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Response to the "comments on Fourier transforms of truncated quasilattices"

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It has been suggested by Srinivasan (1990) that the intensity fluctuations observed by us in the diffraction pattern of finite-size quasilattices are due to the effect of the window function which is well-known. It is shown that, in the present case, the window-function effect is quite negligible, contrary to the suggestion made by Srinivasan. It is also shown that several other features cannot be explained by the window-function whereas these are relevant to the present calculation.

The contribution of the window-function to the intensity fluctuations and the half-widths of the peaks in the diffraction from finite-size quasilattice have been estimated. The details are given below for the peak closest to the origin ($x^* \approx 2$) which will be affected maximum by the window-function. The intensity fluctuations observed with the change in the size of the 1-dimensional quasilattice cannot be quantitatively accounted for by the conventional finite-size effect known in the periodic lattice.

The intensity distribution due to the slit-function (width L) is given by $I(k) = (L(\sin(kL/2)/(kL/2)))^2$. The positions of the secondary maxima are approximately given by $x^* = n/2L$; n:odd$(k = 2\pi x^*)$ (Sommerfeld 1954). At these positions, the intensity is given approximately by $I(x^* \text{sec. max.}) \approx L^2/2n^2$. For the peak closest to the origin ($x^* \approx 2{\cdot}341$), $I(x^* \approx 2)/N^2 \approx 1/32N^2$ where the number of scatterers, $N \approx L$. For $N = 20, I(x^* \approx 2)/N^2 \approx 1/(32 * 400) \approx 0{\cdot}8 \times 10^{-4}$. For $N = 30$, it comes to $0{\cdot}4 \times 10^{-4}$. This gives the intensity fluctuation $0{\cdot}4 \times 10^{-4}$ whereas the corresponding case in the numerical calculation (i.e. 1-dimensional quasilattice) gives $0{\cdot}9 \times 10^{-2}$. This clearly indicates that the observed intensity fluctuations are 100 times more than that allowed by the conventional finite-size effect. In addition, the observed intensity of the peak in the above case is $0{\cdot}3(= I/N^2)$ which is 10^4 times higher than the contribution from the above finite-size effect. This has been checked for the other values of N.

For large values of k, the maxima of the slit-function are given by the maxima of $\sin^2(Lk/2)$. The maxima occur at $Lk/2 = n\pi/2$; n:odd. Near the maximum, $k = k_{max} + \delta k = n\pi/L + \delta k$. It is easily obtained that when $\delta k = \pi/2L$, $\sin^2(Lk/2) = 1/2$. This approximately gives the half-width $\delta x^* = 1/4L$. The estimated half-widths are found to be 1·7 times smaller than the observed values. The variation of the observed half-widths with the size of the quasilattice is found to behave as $L^{-1{\cdot}0}$. On the other hand, for a crystal lattice with scatterers spaced τ apart the calculated half-widths agree very well with the estimated values within 1%. In the quasilattice case there is an extra factor not accounted for by the window-function.

The diffraction pattern has been already calculated from different finite segments of quasilattice having the same width and number of scatterers (figure 12, Balagurusamy *et al* 1990). The peak-positions have been numerically calculated starting from the positions where the peaks would occur in the diffraction from an ideal quasilattice with the smallest interval possible (10^{-6}) and then locating the maxima nearest to them. Although the width is the same, the peak-positions have been found to shift which cannot be explained by the slit-function. This clearly indicates that the arrangement of scatterers plays a crucial role in determining the diffraction pattern.

In the 2-dimensional case, though the real-space tiling (e.g. figure 6 in Baranidharan *et al* 1990) shown is not circular, it has been pointed out in the paper (p. 543) that only scatterers lying in the circular region were used in the Fourier transform calculations.

References

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