**Short Communications**

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.


**Comments on The accuracy of experimental radial distribution functions for metallic glasses by B. J. Thijsse (1984).** By F. HAJDU, Central Research Institute for Chemistry, Hungarian Academy of Sciences, Budapest, POB 17, H-1525 Hungary and G. HERMS, Department of Physics, Wilhelm Pieck University of Rostock, DDR 2500 Rostock, Universitätsplatz 3, German Democratic Republic

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**Abstract**


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A passage of a paper by Thijsse (1984) calls for correction. § V C (p. 70) of the paper (with omission of a few less important words) reads as follows.

'To calculate the best possible approximation to \( G(r) \) on the basis of available data, one computes \( G(r_k) \) using (16).'

[Equation (16) (p. 63 of the paper) reads]

\[
G(r_k) = \frac{2}{\pi} \sum_{i=1}^{N} F(Q_i) \sin(Q_i r_k) \Delta Q \\
\text{for integer } k, \text{ but also for the fractional values } k = \frac{1}{2}, \frac{3}{2}, \ldots
\]

\(Q_i = i \Delta Q, r_k = k \Delta r, Q_N = N \Delta Q = 4 \pi \lambda^{-1} \sin(\theta_{\text{max}}), \lambda = 0.071 \text{ nm and } 2\theta_{\text{max}} = 158^\circ.\]

'The method works as follows. One defines an artificial function \( F'(Q) \) of which only the values at the points \( Q_{N+1}, Q_{N+2}, \ldots, Q_{4N} \) are considered (...). Thus, \( F'(Q) \) is used to represent \( F(Q) \) in the experimentally unaccessible region above \( Q_N \). First, all \( 3N \) numbers \( F'(Q_i) \) are given the value zero. When (16) is applied, ..., and \( N \) is made four times as large, four times as many data points \( G(r_k) \) are obtained, at quarter intervals. This procedure is equivalent to assuming that (16), in its original form, is not only valid for integer \( k \), but also for the fractional values \( k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots \), etc. Although this method is a convenient way of making the graph for \( G(r) \) easier to read (...), only one out of every four points is genuine, i.e. represents experimental information. The other points are merely generated by the implicitly chosen interpolation scheme. ... Nevertheless the method has its merits, as we shall see.'

Our comments on this passage are given below.

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(1) **Comments on the integral formula**

1.1. Mathematically, (16) expresses the simple rectangle rule for numerical integration applied to (9) (p. 62 of the paper):

\[
G(r) = \frac{2}{\pi} \int_{0}^{\infty} F(Q) \sin(Qr) dQ, \text{ where the integrand is multiplied by the data window } [W(Q) = 1 \text{ for } 0 \leq Q \leq Q_N, \text{ and } = 0 \text{ for } Q > Q_N].
\]

From the physical point of view, (16) is an adequate expression for a step-scanning measurement of \( F(Q) \) taken at the points \( Q_i \) and across a rectangular slit of width \( \Delta Q \).

The coincidence of formulas corresponds to the equivalence of two sampling procedures: one carried out on paper (or computer), the other on the diffractometer.

1.2. Both equations, (9) for \( G(r) \) and (16) for \( G(r_k) \), obviously show that the values of \( G(r) \) at any point \( r \) are determined by an integral of the whole (available) function \( F(Q) \) taken over the entire (available) range of \( Q \) (and of course, oppositely in the inverse transformation).

1.3. The points \( r_k \) where \( G(r_k) \) values are computed are optional and independent of \( F(Q) \) or its approximations with broken lines.

1.4. The kernel of the Fourier integrals (9) and (16) is \( \sin(Qr) \). Formally this function is symmetrical for the two reciprocal variables \( Q \) and \( r \), essentially it is not because one of them is the variable of integration while the other is a numerical parameter of the argument and constant for the integral.

(2) **Comment on the resolution of a RDF**

There is a general law for all kinds of optical image-forming procedures concerning their resolving power: this is determined by the maximum of the viewing angle and inversely proportional to the applied wavelength. The variable \( Q \) contains both factors and so the resolution of the RDF is determined by the available \( Q_{\text{max}} \). It must be stressed, however, that the extension of the \( Q \) range has physical sense only when the intensity function in that range has some structure (i.e. an interference pattern), otherwise the extension is 'empty', giving no further details to the image. To contrast with a possible reading of Thijsse's text, it must be emphasized that the limited resolution of an optical procedure never means that the object is well 'seen' at selected points with unseen areas between them. In fact, the image spots of two adjoining object spots get smeared into one and become undiscernible if the object distance between them does not exceed a critical value.

