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An Interactive FORTRAN Program for the Evaluation of Structure Factors and Pair Distribution Functions from Neutron Diffraction Experiments

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An Interactive FORTRAN Program for the Evaluation of Structure Factors and Pair Distribution Functions from Neutron Diffraction Experiments

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Abstract

This report describes an interactive program to evaluate neutron diffraction data using the Graphic System (GS) under MVS(TSO). Different evaluation steps may be directed by a CLIST. The present program is limited to cylindrical sample geometry. From the fully corrected static structure factor the pair correlation function g(r) and the radial density function may be calculated from which the mean coordination number can be obtained by numerical integration over the main peak. Producing a hardcopy output on a mechanical plotter is provided.

Ein Interaktives FORTRAN Programm zur Auswertung von Strukturfaktoren und Paarverteilungsfunktionen aus Neutronenstreuexperimenten

Kurzfassung

Dieser Bericht beschreibt ein Programmsystem zur interaktiven Auswertung von elastischen Neutronenstreudaten durch die Verwendung des Graphischen Systems (GS) unter MVS(TSO). Der Aufruf der verschiedenen Auswerteprogramme wird über eine CLIST-Prozedur durchgeführt. Die Auswertung ist auf zylindrische Probengeometrie beschränkt. Aus dem korrigierten statischen Strukturfaktor kann die Paarverteilungsfunktion g(r) und die radiale Verteilungsfunktion ermittelt werden, aus der die mittlere Koordinationszahl durch numerische Integration über den ersten Peak angenähert bestimmt werden kann. Die erzeugten Bilder können über einen mechanischen Plotter ausgegeben werden.

CONTENTS

1. Introduction

Neutron diffraction methods have been used extensively to investigate the structure of amorphous solids and liquids.

Based on /1/ a system of programs has been developed to evaluate neutron diffraction patterns in an interactive environment using a dual screen workstation concept, as described in more detail in section 3. The scattering data, which are conveniently measured with the variable 2Θ-method, are usually recorded on tape for each scattering angle.

In order to determine the total structure factor S(Q) from experimental data , the measured intensity must be corrected for background scattering, for container scattering and for absorption in the sample and possibly in the container according to Paalman and Pings/2/. To convert the corrected intensity to an absolute scale the evaluation of a vanadium measurement is included. Corrections for incoherent scattering and multiple scattering/3/ may be applied to the data. Inelastic scattering effects are considered analytically according to Placzek/4,5/.

In the next stage of evaluation the Fourier transform of the total structure factor S(Q) may be performed to get the total pair correlation function g(r) and the radial density function (RDF). The coordination number may be derived by numerical integration over the first (main) peak of the RDF.

The formalism described in the text holds for monatomic systems. If extended to more than one typ of atom appropriate averaging of scattering and absorption cross sections must be made. This program so far cannot be applied to calculate partial distribution functions for amorphous alloys but can easily be extended to do so.

The programs have been written in FORTRAN 77 and have been compiled and tested on the IBM/3033 under OS/VS2 MVS-TSO. For the graphic output the Graphic System (GS)/12/ has been used. The overall use of the programs may be directed by a CLIST which is described in section 3. Some further features pertaining the retrieval of the diffraction data or production of hard copy plots are also outlined. It should be noted, that this modular scheme of program calls allows to enlarge the program system with other application programs for special evaluations or data handling routines, if desired.

2. Data Analysis

The following part of this report is not intended to be exhaustive. Some of the descriptions will represent an oversimplification but will, hopefully, be sufficient to aid the user. Moreover, the evaluation is done conversationally, so that all necessary information required by the programs is requested from the user mostly in a selfexplanatory way.

2.1 Calculation of Corrections

Before starting the evaluation step a correction file which contains all necessary data needed to correct for absorption, multiple scattering and inelastic scattering must be created for an experiment to be evaluated. The related program may be called by selecting the C option on the program selection menu as described in section 3.3. Because these corrections are in our case smoothly varying functions, least-squares polynoms of order of 6 have been fitted to the correction factors. These interpolation polynoms are then used later in the analysis. All analytical corrections are restricted to cylindrical geometry.

2.1.1 Absorption

Corrections have to be done for scattering and absorption in the sample and sometimes in the sample container (i.e. pressure cell etc.). A detailed description of the evaluation of the absorption integrals is given in /2/. Based on this formalism some computer programs have been developed by /6/ and which have been used in our program. With respect to the geometry and scattering power of the sample+container the following geometric absorption factors have been provided as a function of the scattering angle 2Θ (in the notation of /2/):

$A_{s,s}$ (2Θ)	Cylindrical absorption factor for scattering and self-absorption in the sample

$A_{s,sc}$ (2Θ)	Cylindrical absorption factor for scattering in the sample and for absorption in both sample and container
$A_{c,c}$ (2Θ)	Cylindrical absorption factor for scattering in the container and self-absorption in the container
$A_{c,sc}$ (2Θ)	Cylindrical absorption factor for scattering in the container and absorption in both sample and container

2.1.2 Multiple Scattering

The multiple scattering of neutrons in a cylindrical specimen of amorphous materials can be kept rather small and forms an isotropic background which can simply be removed from the corrected intensity. The correction factor has been calculated in the incoherent approximation for a range of R/h, wherein R is the radius and h the height of the cylinder/3/.

2.1.3 Inelastic Scattering and Placzek Correction

For structural investigations a total diffraction experiment is performed in which the integration over the elastic and inelastic scattering is done by the detector. To get the correct neutron intensity for constant Q the data have to be transformed from the Θ-space to the Q-space. Departures from the static approximation have been calculated in this program using the formulas as given in /5/ for a 1/v detector or a detector with an arbitrary energy-dependant efficiency.

2.2 Raw Data Preparation

Before performing the data reduction the user has some possibilities to change the input spectra. Several equivalent measurements may be added to improve the statistics. If desired, a measurement may be multiplied with a constant factor.

2.3 Determination of Total Structure Factor S(Q)

The data reduction program may be made available for execution by entering option S on the program selection menu. There are several experimental runs which are usually included in a diffraction experiment. The input description for the diffaction pattern is outlined in section 3.1. Apart from the immediate graphic representation on the graphic screen, the main results may be saved in a picture data set for producing a hard copy/15/. Scale parameters must be entered by the user and may be modified interactively, where desired.

