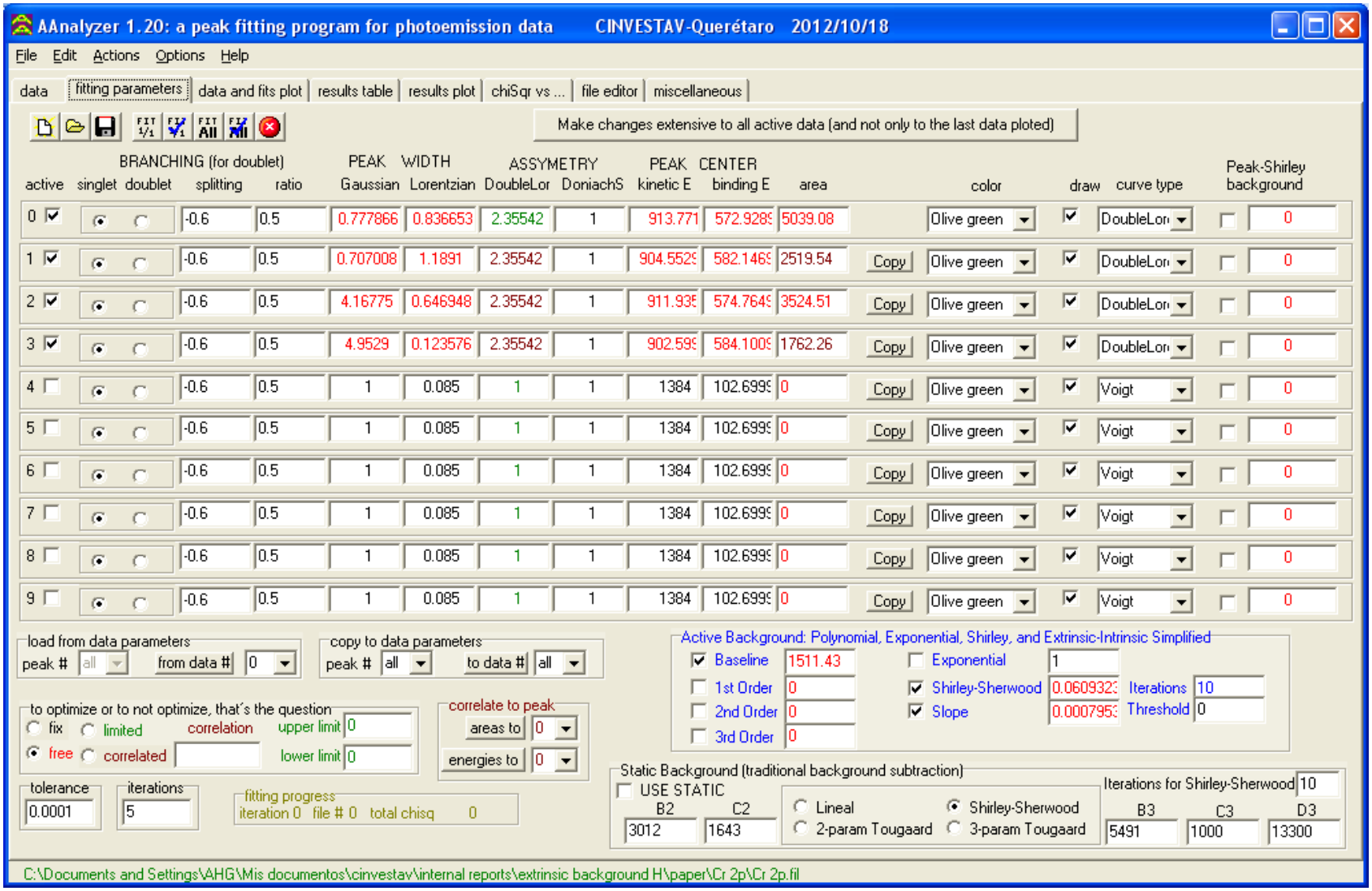
# Cr 2*p*

Other Examples




$$\frac{B}{C^2} = 0.001$$

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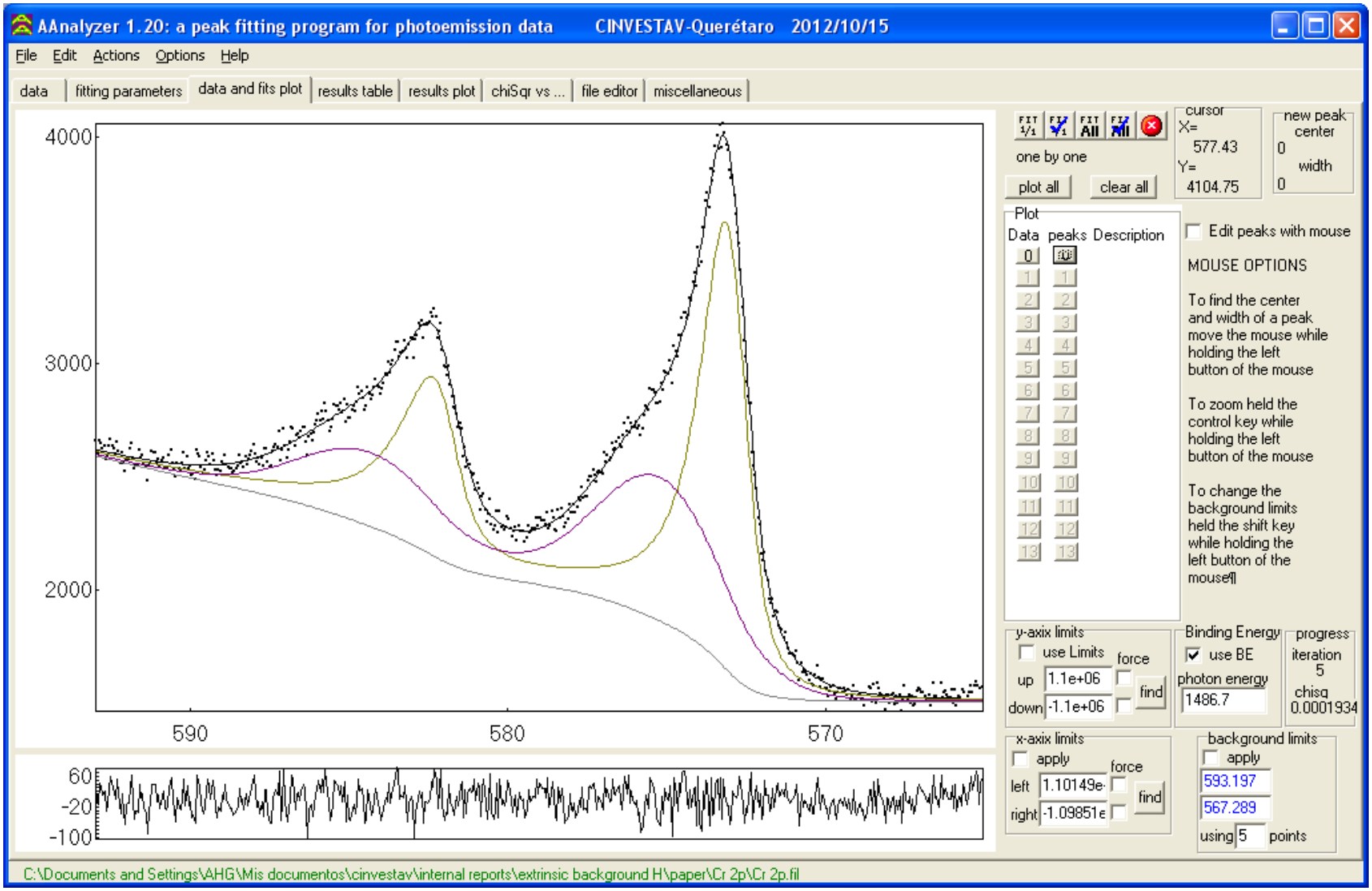
# Cr 2*p*

