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THE DETERMINATION OF SHORT RANGE ORDER AND LOCAL ATOMIC DISPLACEMENTS IN DISORDERED BINARY SOLID SOLUTIONS

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Résumé. — Borie et Sparks ont proposé une méthode d'analyse très générale de l'intensité diffuse des rayons X en vue d'obtenir des informations sur l'arrangement local des atomes dans les solutions solides désordonnées d'alliages binaires. Cette analyse implique une séparation des composantes de l'intensité diffuse en différents termes relatifs à l'ordre local et aux déplacements locaux. Les composantes de l'intensité présentent des relations de symétrie différentes dans l'espace réciproque où l'on peut considérer qu'elles sont périodiques si le rapport des facteurs de diffusion atomique varie légèrement avec $\sin \theta/\lambda$. Ce n'est cependant pas le cas dans la plupart des systèmes d'intérêt pratique et de plus, lorsque cette hypothèse est valable, l'information que l'on peut obtenir sur les déplacements locaux est limitée puisque l'on ne peut séparer les déplacements relatifs aux deux sortes d'atomes.

La méthode d'analyse qui est présentée ici a d'abord été suggérée par Tibballs ; c'est une modification de celle proposée par Borie et Sparks où ces différentes questions sont négligées. Les composantes de l'intensité diffuse due aux déplacements sont séparées en différents termes relatifs aux différentes sortes d'atomes. Ces termes sont alors rigoureusement périodiques dans l'espace réciproque et la variation du rapport des facteurs de diffusion atomique est en fait utilisée pour les séparer.

La diffusion a été simulée sur ordinateur dans le cas de certains alliages binaires et on l'a analysée par cette méthode en tenant compte des erreurs habituelles. (Statistique de comptage, bruit de fond, etc.) L'influence des erreurs sur les valeurs des coefficients de l'ordre à courte distance était du même ordre de grandeur que dans le cas de la méthode de Borie et Sparks et les coefficients des déplacements pour chaque espèce atomique ont été déterminés dans des limites raisonnables d'incertitude. On décrit ici un programme de calcul sur ordinateur en vue d'effectuer de telles mesures.

Abstract. — The most general analysis of diffuse X-ray scattering to obtain information about local atomic arrangements in disordered binary solid solutions has been presented by Borie and Sparks. It involves an expansion of the diffuse intensity into various components, each describing separately the local order or moments of the local displacement distribution. Each of these components has a different symmetry and is periodic in reciprocal space under the assumption that the ratio of atomic scattering factors does not vary drastically with $\sin \theta/\lambda$. This assumption does not hold in many systems of practical interest. Furthermore, even if valid, the information about local displacements is of limited value since the displacements of the two atomic species cannot be determined separately.

Presented here is an analysis of a modification of the Borie and Sparks method, first suggested by Tibballs, which minimizes these problems. The displacement intensity components are broken down further into terms each involving a different atomic species. These new terms are strictly periodic in reciprocal space and the variation of the atomic scattering factor ratio is actually used to separate them.

Diffuse scattering for a number of binary alloys was simulated by computer and subsequently analyzed by this method, including some commonly occurring errors (counting statistics, background errors, etc.). The errors propagating to the final SRO coefficients were never worse than those involved in a Borie and Sparks analysis, and the displacement coefficients for each atomic species could be determined within reasonable errors. An on-line computer program for making measurements with this technique is described.

Introduction. — Only the analysis of scattering can give direct and detailed information about the actual atomic configurations local order and displacements present in an alloy. This scattering may be employed

in some cases by lattice imaging techniques in the electron microscope, but the most detailed information still comes from direct examination of the diffuse scattering of X-rays or neutrons. Here we deal with

the X-ray scattering. Following Borie and Sparks [1] and Gragg [2], the total diffuse intensity from a cubic binary alloy at a point h_1, h_2, h_3 in reciprocal space can be expanded as follows, including up to second moments in the displacements (and in electron units (eu)) :