The intensity function or structure factor S(Q) is directly related to the **coherent differential cross section** in the static approximation by

$$\frac{d\sigma^{(coh)}}{d\Omega} = N\,b^2\,S(Q)$$

wherein for neutrons b is the atomic scattering length and N the number of scattering atoms. Q is equal to $4\pi/\lambda \sin\Theta$ with λ the wave length of the incoming neutrons and Θ the half angle of diffraction. Experimentally, the measured coherent scattering intensity does not give, in principle, the structure factor S(Q) directly, but it is proportional to the effective differential cross section

$$\left(\frac{d\sigma^{(coh)}}{d\Omega}\right)_{eff} = N\,b^2 \int_{-\infty}^{E_0} \varepsilon(k)\,\frac{k}{k_0}\,S(Q,\omega)\,d\omega$$

with Θ constant. $\varepsilon(k)$ is the energy-dependent detector efficiency, k_0 and k are the wave numbers of the incident and scattered neutrons, E_0 the incident neutron energy defined by $(h/2\pi)\,\omega_{max}$. $S(Q,\omega)$ is the van Hove generalized scattering law which is related to S(Q) by

$$S(Q) = \int_{-\infty}^{\infty} S(Q,\omega)\,d\omega$$

wherein Q must be held constant in the integration. The departure of k/k_0 from unity, the influence of the detector efficiency $\varepsilon(k)$ and the curvature of the integration paths in the Q-ω plane give rise to a number of problems in relating the measured intensity to the structure factor S(Q). Therefore, to obtain a S(Q) of a high accuracy, various corrections must be applied to the data, and limitations have to be carefully taken into account. Principal sources of errors have been summarized in the following:

1. Calibration of the equipment
2. Resolution
3. Counting statistics
4. Background
5. Multiple scattering
6. Placzek corrections
7. Finite Q range covered by the experiment
8. Uncertainties in the cross sections
9. Effects of absorption
10. Detector efficiency
11. Effective sample volume
12. Integral relationships for S(Q)

Some of these are of critical importance and must be evaluated as much accurate as possible. More detailed information on some of these corrections is given in section 2.1.

In the following some symbols used below are explained:

f_v	Placzek correction for vanadium
f_s	Placzek correction for the sample
Δ_v	Multiple scattering for vanadium
Δ_s	Multiple scattering for the sample
I_c	Scattering intensity of container
I_v	Scattering intensity of vanadium
I_{c+s}	Scattering intensity of sample with container
I_s	Scattering intensity of sample
N_s	Number density for sample
N_v	Number density for vanadium
A_v	Absorption coefficient $A_{s,s}$ for vanadium
σ_s	Scattering cross section (barn)
σ_c	Coherent scattering cross section (barn)

σ_i	Incoherent scattering cross section (barn)
γ	Normalisation factor which converts absolute intensity to an measured intensity
σ_i^v	Incoherent scattering cross section (barn) for vanadium

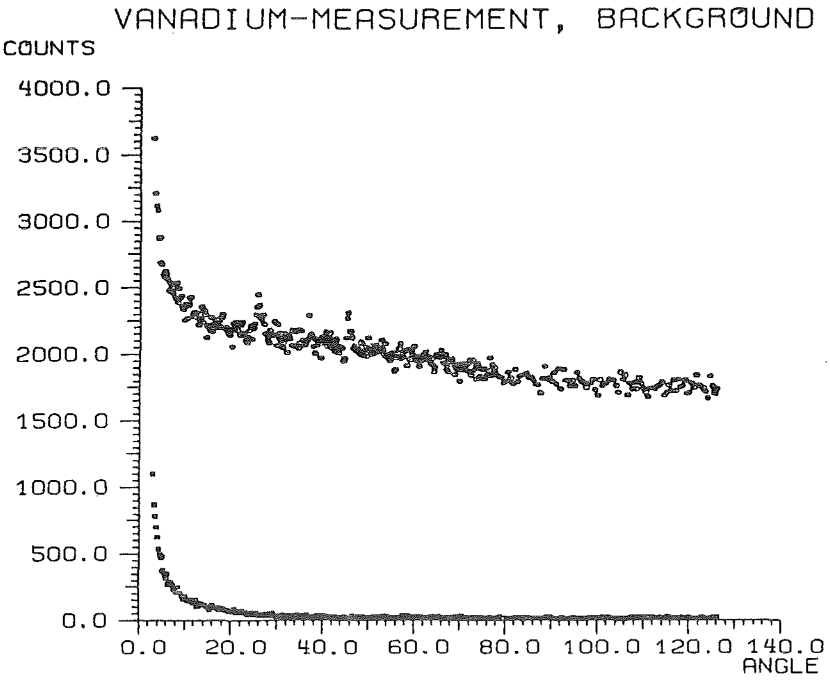

Fig. 1. Vanadium and Background Measurement

For neutrons $\sigma_i^v/\sigma_c^v = 170$ for vanadium which makes it an ideal calibration substance for diffraction experiments. First, the measured vanadium intensities defined by

$$I_v(2\Theta) = \gamma(2\Theta)\, N_v\, \sigma_i^v\, (\, 1 + f_v(2\Theta)\,)\, (\, 1 + \Delta_v(2\Theta)\,)\, A_v(2\Theta)$$

are calculated and corrected for absorption and multiple scattering. To get the normalisation curve the vanadium may be smoothed by a polynomial fit. For more details the user is referred to /1/. Fig. 1 shows the vanadium together with the background measurement.