Other Examples



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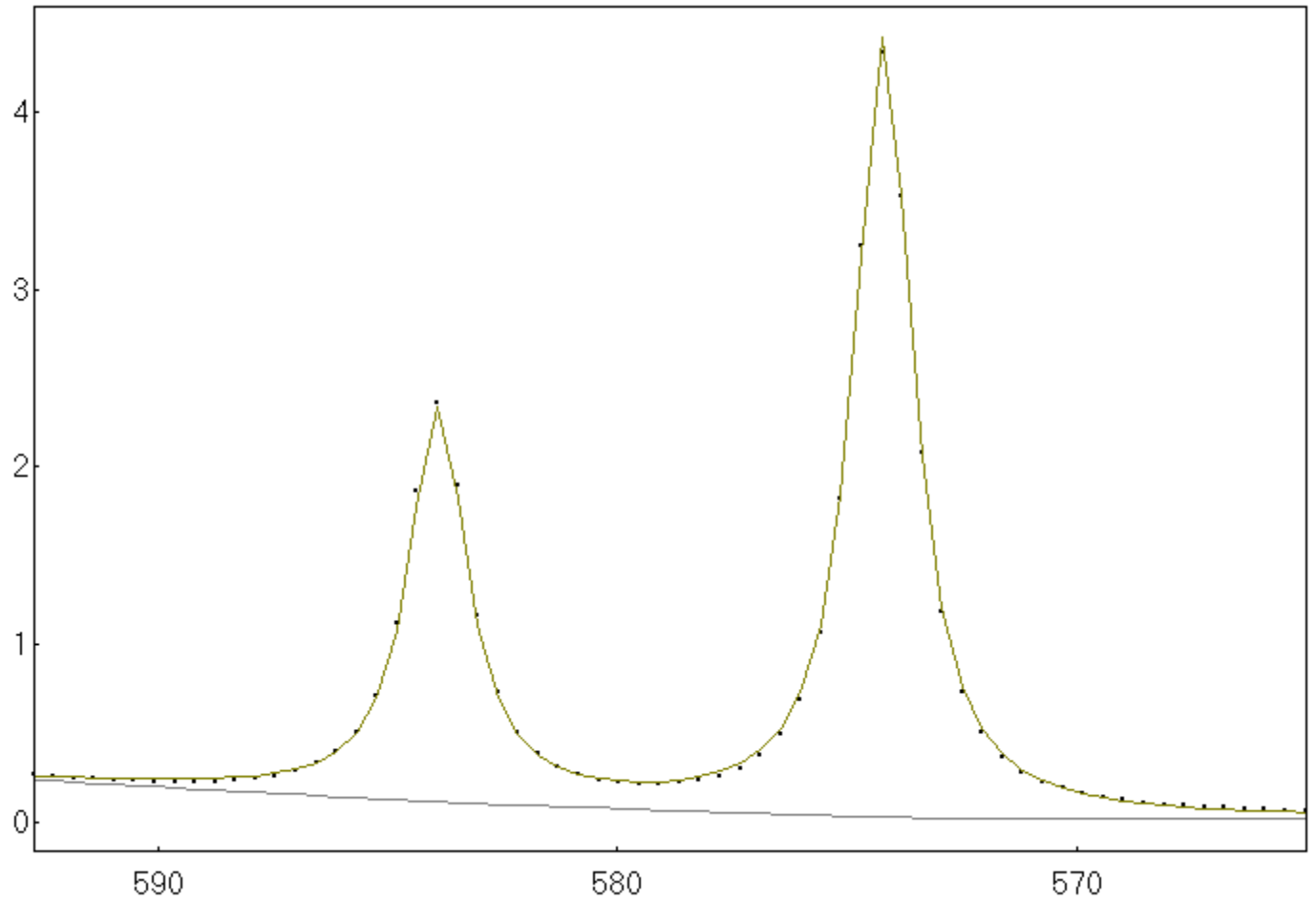
## Comparison with the Cr 2*p* simulated spectrum from ***SESSA***



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# Comparison with the Cr 2*p* simulated spectrum from ***SESSA***

Other Examples

AAnalyzer 1.20: a peak fitting program for photoemission data  CINVESTAV-Querétaro  2012/10/18

File  Edit  Actions  Options  Help

data | fitting parameters | data and fits plot | results table | results plot | chiSqr vs ... | file editor | miscellaneous

Make changes extensive to all active data (and not only to the last data ploted)

| active | singlet | doublet | BRANCHING (for doublet) splitting | ratio | PEAK WIDTH Gaussian | Lorentzian | ASSYMETRY DoubleLor | DoniachS | PEAK CENTER kinetic E | binding E | area | | color | draw | curve type | Peak-Shirley background |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ○ | ● | -9.69914 | 0.5 | 1 | 1.53466 | 1 | 1 | 912.4971 | 574.2027 | 15.6329 | | Olive green | ☑ | Lorentzian | ☐ 0 |
| 1 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 2 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 3 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 4 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 5 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 6 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 7 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 8 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |
| 9 | ● | ○ | -0.6 | 0.5 | 1 | 0.085 | 1 | 1 | 1384 | 102.6995 | 0 | Copy | Olive green | ☑ | Voigt | ☐ 0 |

load from data parameters: peak # all  from data # 0

copy to data parameters: peak # all  to data # 0

to optimize or to not optimize, that´s the question: ○ fix ○ limited  correlation  upper limit 0  ● free ○ correlated  lower limit 0

correlate to peak: areas to 0  energies to 0

tolerance 0.0001  iterations 5

fitting progress: iteration 3  file # 0  total chisq 0.0007093

Active Background: Polynomial, Exponential, Shirley, and Extrinsic-Intrinsic Simplified

☑ Baseline 0.0185982  ☐ Exponential 1
☐ 1st Order 0  ☑ Shirley-Sherwood 0  Iterations 10
☐ 2nd Order 0  ☑ Slope 0.0008969  Threshold 0
☐ 3rd Order 0

Static Background (traditional background subtraction)

☐ USE STATIC  B2 3012  C2 1643

○ Lineal  ● Shirley-Sherwood
○ 2-param Tougaard  ○ 3-param Tougaard

Iterations for Shirley-Sherwood 10  B3 5491  C3 1000  D3 13300

C:\Documents and Settings\AHG\Mis documentos\cinvestav\internal reports\extrinsic background H\paper\Cr 2p sessa\Cr 2p sessa.fil

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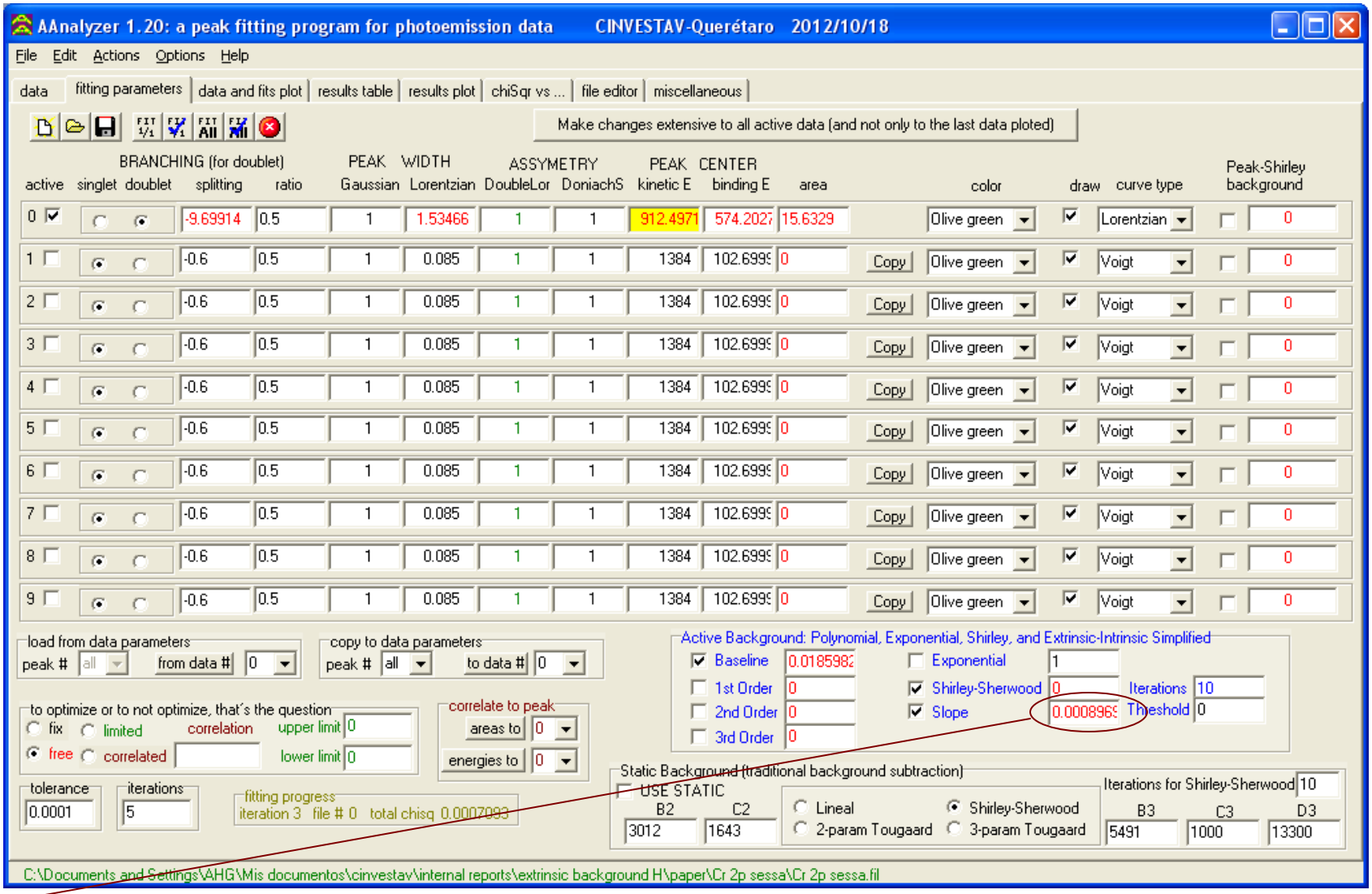
# Comparison with the Cr 2*p* simulated spectrum from ***SESSA***

