

## Edge Measurements using a Complementary Error Function

The Heaviside step function

$$H_c(x) = \begin{cases} 1 & x > c \\ 1/2 & x = c \\ 0 & x < c \end{cases}$$

is the mathematical description for an ideal edge. Physical edges however are less well defined, where the shape observed in measured data is often a blend of the underlying edge structure and also the instrumental response inherent in the measurement process. One means of defining the Heaviside step function is to define the function as the following limit:

$$H_c(x) = \frac{1}{2} \lim_{t \rightarrow 0} \operatorname{erfc}((c-x)/t)$$

When defined in this way, the complementary error function *erfc* provides a means of understanding the observed data. The parameters *t* and *c* can be related to a Gaussian used to compute the *erfc* function.

$$\operatorname{erfc}((c-x)/t) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-\frac{(c-y)^2}{t}} dy$$

While the *erfc* function models the shape of the measured edge, the deviation from an ideal edge is characterised by the width of the Gaussian used in the integral and the position of the edge is the centre of the same Gaussian.

A further observation cementing the relationship between the Heaviside step function and the complementary error function is that the complementary error function can be viewed as a convolution of a Gaussian with the Heaviside step function. A convolution is again the mathematical tool used to blend the contributions of two distributions to form an observed data envelope. For example, the Voigt function used to describe photoelectric line-shapes is a convolution of a Gaussian with a Lorentzian function. The latter representing the life-time broadening of a transition, while the former attempts to introduce an instrumental influence on the observed peaks in an XPS spectrum.

Fitting a complementary error function to an edge, in a least squares sense, provides a tool for characterising a step in the data. Modelling a step using the complementary error function is performed in CasaXPS by using one of two background types. The backgrounds are defined using four parameters as follows:

$$BG(KE) = \frac{a_0}{2} \operatorname{erfc}\left(\frac{a_1 - KE}{a_2}\right) + a_3$$

Where  $a_0$  measures the magnitude of the step,  $a_1$  identifies the location of the step,  $(2\sqrt{\ln 2})a_2$  is the full width at half maximum (FWHM) of the Gaussian used to compute the complementary error function and  $a_3$  represents a constant offset. These four parameters are specified using the four values displayed in the Cross Section fields on the Regions property page. After the region is created using either the “Step Up” (“Su”) or “Step Down” (“Sd”) background types, the  $a_i$  can be optimised by pressing the Region column button on the scrolled-list on the Regions property page.

