About Debye-Waller Factor

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Basically there are two factors to describe the attenuation of scattering – the Lamb-Mössbauer factor (LMF, or the *elastic incoherent structure factor*) and Debye-Waller (DW) factor. The LMF factor is the ratio of elastic scattering to the total scattering for incoherent neutron scattering (or, specifically for Mössbauer spectroscopy). However, the DW factor refers to X-ray scattering or elastic neutron scattering. Also the DW factor is often used in a more generic way to include the incoherent case as well. For detailed description about the above information, see the 'Lamb-Mössbauer factor' Wikipage.

Before going on, it should be made clear the difference between coherent and incoherent neutron scattering (here incoherent scattering of X-ray is not talked about since it is not that important as it is for neutron scattering). Briefly, the coherent scattering is direction specific, but the incoherent scattering is distributed uniformly in all scattering directions. Also it should be pointed out that no matter for coherent or incoherent scattering, there will always be energy loss for part of the scattering, where the LMF and DW factor comes to help characterizing the energy loss for incoherent and coherent scattering, respectively.

For coherent scattering, the DW factor (DWF) is scattering direction specific, thus DWF can be written as the function of scattering vector $\vec{q}$ ($\vec{q} = \vec{k}_s - \vec{k}_i$, where $\vec{k}_i$ and $\vec{k}_s$ is the wave vector of the incoming and scattered beam, respectively), i.e. $DWF(\vec{q})$. The expression of $DWF(\vec{q})$ is:

$$DWF(\vec{q}) = \langle exp(i\vec{q}\cdot\vec{u})\rangle^2 \tag{1}$$

where $\vec{u}$ is hte displacement of the scattering center. The scattering vector and lattice vector determines the phase difference between the incoming and scattered beam, and corresponding phase factor is defined as:

$$F(\vec{q}) = 1 + exp(i\vec{q}\cdot\vec{r}) \tag{2}$$

The if there is a shift of the scattering center, the corresponding phase factor will be changed accordingly, which will, in turn, decrease the intensity of coherent scattering (since coherent scattering is direction specific). The final result is the distribution of scattering center position leads to the scattering intensity shifts away from the original maximum, which then finally gives the diffraction peak with diffuse background.

Back to the definition of DWF, and from the perspective of probability theory, DWF is actually the characteristic function of the distribution of $\vec{q}\cdot\vec{r}$. Then what is characteristic function? In probability theory, we have two different methods to describe any specific distribution – the first one is the cumulative distribution function and the other one is the corresponding characteristic function. The definition of the above two functions is as following:

$$F_X(x) = E[1_{\{X\leq x\}}] \tag{3}$$

$$\phi_X(t) = E[exp(itX)] \tag{4}$$

where 'E' represents the expectation value. Here it should be pointed out that the symbol X is an ensemble notation, referring to the whole data set corresponding to any given distribution. Thus 'X' here is only a SYMBOL, and the actual independent variable for F_X and ϕ_X is 'x' and 't', respectively. Moreover we have:

$$\phi_X(t) = E[exp(itX)] = \int_R e^{itx} dF_X(x) = \int_R e^{itx} f_X(x)dx \tag{5}$$

where we have:

$$f_X(x) = \frac{F_X(x)}{dx} \tag{6}$$

and $f_X(x)$ is the probability density function of the random variable X. Therefore from (5) and (6), it can be found that the cumulative distribution function $F_X(x)$ and the characteristic function $\phi_X(x)$ contains exactly the same information for random variable X - both of the two functions are directly linked to $f_X(x)$.

Back to the definition of DWF, if assuming $\vec{q}\cdot\vec{u}$ obeys the standard normal distribution (which is implied by the assumed Boltzman distribution, see the 'Debye-Waller Factor' Wikipage), the expression for DWF can be further written down as:

$$DWF = exp(-\langle[\vec{q}\cdot\vec{u}]^2\rangle) \tag{7}$$

The derivation of (7) is as following: since we already know the characteristic function of the normal distribution $N(\mu,\sigma^2)$ as following:

$$N(\mu,\sigma^2) \underset{\text{function}}{\overset{\text{characteristic}}{\longleftrightarrow}} e^{it\mu-\frac{1}{2}\sigma^2t^2} \tag{8}$$

For details about characteristic function, see 'characteristic Fucntion' Wikipage). Furthermore, for the previously assumed standard normal distribution for $\vec{q}\cdot\vec{u}$, we should have $\mu = 0$ and $\sigma = 1$. Thus the corresponding characteristic function becomes $exp(-\frac{1}{2}t^2)$, and then DWF becomes:

$$\begin{aligned} DWF(\vec{q}) &= \langle exp(i\vec{q}\cdot\vec{u})\rangle^2 \\ &= [exp(-\frac{1}{2}\langle[\vec{q}\cdot\vec{u}]^2\rangle)]^2 \\ &= exp(-\langle[\vec{q}\cdot\vec{u}]^2\rangle) \end{aligned} \tag{9}$$

The expression (9) for DWF is the form that is commonly used in practice.