Other Examples




0.0089 $eV^{-2}$, close to the 0.0079 $eV^{-2}$ value found for the real data

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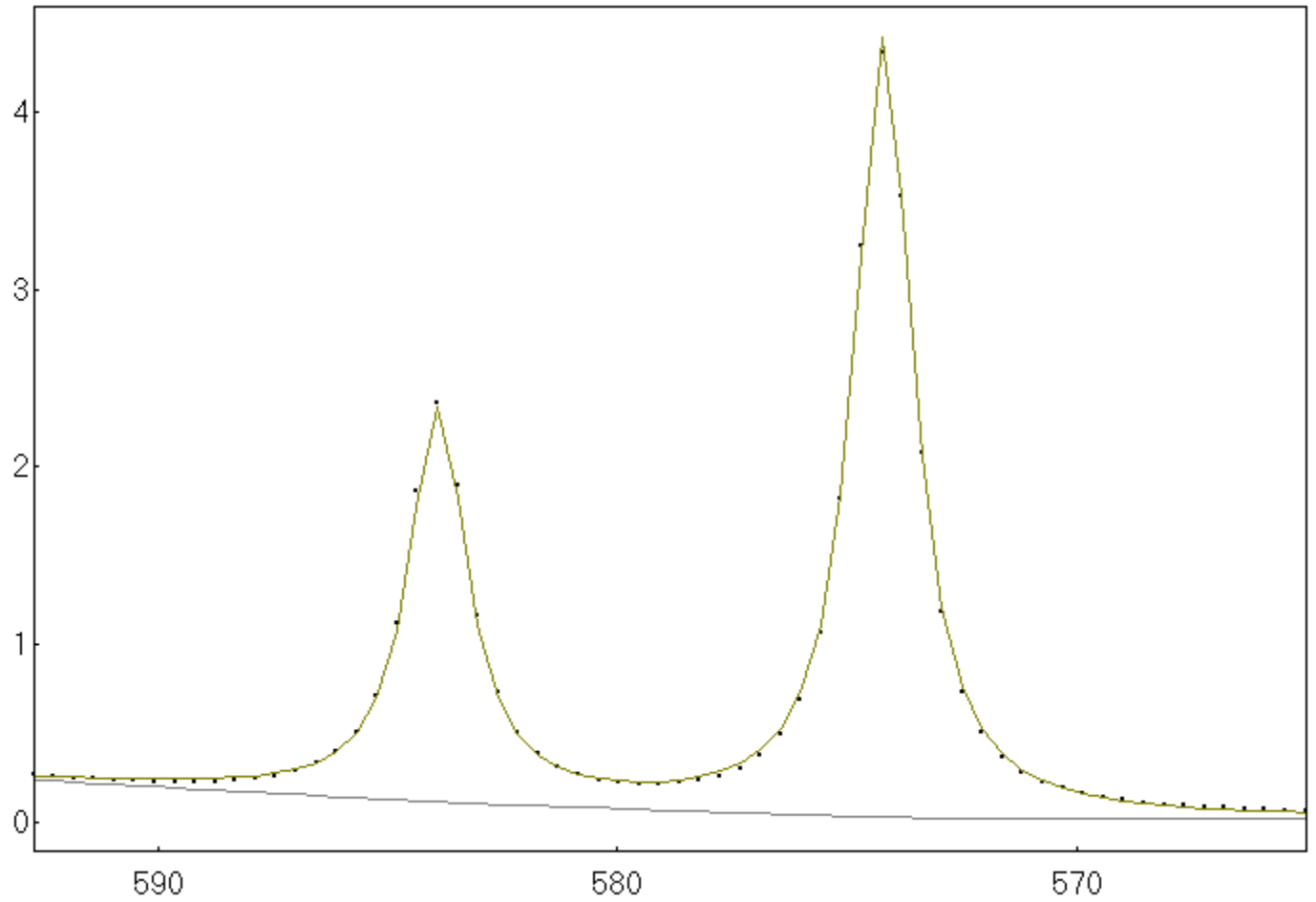
Other Examples

## Comparison with the Cr 2*p* simulated spectrum from ***SESSA***



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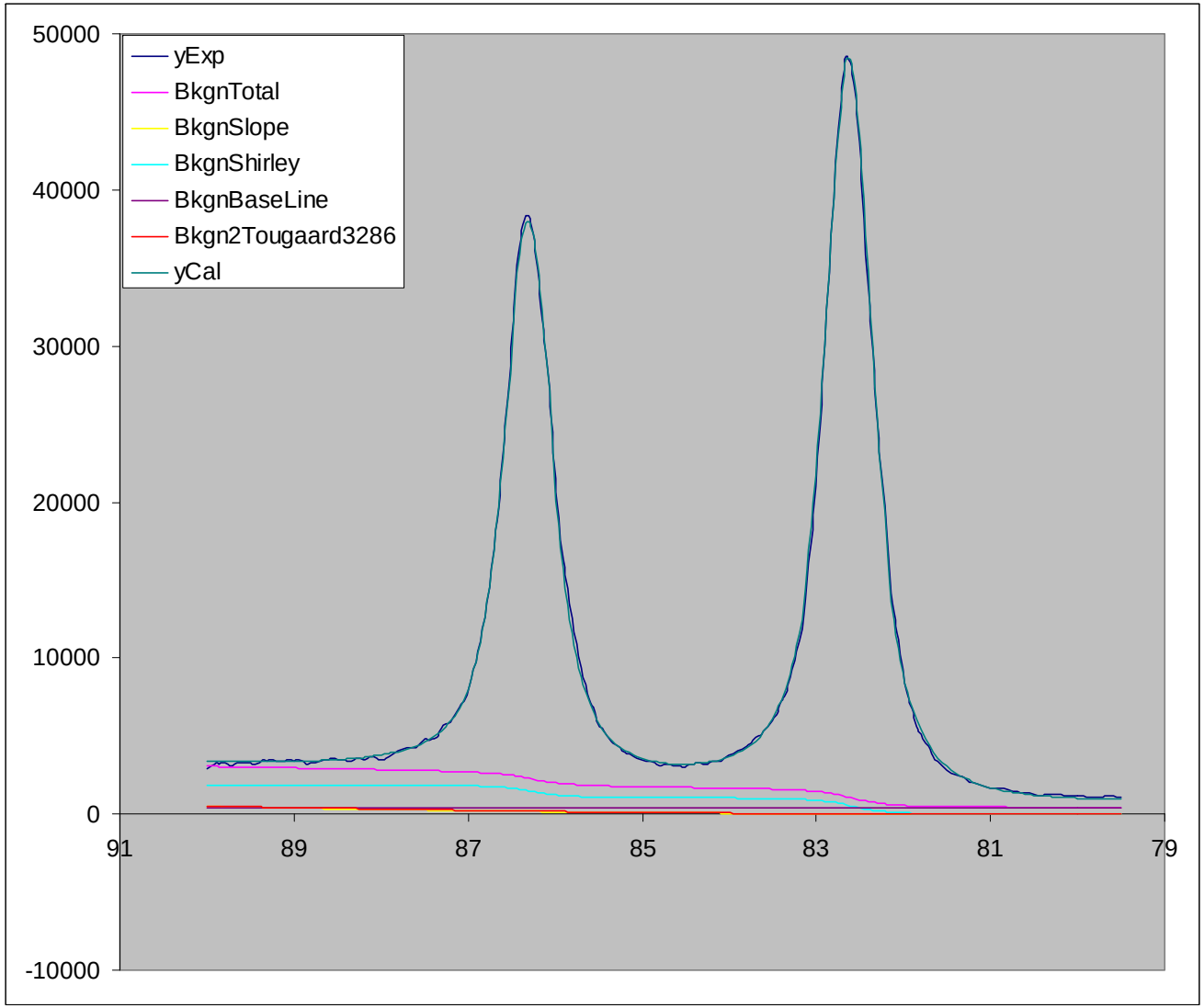