Next, the container will be corrected for background. The sample and the background measurements may be corrected for air scattering behind the sample with a cadmium measurement. The correction of the sample intensity for container and absorption can be done using the relation of /2/

$$I_s(2\Theta) = \left[I_{c+s}(2\Theta) - \frac{A_{c,sc}(2\Theta)}{A_{c,c}(2\Theta)} I_c(2\Theta) \right] \frac{1}{A_{s,sc}}$$

The scattered intensity (coherent + incoherent) can be evaluated in the program using the relation

$$I_s(2\Theta) = \gamma(2\Theta)\, N_s \left[\sigma_c(S(2\Theta) + f_s(2\Theta)) + \sigma_i(1 + f_s(2\Theta)) \right]$$

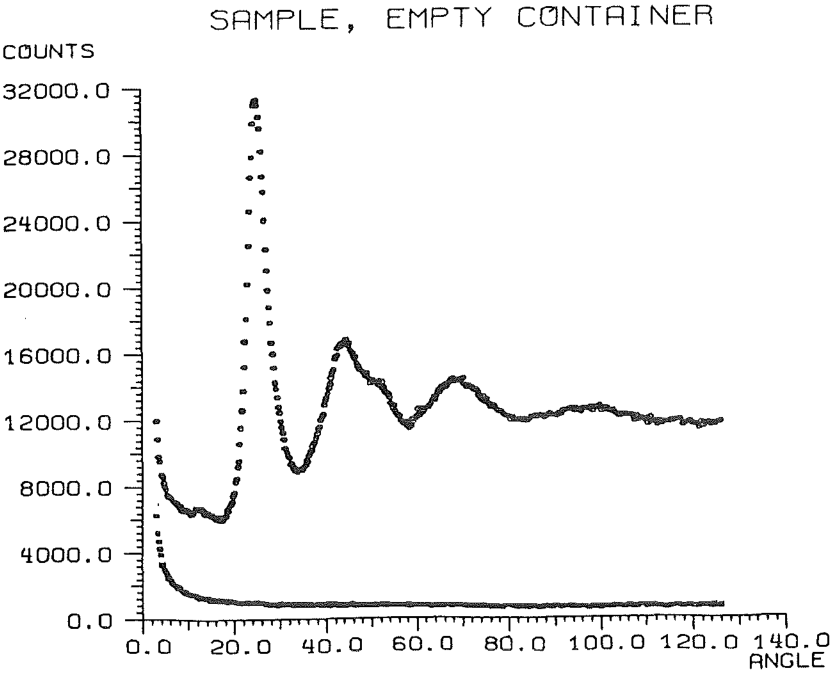

Fig. 2. Raw Data and Empty Container Measurement

In a typical experimental run the counts are recorded at specific intervals for 2Θ between two limiting values for the diffraction angle. Fig.2 shows the raw data for amorphous $Cu_{56}Zr_{44}$ and the empty container measurement. From I_V the normalisation factor $\gamma(2\Theta)$ may be derived to convert the observed intensity to an absolute scale. From the above expression for $I_s(2\Theta)$ which includes multiple scattering we have the total structure factor written for the scattering angle 2Θ (or Q)

$$S(2\Theta) - 1 = \frac{I_{s(2\Theta)}}{\gamma(2\Theta)\ N_s\ \sigma_c} - \frac{\sigma_s}{\sigma_c}\ (\ 1 + f_s(2\Theta)\ )\ (\ 1 + \Delta_s(2\Theta)\ )$$

after rearranging and substituting $\sigma_s = \sigma_c + \sigma_i$. The most important correction is that due to Placzek. Fig.3 represents the experimental results for S(Q) after all corrections have been applied.

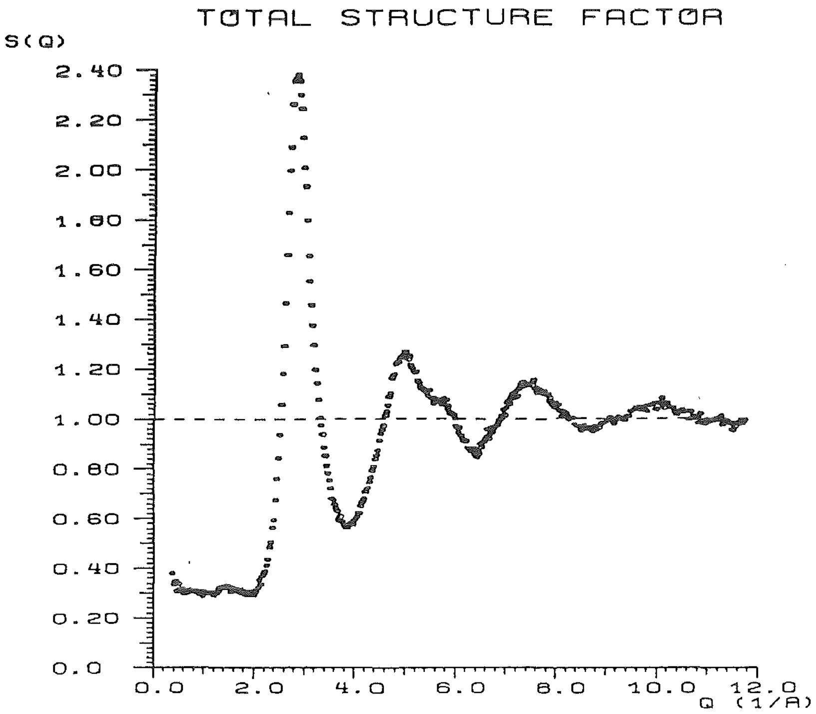

Fig. 3. Fully Corrected Structure Factor S(Q) for $Cu_{56}Zr_{44}$

2.4 Calculation of the Pair Correlation Function g(r)

This section describes how one can extract the pair correlation function from the experimental structure factor S(Q).

The structure factor S(Q) for an **isotropic system** may be related to the local density $\rho(r)$ by the well-known formula

$$S(Q) = 1 + \int_0^\infty 4\pi r^2 \rho(r) \frac{\sin Qr}{Qr} dr$$

wherein $R(r) = 4\pi r^2 \rho(r)$ represents the radial density function (RDF). With the mean atomic density ρ_0 of the scattering system S(Q) becomes then

$$S(Q) = 1 + \frac{4\pi\rho_0}{Q} \int_0^\infty (g(r) - 1) r \sin Qr \, dr$$

wherein $g(r) = \rho(r)/\rho_0$ is the pair correlation function. If we write the reduced interference function

$$F(Q) = (S(Q) - 1) Q$$

the structure factor S(Q) and the pair correlation function g(r) are interrelated by the Fourier transform pair

$$g(r) = 1 + \frac{1}{2\pi^2 r\rho_0} \int_0^\infty F(Q) \sin Qr \, dQ$$

$$F(Q) = 4\pi\rho_0 \int_0^\infty (g(r) - 1) r \sin Qr \, dr$$

In practice, however, we do not have experimental data for S(Q) from zero to infinity as required by the transform given above. The lower and upper integration limits Q_{min} and Q_{max} are are given by the 2Θ range covered by the diffraction experiment.

