generate the profiles, but allows the refinement of all model parameters. [*DIFFaX+* is available from the author (matteo.leoni@unitn.it) on request.]

3.6.2.6.8. *Antiphase domain boundaries*

In the diffraction pattern of an ordered alloy, a dissimilar broadening can often be observed for structure and superstructure peaks (with the former being present in both the ordered and disordered states). The superstructure peaks, in fact, bear microstructural information on the interface between the ordered regions in the material: broadening occurs when domains meet out of phase, creating an antiphase domain boundary (APB or APDB). A general formula for APDB-related broadening does not exist: for a given ordered structure, the Fourier coefficients correspond to the normalized value of $A_{\mathrm{APDB},hkl}(L) = \overline{F(0)F^*(L)}$, where $F(0)$ is the structure factor of a cell positioned at $L = 0$ and $F^*(L)$ is the complex conjugate of the structure factor of a cell at a distance L along the direction $[hkl]$. Being the result of a combination of probabilities, the peak is always expected to be Lorentzian.

Explicit formulae have been derived for the Cu_3Au ordered alloy ($L1_2$ phase; Wilson, 1943; Wilson & Zsoldos, 1966; Scardi & Leoni, 2005). Several types of boundaries can form, depending on the way that the domains meet: the broadening depends both on the boundary plane and on the local arrangement of Au atoms leading to conservative (no Au atoms in contact) or nonconservative (Au atoms in contact) boundaries. By arranging the indices in such a way that $h \geq k \geq l$ and that l is always the unpaired index, the broadening of the superstructure reflections can be described as (Scardi & Leoni, 2005)

$$A^{\mathrm{APDB}}(L) = \exp[-2L\delta f(h, k, l)]. \tag{3.6.51}$$

In this formula, $\delta = \gamma_{\mathrm{APDB}}/a_0$ is the probability of occurrence of an APDB, a_0 is the unit-cell parameter and $f(h, k, l)$ is a function of hkl defined in Table 3.6.2, obtained from the results of Wilson (1943) and Wilson & Zsoldos (1966).

The average distance between two APDBs is given by $1/\delta$. For a random distribution of faults, the broadening is Lorentzian and $A^{\mathrm{APDB}} = \exp(-4L\delta/3)$.

3.6.2.7. *Assembling the equations into a peak and modelling the data*

As previously mentioned, the broadening contributions briefly illustrated in the previous sections are employed to generate the powder peak profile for reflections from the set of planes $\{hkl\}$ using equations (3.6.11) and (3.6.12) and where

$$\begin{aligned} I_{hkl}(s) &= k(d^*) \int_{-\infty}^{\infty} C(L) \exp(2\pi i L s)\, \mathrm{d}L \\ &= k(s) \int_{-\infty}^{\infty} T^{\mathrm{IP}}_{\mathrm{pV}}(L) A^S_{hkl}(L)[A^D_{hkl}(L)\cos(2\pi L s) + iB^D_{hkl}(L)\sin(2\pi L s)] \\ &\quad \times \ldots \times [A^F_{hkl}(L)\cos(2\pi L s) + iB^F_{hkl}(L)\sin(2\pi L s)]\, \mathrm{d}L. \end{aligned} \tag{3.6.52}$$

Table 3.6.2
Models for antiphase domain boundaries for the Cu_3Au case

$N = h^2 + k^2 + l^2$.

ID	Model	$f(h, k, l)$
1	Random	2/3
2	{100} planes	$\frac{2}{3}\frac{h+k+l}{\sqrt{N}}$
2.I	{100} planes, no Au–Au contacts	$(k+l)/\sqrt{N}$ if h is the unpaired index $(h+l)/\sqrt{N}$ if k is the unpaired index $(h+k)/\sqrt{N}$ if l is the unpaired index
2.II	{100} planes, only Au–Au contacts	$\frac{2h+k+l}{2\sqrt{N}}$ if h is the unpaired index $\frac{h+2k+l}{2\sqrt{N}}$ if k is the unpaired index $\frac{h+k+2l}{2\sqrt{N}}$ if l is the unpaired index
3	{110} planes	$\frac{2}{3}\frac{4h+2k}{\sqrt{2N}}$
3.I	{110} planes, Au displacement parallel or perpendicular to plane normal	$\frac{4h}{\sqrt{2N}}$ if h is the unpaired index $\frac{2h+2k}{\sqrt{2N}}$ otherwise
3.II	{110} planes, Au displacement at 60° to plane normal	$\frac{2h+2k}{\sqrt{2N}}$ if h is the unpaired index $\frac{3h+k}{\sqrt{2N}}$ otherwise
4	{111} planes	$\frac{8h}{3\sqrt{3N}}$ if $h \geq (k+l)$ $\frac{4(h+k+l)}{3\sqrt{3N}}$ otherwise