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Other Examples

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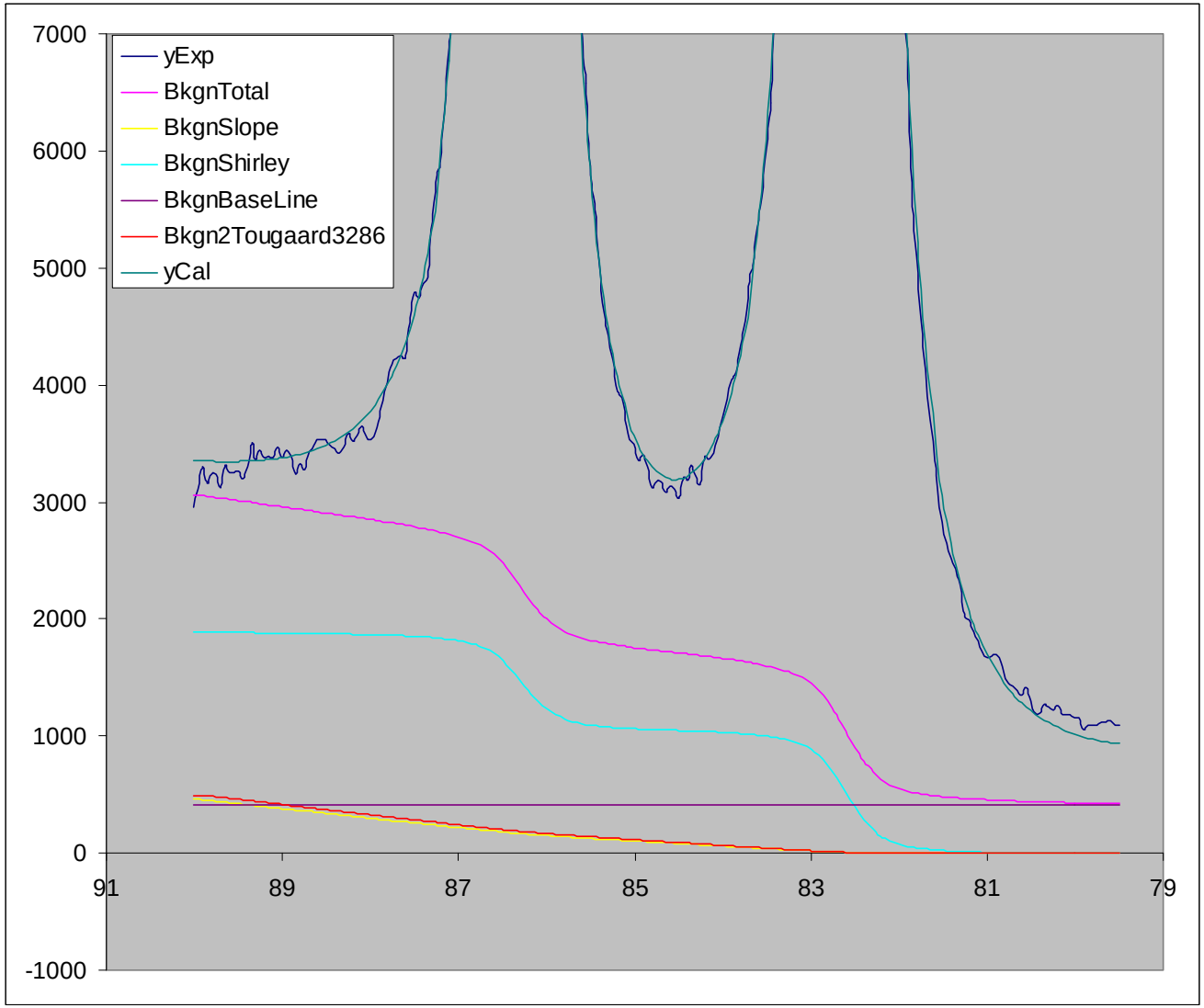

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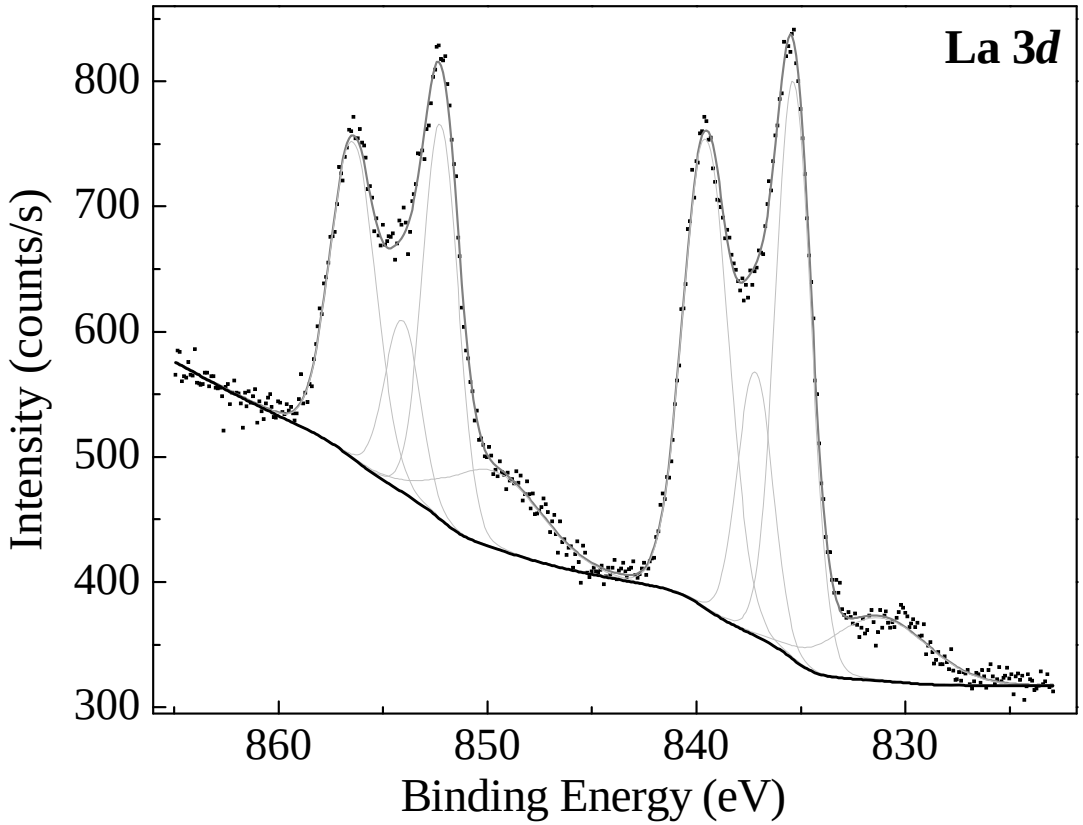
Other Examples

## Sr 3*d*



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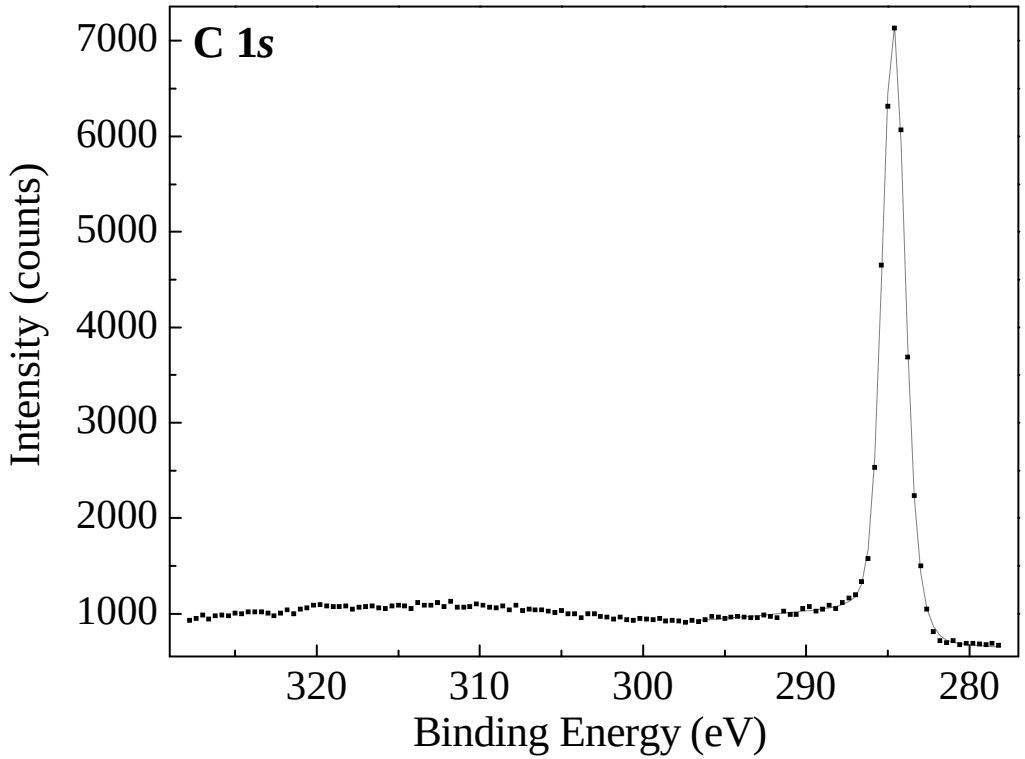
# C 1*s*