In the referenced passage the RDF resolution may be a
misplaced term for the limited resolution of the X-ray measurement and this is the main reason for the present comments.

(3) Comments on sampling

Sampling methods and digital techniques are inseparable features of measuring, recording and computing continuous functions of space or/and time. In the present case sampling appears in three different items.

3.1. The step-scanning operation of a diffractometer means a sampling measurement of the intensities \( f(Q) \). The intervals \( \Delta Q \) must be sufficiently short so as not to lose any features of the reduced intensities \( G(r) \).

3.2. It follows from the principle of Fourier transformation that the transform \( [G(r)] \) is necessarily a sampled function. The sampling points are optional and they should be chosen so as to make all features of \( G(r) \) visible.

3.3. The \( \sin \) function enters (16) also in sampled form. The intervals are not simply \( \Delta Q \) but \( r_k \Delta Q \), where \( 0 \leq r_k \leq r_{\text{max}} \). \( r_{\text{max}} \) is an optional limit of \( r \) where one finishes computation. \( \Delta Q \) should be so small that, if multiplied by \( r_{\text{max}} \), it should allow the appearance of all maxima, minima and zero points of \( \sin(Q) \).

From these it can be concluded that an inherently good experiment can be well exploited by the proper choice of \( \Delta Q \) and \( \Delta r \), or not, in the opposite case.

(4) Comment on fast Fourier transformation

The fast Fourier transformation is an algorithm to perform a Fourier transformation on the computer. It is based on a scheme of the possible arguments of the function \( \sin (rQ) \). If it offers an insufficient fine division for the argument then it must be either changed or abandoned. The formal extension of the \( Q \) range is one way to improve the fineness of the scheme. The 'new' \( r_k \) points obtained by this are as good as the 'original' ones and the \( G(r_k) \) values do not have to be divided into groups of 'genuine' and 'interpolated'. The effect of an artificial extension of \( F(Q) \) (the Lanczos function) must be treated with precaution. Also, the extension of \( G(r) \) beyond a physically sensible limit calls for a critical attitude.

The authors hope that the present revised text reflects to some extent the mutually acceptable points which have come to light by direct correspondence with B. J. Thijsse who is thanked for his collegial attitude to our critical comments.

Reference


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Abstract


Unfortunately some confusion over the functions \( G(r) = \int_0^\infty f(Q) \sin(Qr) \, dQ \) and \( G_I(r) = \int_0^\infty f(Q) \sin(Qr) \, dQ \) appears to be present in the comments by Hajdu & Herm (1986) [H & H]. The latter function is, in the least-squares sense, the best possible approximation of the first one, out of all possible functions of the type \( \int_0^\infty f(Q) \sin(Qr) \, dQ \). In other words, one cannot hope to compensate for the lack of knowledge of \( F(Q) \) above \( Q_N \) by cleverly modifying \( F(Q) \) below \( Q_N \). But, since \( G_I(r) \) is - by definition - a band-limited function, it is completely determined by its values at a discrete set of abscissae \( r_k \) with a spacing \( \Delta r = \pi/Q_N \).

Of course, since \( G_T \) is an ordinary function of \( r \), one is at liberty to calculate \( G_T(r) \) for \( r \) values not belonging to this set as well [H & H, §§ 1.2 and 1.3], but one does not obtain extra information on \( G_T(r) \), or on \( G(r) \), in this way. This is the crucial point of the matter. In fact, one does not even need to know \( F(Q) \) to calculate \( G_T(r) \) between the points \( r_k \). This is why I have called the set of values \( G_I(r_k) \) 'genuine' data points, since they represent all of the available information (perhaps 'sufficient' would have been a better word?). It does not imply, however, that there are 'unseen areas between them' [H & H, § 2], and I have nowhere suggested this. Rather, it implies that these areas 'give no further details to the image'; a statement, strangely enough also made by Hajdu & Herm [H & H, § 2].

Finally, I do not agree with comments 3.2 and 3.3: neither \( G_T(r) \) nor \( G(r) \) are necessarily sampled functions (in fact they are not), and both \( r_{\text{max}} = \pi/\Delta Q \) and \( \Delta r = \pi/Q_N \) are determined by the experimental conditions: for instance, one cannot trade the rather useless values of \( G_I \) at high \( r \) values for the much more interesting in-between values at low \( r \).

References