# Appendix 1: Relationship of the stacking uncertainty σij and Biso

The uncertainty in stacking vector is implemented in DIFFaX in a method discussed separately by Drits and Treacy. (Drits & Tchoubar, 1990; Treacy, Newsam & Deem, 1991) In the DIFFaX user’s manual, Treacy introduces this uncertainty as a Debye-Waller-like term, dubbed “Fats-Waller” with coefficients Cij. The relationship between this Debye-Waller like term and a real space distribution describing the spatial correlations of discrete lamellar sheets is discussed below.

The phase term of the scattered wave is modified to account for the uncertainty **εj** associated with the stacking vector **R**j of the jth transition type. Consequently the position of the atoms in a general layer will be given by the sum of the basis vector **r**j and the stacking vector :

|  |  |  |
| --- | --- | --- |
|  |  | 10 |

In constructing the phase argument of the scattered wave amplitude we will consequently obtain terms (in three dimensions) of the form :

|  |  |  |
| --- | --- | --- |
|  |  | 11 |
|  |  | 12 |

Where αij is the transition probability, **s** is the scattering vector and the last term suggests a Debye-Waller-like factor. We will assume (a) the uncertainties are uncorrelated (i.e. stacking disorder of the second type (Drits & Tchoubar, 1990)) and (b) the uncertainty in the stacking vector is proportional to the mean square displacement (MSD) of the sheet. If the crystal obeys the harmonic approximation, then it is reasonable to assume that the MSD is normally distributed.

Making use of a general expression for the Debye-Waller Factor:

|  |  |  |
| --- | --- | --- |
|  |   | 13 |
|  |  | 14 |

Where <**u**2> is the mean square atomic displacement about u0 = 0 for some atom in some sheet. Uij and Bij have their typical meaning :

|  |  |  |
| --- | --- | --- |
|  |  | 15 |

We proceed by assuming that the MSD of the constituent atoms are representative of the MSD of the sheet, and that it follows a standard normal distribution. The value of <**u**2> can then be calculated as:

|  |  |  |
| --- | --- | --- |
|  |  | 16 |
|  |  | 17 |

Where N is the normalization factor, and **μ** and **σ** have their typical meanings and have components in three dimensions. Assuming that the displacement is isotropic and with reference to the atom position, the exponential terms become equivalent and μ becomes zero. Further, it can be shown that N for any dimension D is:

|  |  |  |
| --- | --- | --- |
|  |  | 18 |

Making the appropriate substitutions, collecting terms, and exchanging the discrete sum for an integral over all space, we have:

|  |  |  |
| --- | --- | --- |
|  |  | 19 |

With the change of variables:

|  |  |  |
| --- | --- | --- |
|  |  | 20 |

And recognizing the integrand as a symmetric function, the integral becomes:

|  |  |  |
| --- | --- | --- |
|  |  | 21 |

In which the integral is readily recognized as the Γ-function Γ(3/2):

|  |  |  |
| --- | --- | --- |
|  |  | 22 |

After substitution and collection of terms, we obtain the result that in the isotropic case, the MSD is equal to the square of the standard deviation, i.e.:

|  |  |  |
| --- | --- | --- |
|  |  | 23 |
|  |  | 24 |

Where convenient, the following expressions should be equivalent:

|  |  |  |
| --- | --- | --- |
|  |  | 25 |

Thus we can see there is an equivalence between the statistically distributed sheet correlations and the Debye-Waller-like effect approximating the uncorrelated position fluctuations of layers in a stacking disorder model.