The Slope Background for decaying intensities



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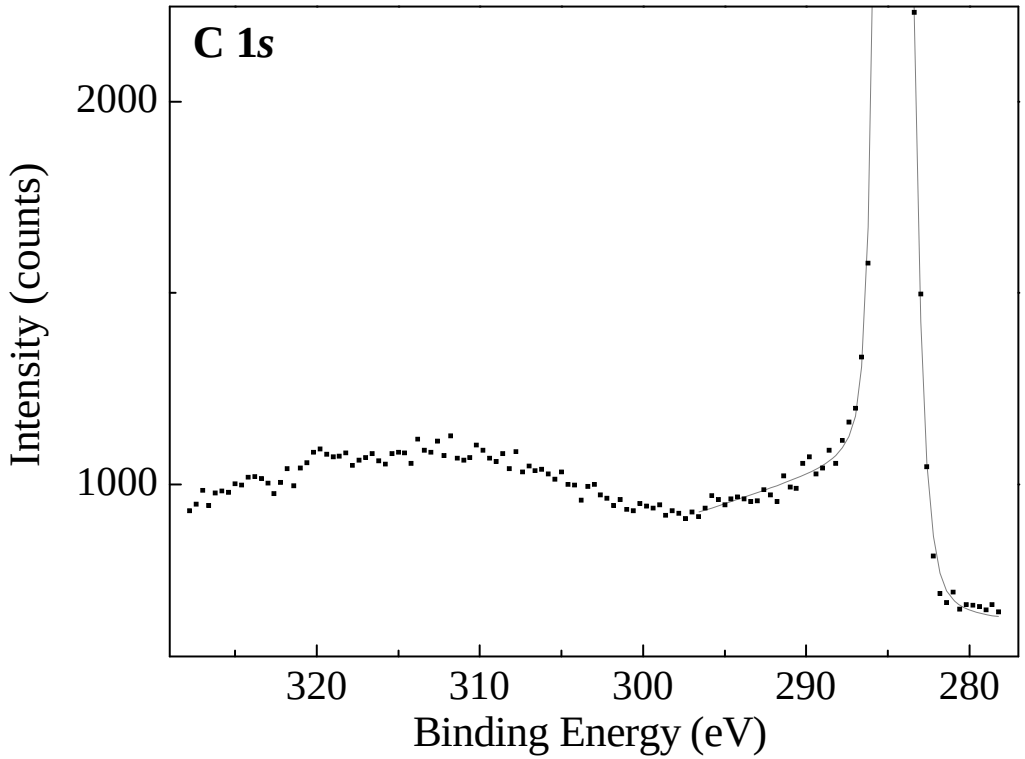

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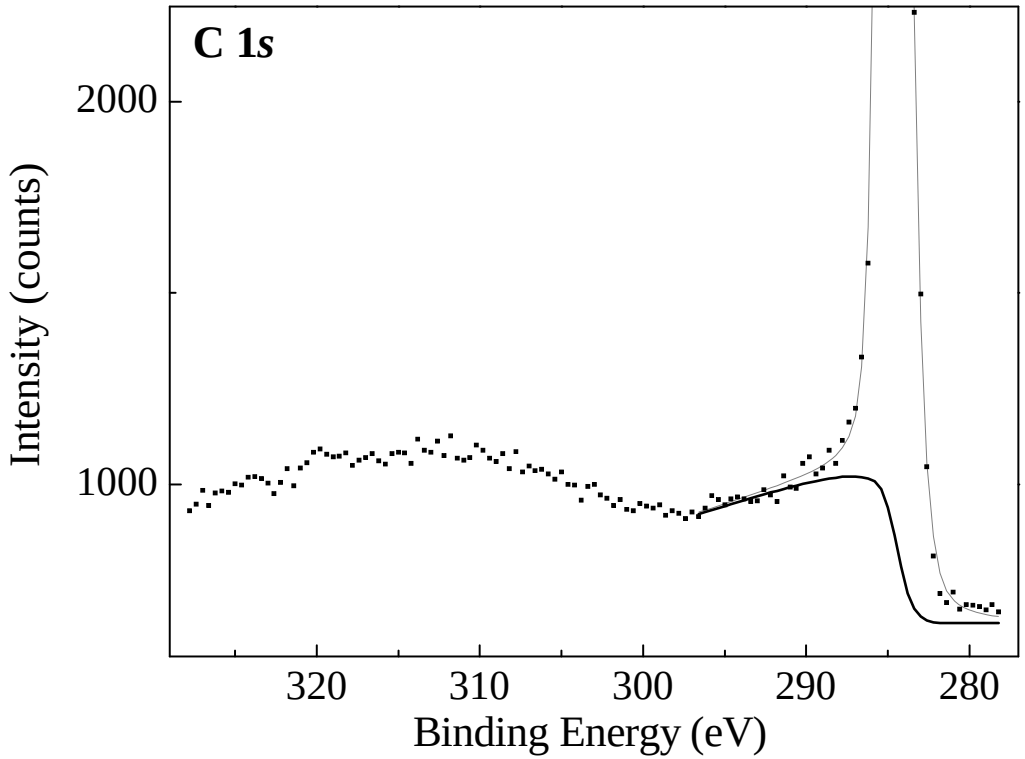

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  - Au 4*f*
  - Sr 3*d*
- Application of the Slope Background to decaying intensities
  - C 1*s*
  - Au 4*d*
- Conclusions

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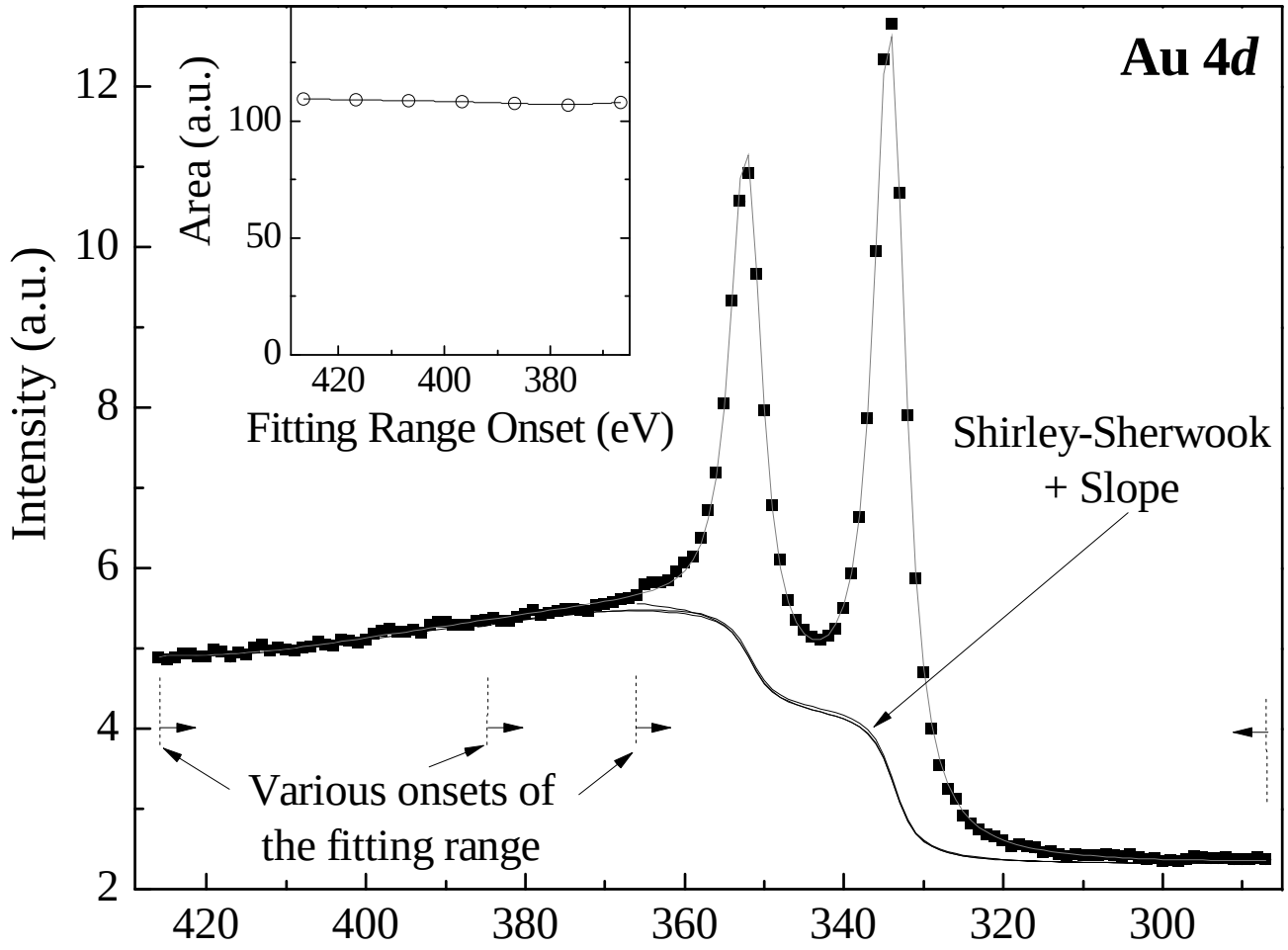
The Slope Background for decaying intensities