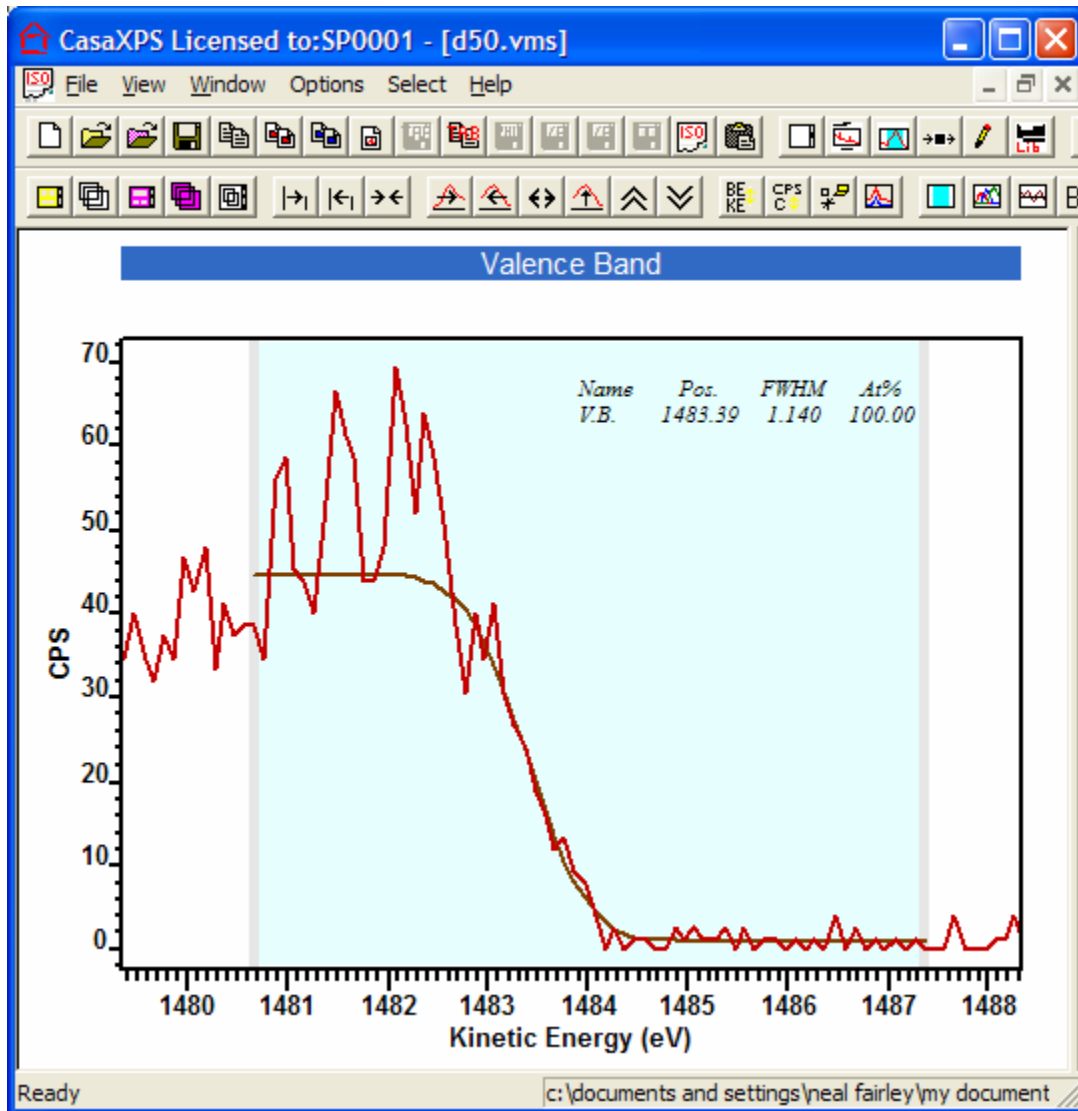


Figure 1: An example of a Step Down background type supplied by Duke University [2].

Figure 1 shows an example of the Step Down background type (the Step Down background is a reflection in the vertical line  $KE = a_1$  of the Step Up background) used to model the valence band edge in an XPS spectrum. Once fitted to the data, the Step Down

and Step Up background types report the position of the edge  $a_1$  and the FWHM  $(2\sqrt{\ln 2})a_2$  on the Regions property page shown in Figure 2.

A further parameter sometimes of interest [1][2] is the position of the intersection of the horizontal offset line  $y = a_3$  with the line representing the linear portion of the step. When approximated using the complementary error function, a line representing the “linear portion” of the step can be defined as the tangent line at the position of the edge. The intersection of the tangent line with the horizontal offset line occurs at  $KE = a_1 \pm a_2$  where the  $\pm$  refers to the Step Down or the Step Up background type. Given that the background type is either Step Up or Step Down, then the intersection of these two lines is reported as the Position Constraint in a configured Regions Standard Report, where the field POSITION\_CONST must be added to the RegionQuantTable.txt file in the CasaXPS.DEF directory (see page 143 in The Casa Cookbook). Alternatively  $a_1$  and  $a_2$  can be read from the second and third entries in the Cross Section field on the Regions property page (Figure 2).