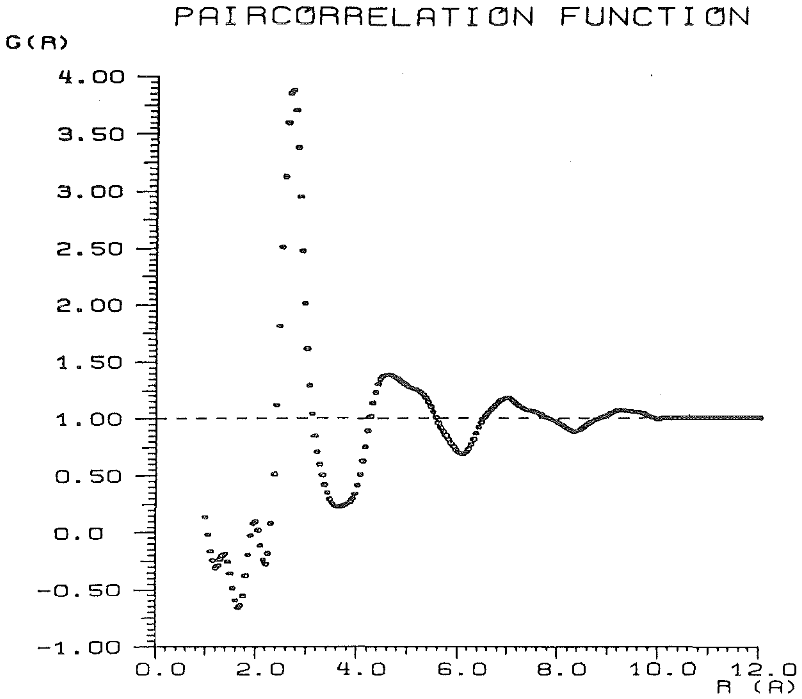

Fig. 4. Pair Correlation Function g(r) for $Cu_{56}Zr_{44}$

The Fourier transformation has been performed numerically by means of Romberg's integration method. The pair correlation function g(r) may be calculated for an equidistant r-scale, starting with $r_1 \geq 0$ and going up to r_2 by the stepsize Δr as required from the user via the alphanumeric keyboard during an evaluation run. The scale may be expanded to a $r_{max} \geq r_2$ as defined by input. Then we have (Fig.4)

$$g(r) = 1 + \frac{1}{2\pi^2 r\rho_0} \int_{Q_{min}}^{Q_{max}} (S(Q) - 1) Q \sin Qr \, dQ \, , \quad r_1 \leq r \leq r_2$$

$$g(r) = 1 \quad , \qquad r_2 < r \leq r_{max}$$

The truncation leads to the so-called termination errors in the

correlation functions, i.e. the distributions may exhibit unphysical oscillations especially at small values of r; the cut of the S(Q) at Q_{max} introduces a broadening of the peaks and oscillations with a pseudoperiod of $2\pi/Q_{max}$ called **termination ripples**.
In order to minimize the influence of the cut-off in the experimental data on the Fourier transform, various modification functions M(Q) are sometimes used in the range of r between 0 and Q_{max}. This, however, may lead to a smearing out of structure which may have physical significance and g(r) can be written as:

$$g(r) = 1 + \frac{1}{2\pi^2 r\rho_0} \int_0^{Q_{max}} (S(Q) - 1) \, Q \, M(Q) \sin Qr \, dQ$$

Instead of the step function M(Q) = 1 the following **window functions** may be chosen by the interactive user. The first window function is represented by the artificial temperature factor/7/

$$M(Q) = e^{-\alpha Q^2} \qquad \text{with} \quad \alpha = \ln \frac{10}{Q_{max}^2} .$$

An alternative giving better results is the peak shape function as suggested by Lorch/8/,

$$M(Q) = \frac{\sin \Delta r \, Q}{\Delta r \, Q}$$

wherein $\Delta r = \pi/Q_{max}$ represents a resolution length in real space.

On the other hand, refinement techniques based on **iterative procedures** are also applied; from R(r) one gets

$$G(r) = 4\pi\rho_0 (g(r) - 1) r = \frac{2}{\pi} \int_0^{\infty} F(Q) \sin Qr \, dQ$$

which has been used by some authors to remove the spurious ripples at small r by Fourier transformation and inverse Fourier transformation between g(r) and S(Q)/9/. But such a procedure has not yet been included in this program.

The absolute value of S(Q) may be further refined by the following integral relationships. The limiting value for S(Q) when Q approaches zero may be obtained directly from the above expression for S(Q). So we have from the compressibility equation/10/

$$S(0) = \rho_0 \, k_B T \, \chi_T$$

where k_B is the Boltzmann constant, T the absolute temperature, χ_T the isothermal compressibility and ρ_0 the average number density of the system. This value may be then used as a guide of view to extrapolate the experimental S(Q) smoothly to small Q. However, substantial errors may be introduced, because it is often difficult to determine the true functional form of S(Q) in the region of small Q outside the range of measurement due to statistics. Because the value for χ_T is not generally known this relation has not been used so far in the reported program. As a consequence of the fact that g(0) is zero due to the strong interatomic repulsion at short range, the **sum rule** given below follows at once from g(r)

$$\int_0^\infty Q^2 \, (\, S(Q) - 1 \,) \, dQ = - 2\pi^2 \rho_0$$

This relation must be satisfied by the correct structure factor S(Q). It may be, therefore, used either as a check, if the intensity may be considered to have already reached a constant value for the finite upper value Q_{max}, or as a normalisation. The value of the integral will be displayed for inspection and might be taken into account for a supplemental calibration of S(Q), if desired.