## Au 4*d*



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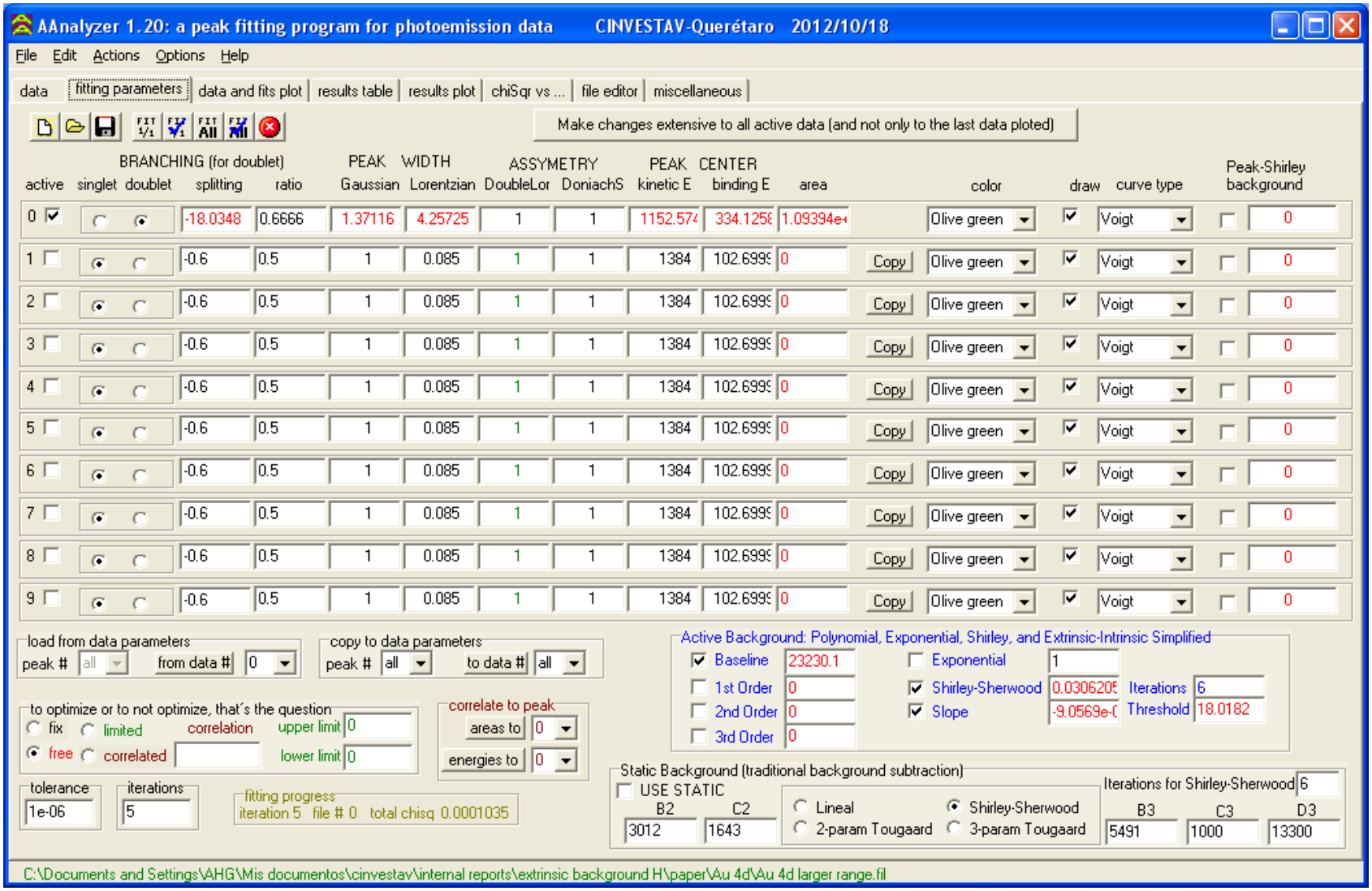
# Au 4*d*

The Slope Background for decaying intensities



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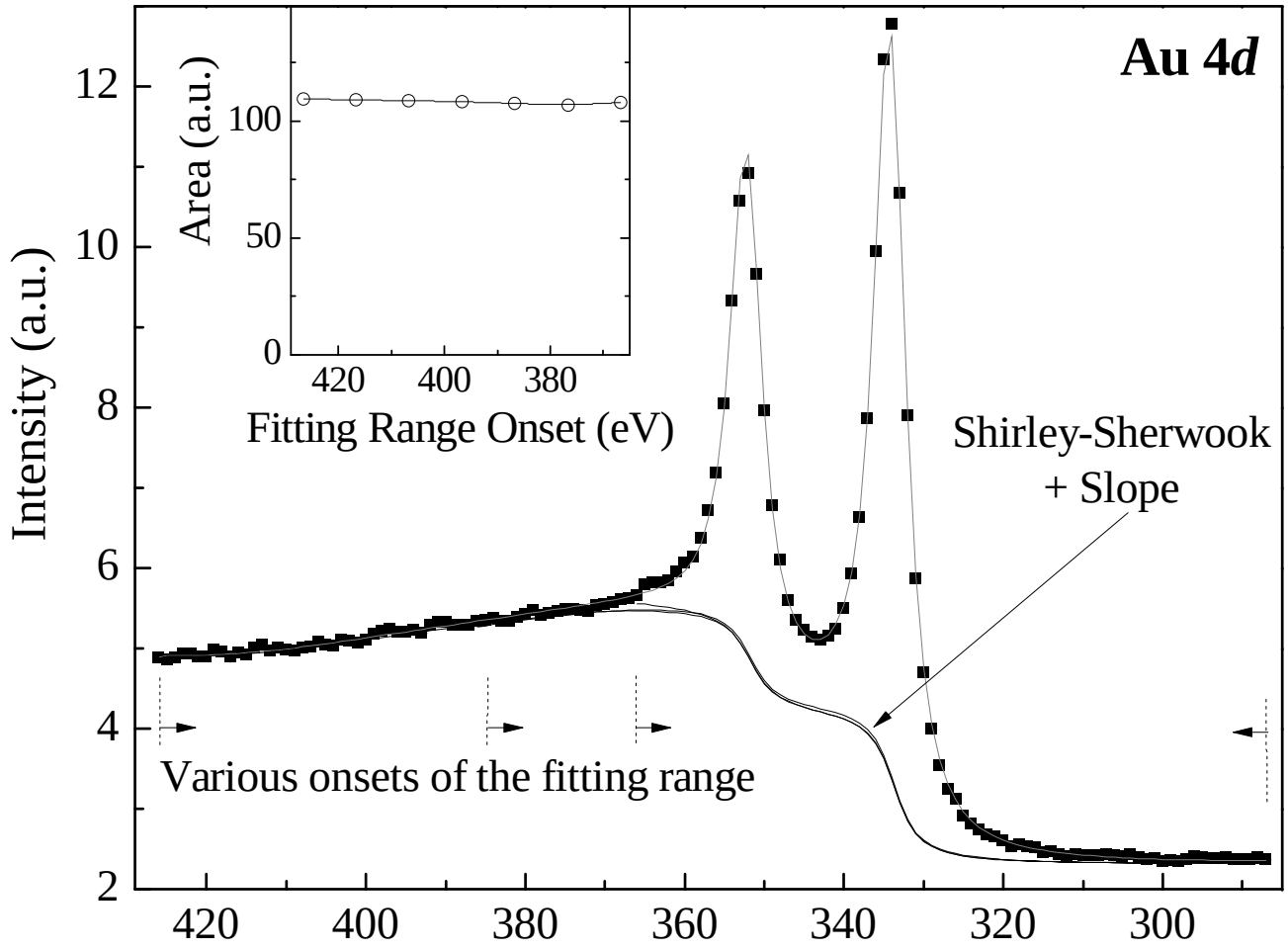
The Slope Background for decaying intensities

