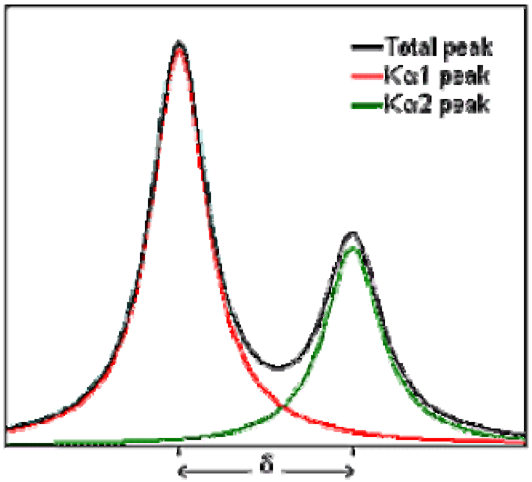
Kα2 Strip Algorithm

$K\alpha$2 Strip Algorithm

In X'Pert HighScore two algorithms are implemented for $K\alpha_2$ stripping:

Rachinger method: The RACHINGER method uses the exact wavelengths of the $K\alpha_1$ and $K\alpha_2$ lines and their intensity ratio. The intensity measured at the first point in the profile is assumed to be entirely stemming from $K\alpha_1$. The d_{hkl} causing the diffraction at this 2θ angle will, of course, also diffract the $K\alpha_2$ at the angle proscribed by Bragg's law. Because the intensity ratio of the $K\alpha_1$: $K\alpha_2$ reflections is exactly 2 : 1, half of the intensity measured at the low-angle 2θ can be subtracted from the higher angle intensity, where the $K\alpha_2$ wavelength diffracts.



The Rachinger method is a good first approximation to $K\alpha_2$ deconvolution; however, it assumes that the profile of $K\alpha_1$ is identical to the $K\alpha_2$ profile. In fact, the $K\alpha_2$ peak occurs at a higher angle and is somewhat broader than the $K\alpha_1$ peak. This difference in profile shape gets more pronounced as 2θ increases.

Modified Rachinger method: According to DELHEZ and MITTEMEIJER the doublet separation, δ_R, is calculated as a 2θ dependent parameter as shown in the formulas below:

$$I_{\alpha 2}(2\theta) = R_{int} I_{\alpha 1}(2\theta - \delta_R)$$

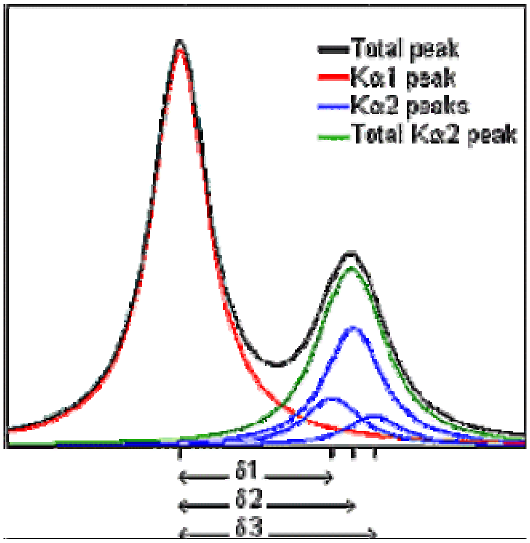
$$R_{int} = 0.5$$

$$\delta_R = 2\arcsin e(R_{wav} \sin\theta_1) - 2\theta_1$$

$$R_{wav} = \lambda_2 / \lambda_1$$

Ladell method: LADELL et al. carefully determined the profiles of $K\alpha_1$ and $K\alpha_2$ peaks of resolved lines. They also calculated how the difference in peak shape varies with 2θ, using Fourier techniques. Based on this analysis, a table, which is used to subtract a portion of the $K\alpha_2$ intensity from a series of adjacent 2θ points was created.

This method describes the $K\alpha_2$ profile as the summation of 3, 5 or 7 sub profiles instead of only 1 sub profile as in other modified Rachinger methods. The sub profiles are indicated with levers (positions as wavelength ratios) and weights (intensity ratios). The algorithm of X'Pert HighScore uses 3 sub profiles.



First the sum of the weights is normalized to 0.500 (see table below). Secondly, each weight, W_i, is changed with one parameter, R_{int}, using the formula (factory default R_{int}=0.500):

$$W_{i,new} = W_{i,old} \times (R_{int} / 0.5)$$

Thirdly, each lever, L_i, is also changed with only one parameter, δR_{wav}, using the formula (factory default δR_{wav}=0):

$$L_{i,new} = L_{i,old} \times (1+\delta R_{wav})$$

As the change in wavelength parameter δR_{wav} is very subtle, values are entered in ppm units (parts per million) rather than a number like 0.000036 (i.e. 36 ppm).

Weights and levers for radiations other than Cu are available (see table below). If no weights and levers for Ladell (choice 2) are available only the modified Rachinger method is available.

Table for the normalized levers and weights for Cu, Co, Cr and Fe (Fe is interpolated; Mo is not available):

Cu		Co		Cr		Fe	
Levers	**Weights**	**Levers**	**Weights**	**Levers**	**Weights**	**Levers**	**Weights**
1.0023535	0.1436782	1.0020914	0.1549299	1.0014772	0.1303546	1.0019560	0.1492976
1.0024536	0.2527030	1.0021705	0.1766405	1.0017061	0.1916853	1.0020351	0.1817179
1.0025788	0.1036188	1.0022506	0.1684296	1.0018215	0.1779601	1.0021152	0.1689845
Sum W =	0.5000000	Sum W =	0.5000000	Sum W =	0.5000000	Sum W =	0.5000000
Average L =	1.002451	Average L =	1.002173	Average L =	1.0016875	Average L =	1.002039

For both methods you can change the intensity ratio and the wavelength ratio correction δ (i.e. doublet separation). This is not shown in the pictures.

See also:
Kα2 Stripping