2.5 Calculation of the Radial Density Function R(r)

If we substitute $\rho(r)=\rho_0 g(r)$, the radial density function R(r) becomes then

$$R(r) = 4\pi r^2 \rho_0 + \frac{2r}{\pi} \int_0^\infty F(Q) \sin Qr \, dQ$$

Fig. 5 shows the radial density function R(r) which represents the number of atoms in a spherical shell of radius r and thickness unity. Therefore, the RDF reflects the atomic distribution more directly then the pair correlation function g(r) and allows some interpretations about the **short-range topological order** of the system. This function is zero for values of r less than the hard-sphere diameter of the atoms, oscillates around $4\pi r^2 \rho_0$ and tends towards $4\pi r^2 \rho_0$ for larger r.

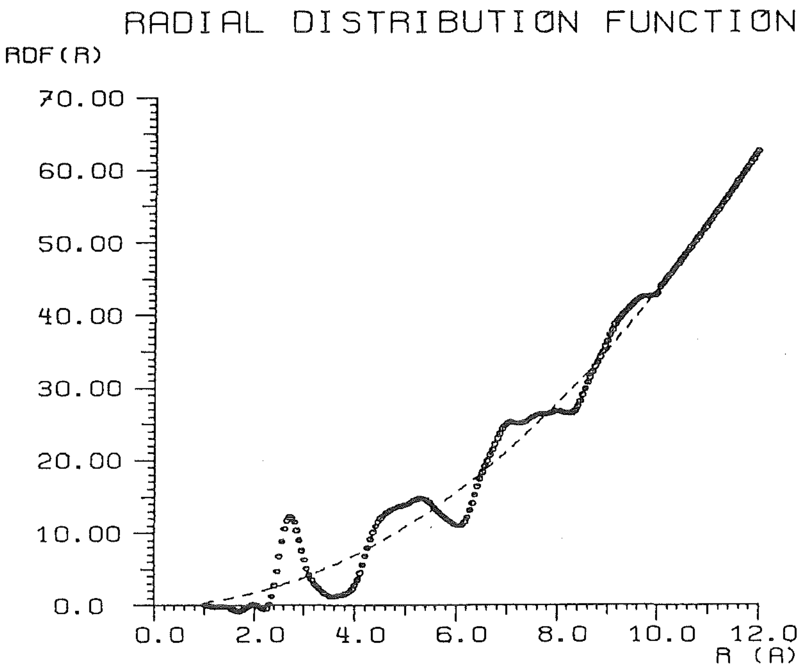

Fig. 5. Radial Density Function R(r) for $Cu_{56}Zr_{44}$

From the radial density function $4\pi r^2 \rho(r)$ a preliminary coordination number C_i may be derived by integration over a selected interval

$(r_i-\delta_1, r_i+\delta_2)$ around pronounced peaks i.

$$C_i = \int_{r_i-\delta_1}^{r_i+\delta_2} 4\pi r^2 \rho_0 g(r)\, dr$$

However, the determination depends considerably on the way in which the peaks can be separated from subsequent peaks, because well separated peaks are not always apparent and overlapping is generally observed. Therefore, several methods may be used to obtain the number of the first, second, etc. neighbours about a given atom/11/.

One method consists in an extrapolation of the right-hand side of the peak to the abscissa. Another method is based on the assumption that the coordination shells are symmetrical about a radius defined by the peak position in the RDF, so the integration has to be done between the left-hand side of the peak and its maximum and multiplied by two. It should be noted that there may be an asymmetric contribution with respect to the mean distance for amorphous metals, so this method may give too low values for C_i. Third, the coordination number may be derived approximately by integrating the area under the peaks in the (smoothly corrected) RDF. However, if termination ripples are present, this method may also give probably unreliable results.

3. Executing on OS/VS2 MVS-TSO

3.1 Description of the Graphic Workstation

The program uses the Graphics System (GS) of the KFK, which permits to attach a non-IBM graphic storage display monitor to the IBM/3277 Model 2 display terminal (Fig.6). In our case a TEKTRONIX 618 storage display unit has been used. For detailed informations about this special approach to interactive graphics the user is referred to /12/.

```
                                       -----------
                                      |           |
                                      | IBM/3277  |
                                      |    GA     |
                                      |           |
 ----------                            -----*-----
|          |          -------               |
| IBM/3033 |         |       |              |
|   MVS    |<=======>|  GS   |<============>+
|  (TSO)   |         |       |              |
|          |          -------               |
 ----------                            -----*-----
                                      |           |
                                      | TEKTRONIX |
                                      |    618    |
                                      |           |
                                       -----*-----
                                            |
                                       -----------
                                      | Joystick  |
                                       -----------
```

Fig. 6. Dual Screen Workstation

Wherein the alphanumeric screen may be used for function menuing, alphanumeric data entry and message prompting, all graphic data are displayed separately on the storage display TEKTRONIX 618 having intrinsic storage and refresh capability. For graphic input a cursor control joystick (crosshair cursor) is provided.

3.2 Storage and Retrieval of Diffraction Data

Several FORTRAN files are used for permanent or temporary data gathering during a program run. In a data reduction run several measurements must be sometimes corrected or smoothed due to experimental uncertainties. Such manipulations may be, for example, performed easier, if all data are saved in a partitioned data set and the TSO-ISPF/PDF facilities/13/ have been utilized for editing functions.

The diffraction pattern of each measurement must be therefore saved as members of a user defined partitioned data set. These formatted data contain the scan number, some textual information and pairs of scattering angle and intensity/14/. In some cases measurements were performed with different stepsizes in the scattering angle. Then additional records containing the new stepsize are inserted in the input data set, so that all following angles may be rounded to the true value.

Because measurements are often carried out covering different ranges of the scattering angles due to experimental requirements, an appropriate preparation of input data (compress or expand) is sometimes necessary. On the other hand, the range of the scattering angle may be chosen in such a manner, so that this range will be covered by all to be compared measurements.