## Au 4*d*



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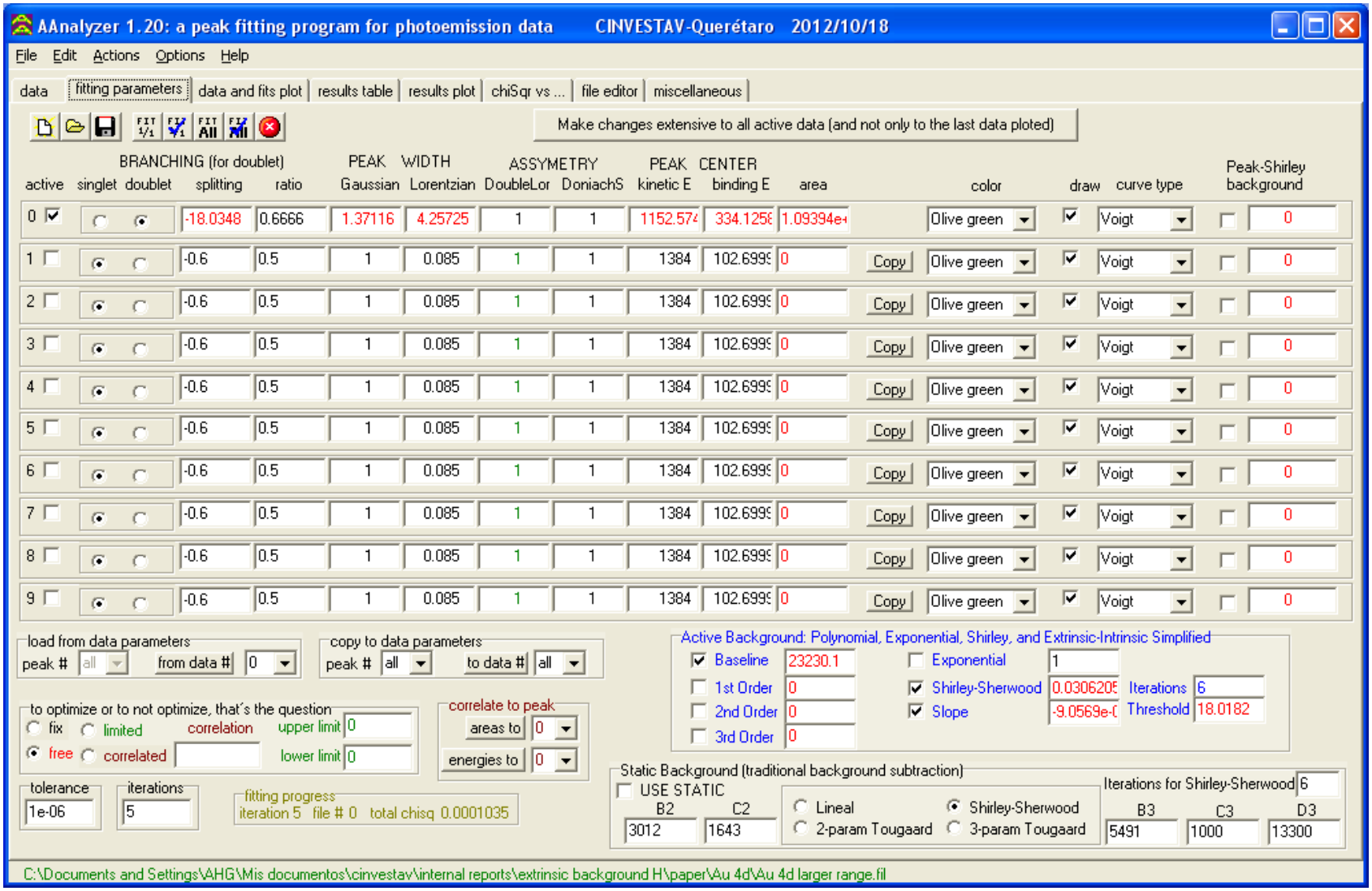
# Au 4*d*

The Slope Background for decaying intensities



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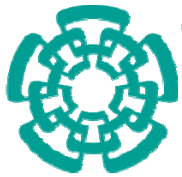
# Content

## The Slope Background for the near-peak regimen of photoemission spectra

- The various regions of the background: Si 2*p* example
- The total background as the sum of various terms
- The Slope Background
- The Slope Background in the Tougaard formalism
  - The near-peak regimen
  - The universal Tougaard cross sections
- Other examples:
  - Cr 2*p*
  - Comparison with Cr 2p simulated data from ***SESSA***
  - Au 4*f*
  - Sr 3*d*
- Application of the Slope Background to decaying intensities
  - C 1*s*
  - Au 4*d*
- Conclusions




# Conclusions

- The Slope Background
  - is applicable in the near-peak regimen,
  - reproduces the slope of the background on the left of the spectrum,
  - provides excellent fits when employed in conjunction with the Shirley-Sherwood background,
  - is predicted under the Tougaard formalism,
  - coincides with ***SESSA*** simulations,
  - is versatile since it can deal with decaying backgrounds,
  - employs only one parameter (blind to the operator) which could be used for “reverse engineering”,
  - makes the fit independent of the operator’s choice of the fitting range limits,
  - is applicable to quantitative analysis since the area of the remaining peaks can be assessed employing integrable curve shapes (symmetric and asymmetric).

Thank you for your attention!

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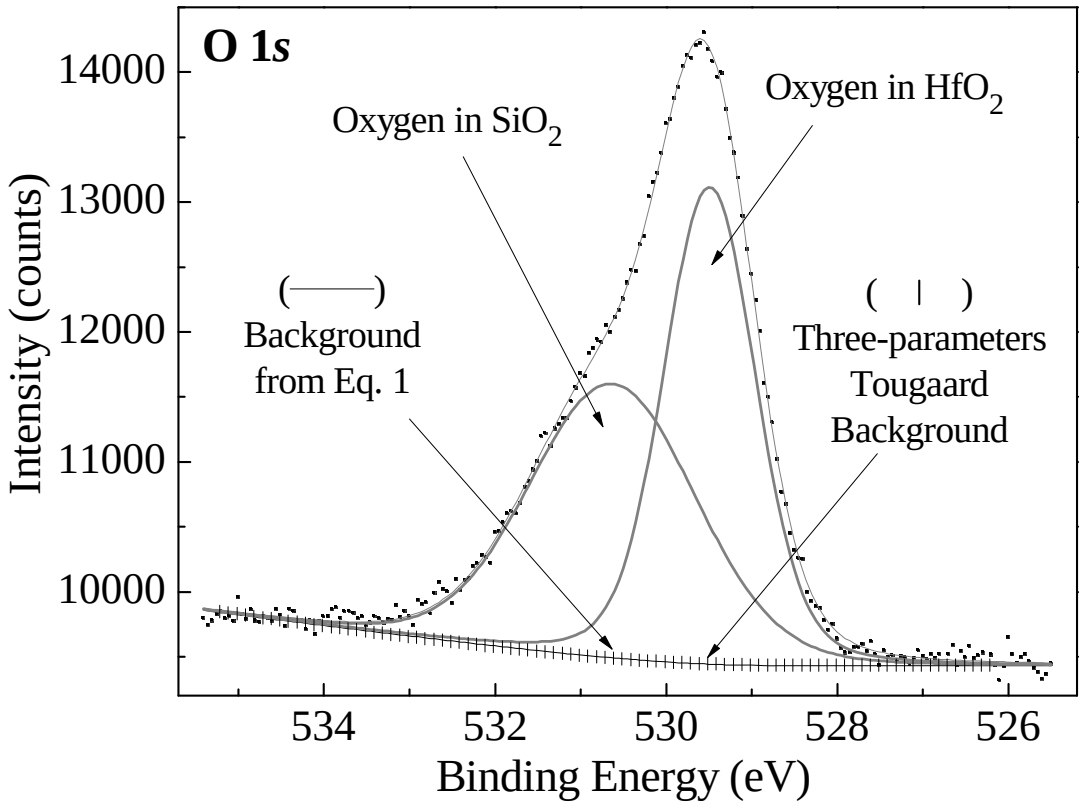
O 1s
Oxygen in SiO2
Oxygen in HfO2
(——)
Background
from Eq. 1
( | )
Three-parameters
Tougaard
Background
Intensity (counts)
14000
13000
12000
11000
10000
534
532
530
528
526
Binding Energy (eV)