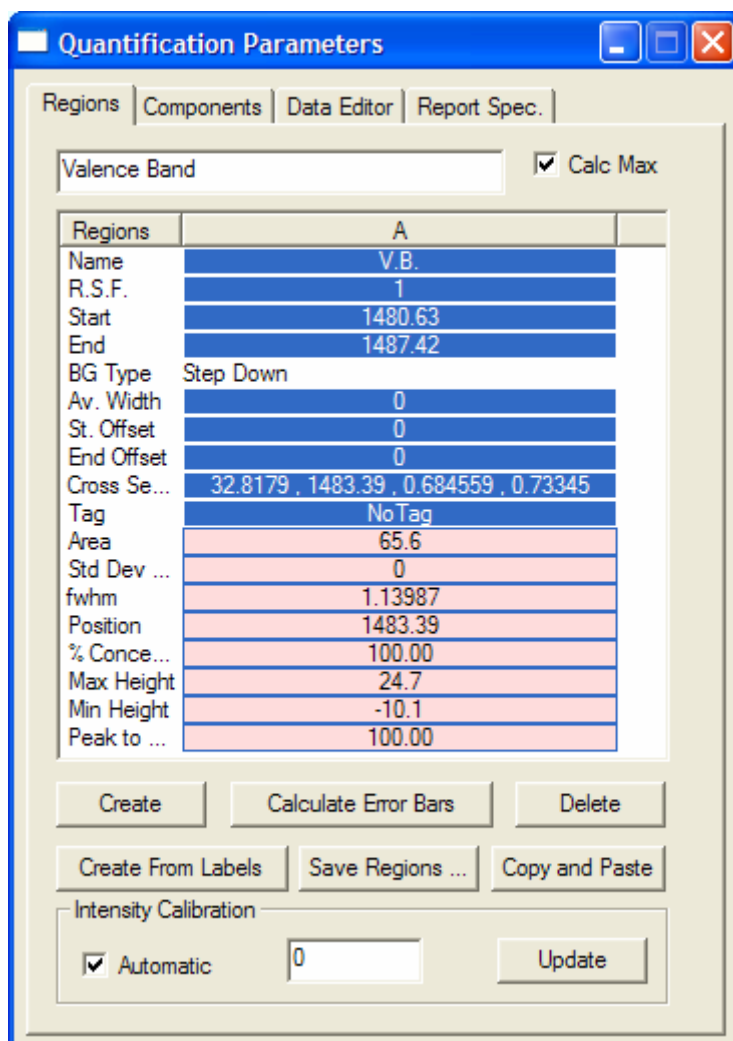


Figure 2: The Regions property page showing the parameters used to fit the data in Figure 1.

## ***Propagating Step Backgrounds***

Step background types can be propagated to other spectra using the Browser Actions dialog window. The region defined in Figure 1 and Figure 2 is propagated to other similar spectra by first selecting the VAMAS blocks in the right-hand-side browser pane, then right-clicking the mouse over the window displaying the spectrum. The Step background types are different from other background types in that the background is both copied to the target data and also a linear least squares optimization determines the four coefficients as part of the propagation.

## ***Image Processing using Step Background Types***

The image processing window provides yet another means of fitting Step backgrounds to sets of data en masse. If a Step background type is defined on each VAMAS block and the VAMAS blocks represent a row of spectra in an image data set, then for all such VAMAS block overlaid in the active tile, the act of pressing the **Convert Regions to Images** button causes the fitting of the background to each and every spectrum, from which an image is created for each of the  $a_0$ ,  $a_1$  and  $a_3$  background parameters [3].

[1] Chambers *et al*, J. Vac Sci Technol. B 22 (4), Jul/Aug 2004

[2] M. Garcia, S.D. Wolter, T. Kim, S. Choi, A. Brown, et. al. /Surface oxide relationships to Fermi level Band Bending in GaN/, Appl. Phys. Lett. Accepted for Publication, (2005)

[3] Renault *et al*, SIA proceeding of ECASIA'05.