3.3 General Description of Program Calls (CLIST)

With respect to an efficient application of the computer codes a CLIST procedure has been developed which performs all necessary data set allocations due to user requirements, calls the programs and releases all data sets where necessary. Furthermore, the JCL card set may be completed and submitted to the background, if desired.

```
---------------------------------------------------------------------


   *******************************************************
   PROGRAM SYSTEM FOR THE ANALYSIS OF NEUTRON DIFFRACTION
   EXPERIMENTS TO EVALUATE THE TOTAL STRUCTURE FACTOR S(Q)
        AND THE TOTAL PAIR CORRELATION FUNCTION G(R)
                     == VERSION 3/84 ==
   *******************************************************


    PROGRAM/OPTION - MENU :

    C - CALCULATE CORRECTIONS FOR SCATTERING AND ABSORPTION
    A - ADD TWO MEASUREMENTS
    M - MULTIPLY A MEASUREMENT WITH A CONSTANT FACTOR
    S - EVALUATE S(Q) AND G(R) AND RDF
    D - DISPLAY RAW DATA
    P - PLOT SAVED PICTURES ON EXTERNAL PLOTTER
    L - ROUTE PRINT-OUT TO PRINTER
    I - GENERAL INFORMATIONS ON USE
    R - SAVE RAW DATA
    T - TERMINATE

    TYPE PROGRAM OPTION =====> _


---------------------------------------------------------------------
```

Fig. 7. Program Selection Menu

After LOGON (with the procedure **F**) the user may call the evaluation programs by entering the following TSO command:

ex 'tso352.tx.clist(sq)'

The CLIST-procedure SQ is listed in Appendix B. First, the program selection menu will be displayed, from which the user is prompted for the name of an option pertaining to the desired evaluation step he wants to perform (Fig. 7).

The picture data sets will be allocated automatically before each call to a program which then uses this data set for saving purposes. If a program will be called many times, the user has to keep in mind the names of each related picture data set for performing a selective plotting using option P, if desired. With respect to the GS picture data structure all hard copy plots may be easily performed using the **BIPLOT**/15/ command allowing some image transformations independently from the creation of the pictures. In this way several plots may be prepared without a recalling of the related evaluation program.

The input spectra may be inspected after entering option D on the program selection menu. If desired, hard copy plots may also be prepared.

If the user wishes to save input data or results, i.e. the whole partitioned data set, on tape, he may use the CLIST **AR**/16 which may be called using option R. However, in most cases it seems to be sufficient to use the different MSS commands for all saving operations/13/.

After program completion the program option menu appears on the alphanumeric screen. Then the user may chose another option to continue or he may select option T for terminating the CLIST. In this case the user has to decide whether a picture data set should be deleted or not. Of course, those data sets must be kept which are used by the submitted job to produce hard copy plots. The printout of the last run may be routed to a local printer after selection of the L option.

Acknowledgement

I would like to thank Dr. F. Gompf and M. Kobbelt for many discussions and valuable comments from a users view point during the development and first application of the program. We are very grateful to M. Kobbelt for providing a data transfer program on the NOVA computer to make the measured diffraction pattern available for evaluation on the IBM computer.

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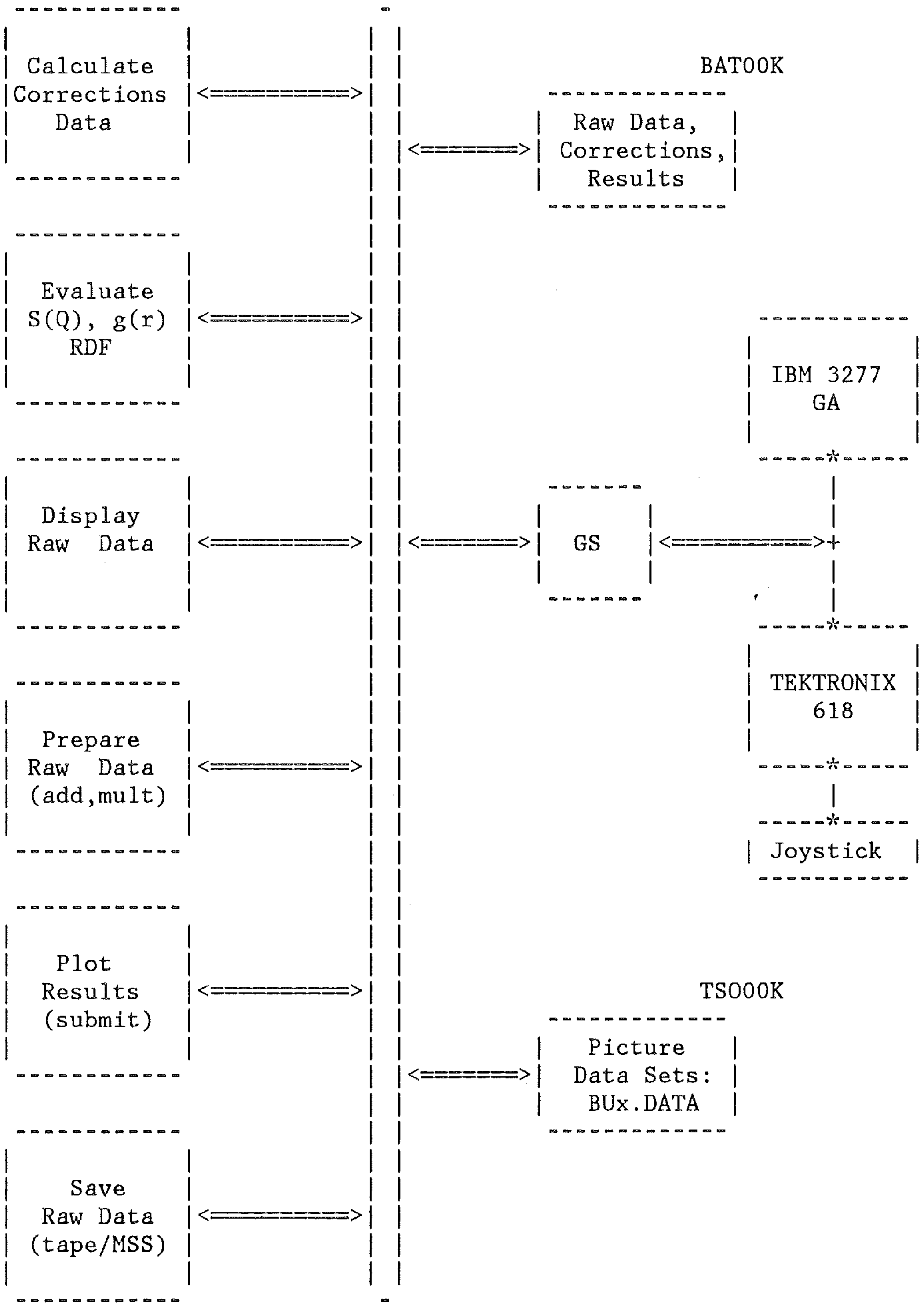
Appendix A: Graphic Representation of the Program System