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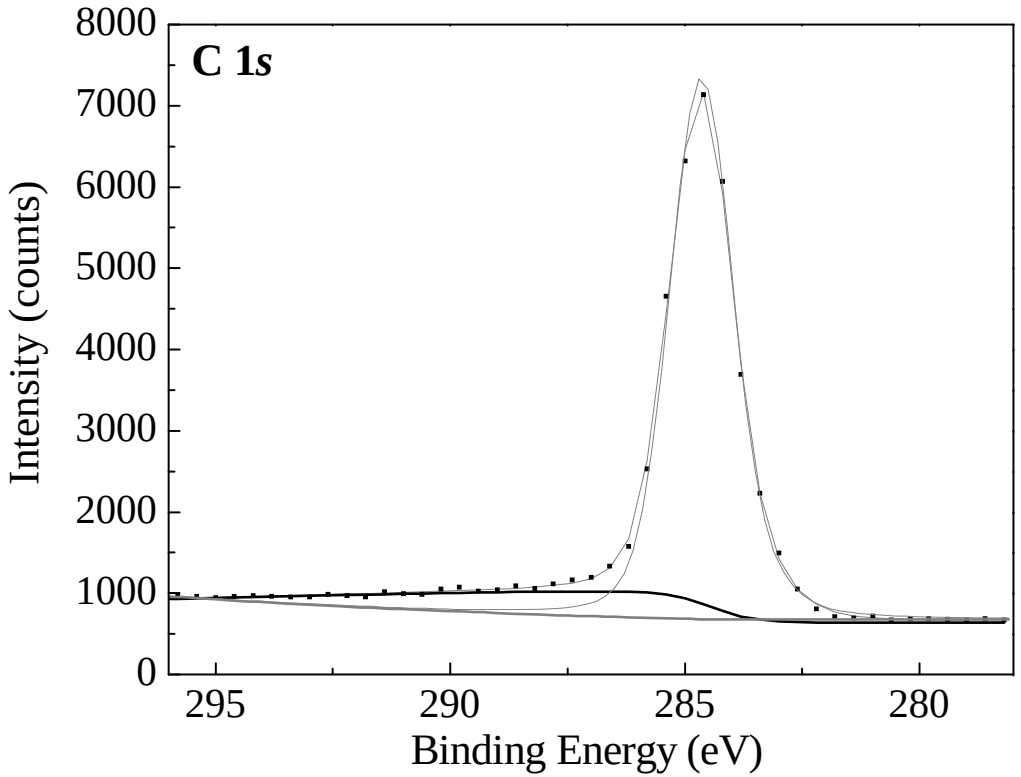
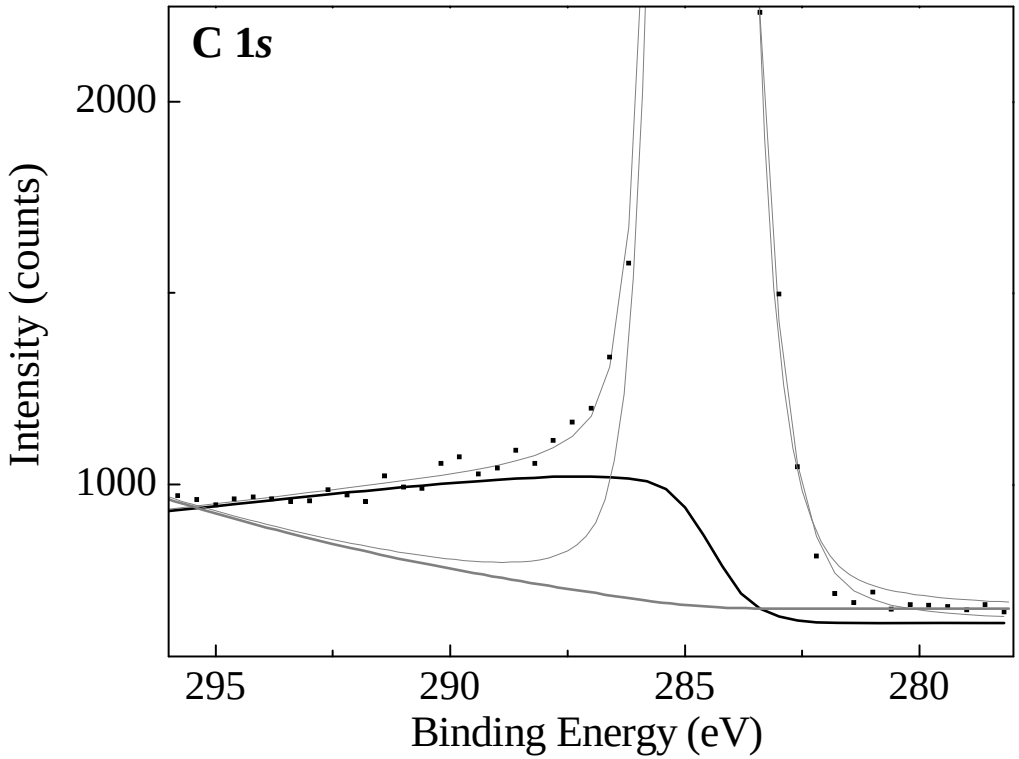

C 1s
Intensity (counts)
8000
7000
6000
5000
4000
3000
2000
1000
0
295
290
285
280
Binding Energy (eV)


C 1s
2000
1000
Intensity (counts)
295
290
285
280
Binding Energy (eV)

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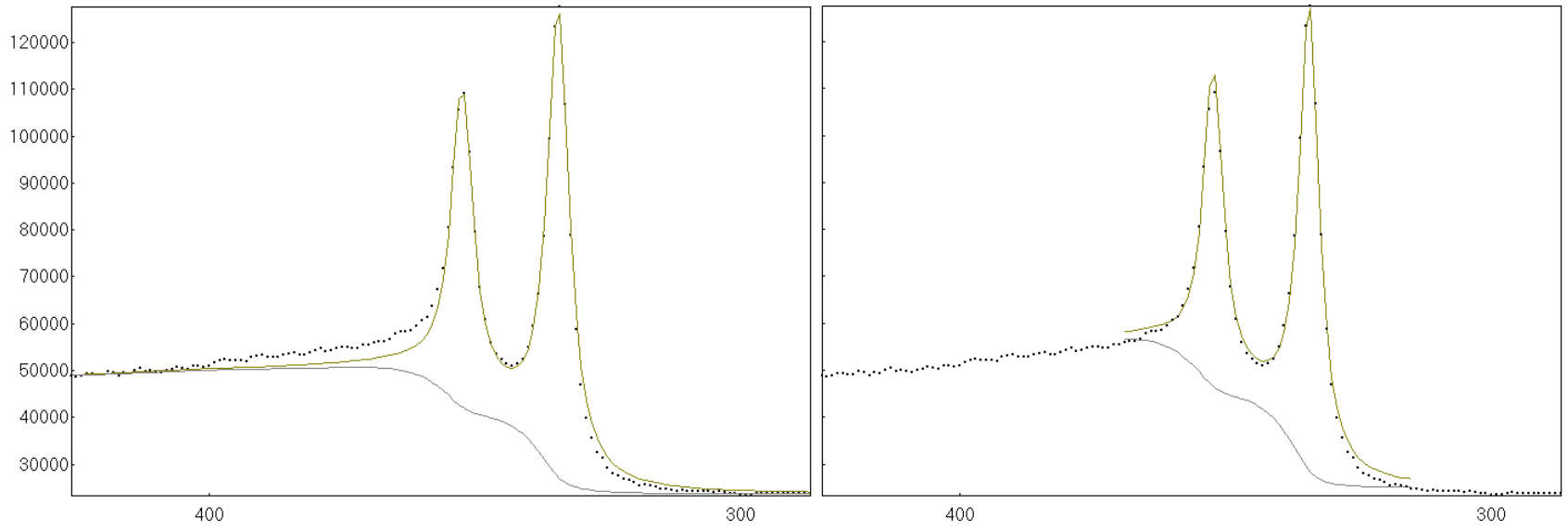
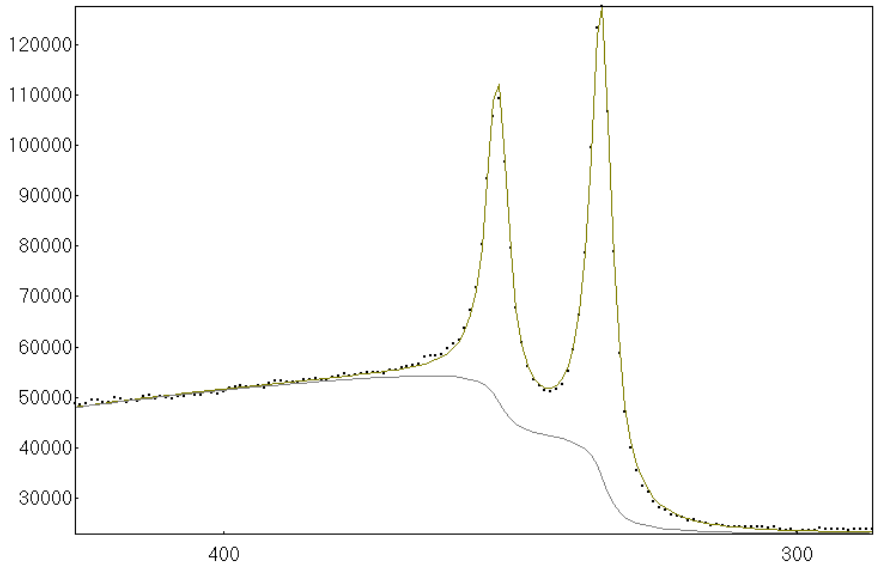

120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
400
300
400
300


120000
110000
100000
90000
80000
70000
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50000
40000
30000
400
300