$$I_D(h_1, h_2, h_3) = N c_A c_B (f_A - f_B)^2 [I_{\text{SRO}} + h_1 Q_x + h_2 Q_y + h_3 Q_z + h_1^2 R_x + h_2^2 R_y + h_3^2 R_z + h_1 h_2 S_{xy} + h_2 h_3 S_{yz} + h_3 h_1 S_{zx}], \quad (1)$$

where N is the total number of atoms under the X-ray beam, c_A and c_B are the atom fractions of the constituents A and B of the alloy, f_A and f_B are the respective atomic scattering factors and for cubic symmetry :

$$I_{\text{SRO}} = \sum_l \sum_m \sum_n \alpha_{lmn} \cos 2\pi h_1 l \cos 2\pi h_2 m \cos 2\pi h_3 n, \quad (2a)$$

$$Q_x = \sum_l \sum_m \sum_n \gamma_{lmn}^x \sin 2\pi h_1 l \cos 2\pi h_2 m \cos 2\pi h_3 n, \quad (2b)$$

and similarly for Q_y and Q_z . (The lmn are coordinates of an interatomic vector.)

$$R_x = \sum_l \sum_m \sum_n \delta_{lmn}^x \cos 2\pi h_1 l \cos 2\pi h_2 m \cos 2\pi h_3 n, \quad (2c)$$

and similarly for R_y and R_z

$$S_{xy} = \sum_l \sum_m \sum_n \varepsilon_{lmn}^{xy} \sin 2\pi h_1 l \sin 2\pi h_2 m \cos 2\pi h_3 n, \quad \text{etc.} \quad (2d)$$

The α_{lmn} are the familiar Warren short-range order parameters and the rest of the Fourier coefficients in (2) are defined as :

$$\gamma_{lmn}^x = -2\pi \left[\eta \left(\frac{c_A}{c_B} + \alpha_{lmn} \right) \langle x_{lmn}^{\text{AA}} \rangle - \zeta \left(\frac{c_B}{c_A} + \alpha_{lmn} \right) \langle x_{lmn}^{\text{BB}} \rangle \right], \quad (3a)$$

$$\delta_{lmn}^x = 4\pi^2 \left[\eta^2 \left(\frac{c_A}{c_B} + \alpha_{lmn} \right) \langle x_0^{\text{A}} x_{lmn}^{\text{A}} \rangle + 2\eta\zeta(1 - \alpha_{lmn}) \langle x_0^{\text{A}} x_{lmn}^{\text{B}} \rangle + \zeta^2 \left(\frac{c_B}{c_A} + \alpha_{lmn} \right) \langle x_0^{\text{B}} x_{lmn}^{\text{B}} \rangle \right], \quad (3b)$$

$$\varepsilon_{lmn}^{xy} = 8\pi^2 \left[\eta^2 \left(\frac{c_A}{c_B} + \alpha_{lmn} \right) \langle x_0^{\text{A}} y_{lmn}^{\text{A}} \rangle + 2\eta\zeta(1 - \alpha_{lmn}) \langle x_0^{\text{A}} y_{lmn}^{\text{B}} \rangle + \zeta^2 \left(\frac{c_B}{c_A} + \alpha_{lmn} \right) \langle x_0^{\text{B}} y_{lmn}^{\text{B}} \rangle \right], \quad (3c)$$

with similar expressions for $\gamma_{lmn}^y, \gamma_{lmn}^z, \delta_{lmn}^y$, etc.

$$\eta = \frac{f_A}{f_A - f_B}, \quad \zeta = \frac{f_B}{f_A - f_B}$$

and the terms in carets are lattice averages of fractional atomic displacements from the ideal lattice sites. That is, $\langle x_{lmn}^{\text{AA}} \rangle$ is the average displacement in the x direction of an A atom, located near site (lmn) , when the origin is occupied by an A atom. The term $\langle x_0^{\text{A}} x_{lmn}^{\text{A}} \rangle$ is a measure of the correlation of displacements between sites ; it is the average of the product of the displacement of an A atom at site (lmn) and that of another A atom at the origin. The method of Borie and Sparks, which is the best known and most commonly employed, makes use of the fact that the intensity components in (1) are pseudoperiodic for X-rays and each one exhibits different symmetries in reciprocal space. Inspection of (3) shows that indeed, if η and ζ are constant or very weak functions of $\sin \theta/\lambda$, this statement is true.