Appendix B: CLIST Procedure

```
PROC 0
CONTROL END(ENDO) NOFLUSH NOMSG
GLOBAL &USER &NAME &ACCT
GLOBAL &USED &ALLOC &DSORG &VOLUME
ERROR DO
      WRITE SQ ERROR : CC=&LASTCC, CMD= &SYSPCMD &SYSSCMD
      RETURN
      ENDO
ATTN  DO
      GOTO P6
      ENDO
EX 'TSOSYS.CMDPROC.CLIST(MSSCLEAR)'
WRITE *******************************************************
WRITE PROGRAM SYSTEM FOR THE ANALYSIS OF NEUTRON DIFFRACTION
WRITE EXPERIMENTS TO EVALUATE THE TOTAL STRUCTURE FACTOR S(Q)
WRITE      AND THE TOTAL PAIR CORRELATION FUNCTION G(R)
WRITE             == KARLSRUHE  VERSION 7/84 ==
WRITE *******************************************************
SET &JCL=0
SET &PRI=0
SET &NBUCH=0
SET &IGA=0
ATTRIB DCB2 LRECL(133) BLKSIZE(3857) RECFM(F B A)
ERROR DO
      WRITE DATA SET ALREADY EXISTS, IT WILL BE REUSED
      RETURN
      ENDO
ALLOC DA(SQ$LPT.DATA) USING(DCB2) SPACE(5,2) TR NEW
ERROR OFF
FREE ATTRLIST(DCB2)
FREE F(FT06F001)
ALLOC F(FT06F001) DA(SQ$LPT.DATA)
ALLOC F(FT08F001) DA(*)
ALLOC F(FT09F001) DA(*)
GOTO S0
/********************************************************************/
P0: +
EX 'TSOSYS.CMDPROC.CLIST(MSSCLEAR)'
WRITE
WRITE
WRITE
WRITE
WRITE
WRITE
S0: +
WRITE
WRITE  PROGRAM/OPTION - MENU :
WRITE
WRITE  C - CALCULATE CORRECTIONS FOR SCATTERING AND ABSORPTION
WRITE  A - ADD TWO MEASUREMENTS
WRITE  M - MULTIPLY A MEASUREMENT WITH A CONSTANT FACTOR
WRITE  S - EVALUATE S(Q) AND G(R) AND RDF
WRITE  D - DISPLAY RAW DATA
WRITE  P - PLOT SAVED PICTURES ON EXTERNAL PLOTTER
WRITE  L - ROUTE PRINT-OUT TO PRINTER
WRITE  I - GENERAL INFORMATIONS ON USE
```

```
WRITE  R - SAVE RAW DATA
WRITE  T - TERMINATE
WRITE
WRITE
WRITE
WRITENR  TYPE PROGRAM OPTION =====>
READ &PROG
EX 'TSOSYS.CMDPROC.CLIST(MSSCLEAR)'
/* VERTEILER */
IF &PROG=&STR(C) THEN GOTO P1
IF &PROG=&STR(S) THEN GOTO P2
IF &PROG=&STR(P) THEN GOTO P3
IF &PROG=&STR(R) THEN GOTO P4
IF &PROG=&STR(L) THEN GOTO P5
IF &PROG=&STR(T) THEN GOTO P6
IF &PROG=&STR(I) THEN GOTO P7
IF &PROG=&STR(D) THEN GOTO P8
IF &PROG=&STR(A) THEN GOTO P9
IF &PROG=&STR(M) THEN GOTO PA
WRITE PROGRAM OPTION NOT DEFINED, REENTER
GOTO S0
/*********************************************************************/
P1: +
WRITE
/* EXEC PROGRAM TO CALCULATE CORRECTION DATA */
FORT77 SQ.FORT(SQ1) GO LIBDD(SYSLIB)
GOTO P0
/*********************************************************************/
P2: +
WRITE
/* EXEC DATA REDUCTION */
IF &IGA=0 THEN EX 'TSO352.TX.CLIST(GSA)'
SET &IGA=1
SET &NBUCH=&NBUCH+1
ATTRIB D RECFM(U) BLKSIZE(2048)
ERROR DO
      WRITE DATA SET BU&NBUCH..DATA ALREADY EXISTS, DATA SET IS REUSED
      ALLOC F(BUCH) DA(BU&NBUCH..DATA) SHR
      RETURN
      ENDO
ALLOC F(BUCH) DA(BU&NBUCH..DATA) DIR(2) SPACE(40 5) TR USING(D) NEW
ERROR OFF
FREE ATTRLIST(D)
WRITE PICTURE DATA SET IS : BU&NBUCH..DATA
FORT77  SQ.FORT(SQ2) GO LIBDD(SYSLIB) LIB('TSOSYS.GSMAIN.LOAD')
FREE F(BUCH)
GOTO P0
/*********************************************************************/
P3: +
WRITE
/* EXEC HARD COPY PLOT */
WRITENR NUMBER OF CURRENT BOOKS IS &NBUCH
WRITE
SET &I=1
DO WHILE &I<=&NBUCH
WRITE
WRITENR &I.. PICTURE DATA SET : BU&I..DATA
SET &I=&I+1
ENDO
BIPLOT
GOTO P0
```

```
/********************************************************************/
P4: +
WRITE
/* EXEC SAVE ON TAPE */
WRITE (THE MSS COMMANDS MAY BE USED INDEPENDENTLY TO SAVE THE DATA)
WRITE IF YOU ARE INTENDED TO USE THE TAPE FACILITY, TYPE Y, ELSE CR :
READ &ANS
IF &ANS=Y THEN +
DO
WRITE TSO-TAPE-CATALOGUE ALREADY EXISTS FOR THE DV---- TAPE ?  TYPE Y/N
READ &ANS
IF &ANS=N OR &ANS= THEN +
DO
EX 'TSO352.TX.CLIST(ARC)'
ENDO
EX 'TSO352.TX.CLIST(AR)'
ENDO
GOTO PO
/********************************************************************/
P5: +
WRITE
/* EXEC ROUTE OUTPUT */
SET &PRI=0
CONTROL MSG
WRITENR ROUTE JOB-OUTPUT TO PRINTER ? TYPE Y(ES), ELSE RETURN
READ &L
IF &L=  THEN GOTO PO
IF &L=N THEN GOTO PO
WRITENR FOR RJE TYPE 7/9, ELSE RETURN     :
READ &OUT
SET &PRI=1
EX 'TSO352.TX.CLIST(RDACCT)'
COPY 'TSO352.DUMMY.CNTL' XRJCL.CNTL NONUM
EDIT XRJCL CNTL NONUM OLD
TOP
DEL * 500
IN //IAK&USER.PR JOB &ACCT.,&NAME
IF &OUT=7 OR &OUT=9 THEN IN //&STR(*)MAIN ORG=RM00&OUT
IN //OUT EXEC PGM=IEBGENER
IN //SYSUT1 DD DSN=&SYSPREF..SQ$LPT.DATA,DISP=(OLD,DELETE)
IN //SYSUT2 DD SYSOUT=A
IN //SYSPRINT DD DUMMY
IN //SYSIN DD DUMMY
IN //
S
END
SUB XRJCL.CNTL
DEL XRJCL.CNTL
GOTO PO
/********************************************************************/
P7: +
WRITE
WRITE ALLGEMEINE HINWEISE FUER DIE BENUTZUNG DER PROZEDUR
WRITE ===================================================
WRITE
WRITE 1. NUR TSO-DATEIEN FUER DIE SPEKTREN UND AUSWERTUNGEN. AUFRUF
WRITE    NUR VON DER EIGENEN TSO-REGION AUS WEGEN OPEN FILE UND ACCT.
WRITE 2. AUFRUF DES AUSWERTEPROGRAMMS SETZT KORREKTUR-FILE VORAUS.
WRITE 3. AUSFUEHRUNG DES AUSWERTEPROGRAMMS NUR AM GRAPHISCHEN DISPLAY
WRITE    MOEGLICH (IBM3277+TEKTRONIX 618).
WRITE 4. FUER EINE BAND-ARCHIVIERUNG MUSS EINE TSO-DATEI ALS BANDKATALOG
```

```
WRITE    VORHANDEN SEIN, Z.B. TSO___.DVNNNN.DATA (NNNNN = BAND-NUMMER).
WRITE    (SIEHE PROGRESS REPORT KFK 2881, 1979)
WRITE 5. FALLS EINE PLOT-AUSGABE VORGENOMMEN WURDE, DUERFEN DIE
WRITE    BETREFFENDEN BILD-DATEIEN AM SCHLUSS NICHT GELOESCHT WERDEN.
WRITE
WRITE
WRITE
WRITE
WRITE
WRITE
WRITE
WRITE
WRITENR WEITER MIT RETURN/ENTER TASTE :
READ &C
GOTO P0
/**********************************************************************/
P8: +
WRITE
/* EXEC DISPLAY RAW DATA */
IF &IGA=0 THEN EX 'TSO352.TX.CLIST(GSA)'
SET &IGA=1
SET &NBUCH=&NBUCH+1
ATTRIB D RECFM(U) BLKSIZE(2048)
ERROR DO
      WRITE DATA SET BU&NBUCH..DATA ALREADY EXISTS, DATA SET IS REUSED
      FREE F(BUCH)
      ALLOC F(BUCH) DA(BU&NBUCH..DATA) OLD
      RETURN
      ENDO
ALLOC F(BUCH) DA(BU&NBUCH..DATA) DIR(2) SPACE(40 5) TR USING(D) NEW
ERROR OFF
FREE ATTRLIST(D)
WRITE PICTURE DATA SET IS : BU&NBUCH..DATA
FORT77 SQ.FORT(SQ4) GO LIBDD(SYSLIB) LIB('TSOSYS.GSMAIN.LOAD')
FREE F(BUCH)
GOTO P0
/**********************************************************************/
P9: +
WRITE
/* EXEC ADD TWO MEASUREMENTS */
FORT77 SQ.FORT(SQ5) LIBDD(SYSLIB)
GOTO P0
/**********************************************************************/
PA: +
WRITE
/* EXEC MULTIPLICATION OF MEASUREMENTS */
FORT77 SQ.FORT(SQ6) GO LIBDD(SYSLIB)
GOTO P0
/**********************************************************************/
/**********************************************************************/
P6: +
IF &IGA=0 THEN GOTO P99
CONTROL MSG
WRITE STATUS OF THE PICTURE DATA SETS
WRITE
WRITE * IF THE USER HAD SELECTED OPTION P (HARD COPY PLOT), THE RELATED
WRITE * GRAPHIC DATA SETS SHOULD NOT BE DELETED BEFORE THE COMPLETION
WRITE * OF THE PLOT-SUBMIT-JOB.
SET &I=1
DO WHILE &I<=&NBUCH
WRITE
```

```
WRITENR ERASE DATA SET BU&I..DATA ?  TYPE Y(ES), ELSE RETURN
READ &L
IF &L=&STR(Y) THEN DEL BU&I..DATA
SET &I=&I+1
ENDO
CONTROL NOMSG
/**********************************************************************/
P99: +
FREE F(FT06F001 FT08F001)
IF &PROG¬=&STR(P) THEN FREE F(FT09F001)
IF &PRI =0 THEN DEL SQ$LPT.DATA
           ELSE FREE DA(SQ$LPT.DATA)
ALLOC F(FT06F001) DA(*)
WRITE
WRITE == EXEC TERMINATED ==
WRITE
END
```