Now, due to cubic symmetry, the displacement components are related, and hence :

$$Q_x(h_1, h_2, h_3) = Q_y(h_2, h_1, h_3) = Q_z(h_3, h_2, h_1). \quad (4)$$

Similar relations exist between the R and S terms. Thus, by substitution, equation (1) can be rewritten so as to contain only I_{SRO} , Q_x , R_x and S_{xy} . One can now express these components as linear combinations of the total diffuse intensity as follows [1, 2] :

$$S_{xy}(h_1, h_2, h_3) = [I(h_1, h_2, h_3) - I(2 - h_1, h_2, h_3) - I(h_1, 2 - h_2, h_3) - I(2 - h_1, 2 - h_2, h_3)]/4, \quad (5a)$$

$$R_x(h_1, h_2, h_3) = [I(2 + h_1, h_2, h_3) - 2I(h_1, h_2, h_3) + I(2 - h_1, h_2, h_3)]/8, \quad (5b)$$

$$Q_x(h_1, h_2, h_3) = [I(h_1, h_2, h_3) - I(2 - h_1, h_2, h_3) - 4(h_1 - 1)R_x(h_1, h_2, h_3) - 2h_2S_{xy}(h_1, h_2, h_3) - 2h_3S_{xy}(h_3, h_1, h_2)]/2, \quad (5c)$$

$$\begin{aligned} I_{\text{SRO}} = & I(h_1, h_2, h_3) - h_1Q_x(h_1, h_2, h_3) - h_2Q_x(h_2, h_3, h_1) - h_3Q_x(h_3, h_1, h_2) - \\ & - h_1^2R_x(h_1, h_2, h_3) - h_2^2R_x(h_2, h_3, h_1) - h_3^2R_x(h_3, h_1, h_2) - h_1h_2S_{xy}(h_1, h_2, h_3) \\ & - h_2h_3S_{xy}(h_2, h_3, h_1) - h_3h_1S_{xy}(h_3, h_1, h_2). \end{aligned} \quad (5d)$$

The procedure is repeated for a different set of h_1, h_2, h_3 values, until each component is known throughout some minimum volume in reciprocal space, from which it can be reproduced by symmetry to fill one reciprocal unit cell. A Fourier inversion then yields the coefficients a, γ, δ and ϵ .

An extensive error analysis of this method [3] showed it to be quite satisfactory in many cases when reasonable experimental errors are taken into account. However, in many other cases, where η and ζ vary appreciably throughout the $\sin \theta/\lambda$ range of reciprocal space investigated, the method seems to suffer, especially in the case of clustering systems. Furthermore, even in an accurate analysis, when η and ζ are nearly constant, the information gained about local atomic displacements is of rather limited value, since the Fourier coefficients resulting from the analysis involve more than one displacement term.

Another method was devised by Williams [4]. By substituting (2) into (1) and writing out the sums as separate terms, the total diffuse intensity is expressed as a linear combination of ~ 50 coefficients, by judiciously terminating each sum in (2). The intensity is measured in as many points in reciprocal space as possible and the resulting linear system is solved by least-square methods.

Among the advantages of this method is the flexibility in emphasizing certain coefficients, or omitting others that are known or assumed to be small. The disadvantages, however, due to termination may be serious.

This method is, obviously, also plagued by the variation of the scattering factor terms.

A new method. — Following a suggestion by Tibballs [5], equation (1) is rewritten in the following form :

$$\begin{aligned} \frac{I_D}{c_A c_B (f_A - f_B)^2} = & I_{\text{SRO}} + h_1 \eta Q_x^{\text{AA}} + h_1 \zeta Q_x^{\text{BB}} + h_2 \eta Q_y^{\text{AA}} + h_2 \zeta Q_y^{\text{BB}} + h_3 \eta Q_z^{\text{AA}} + h_3 \zeta Q_z^{\text{BB}} + \\ & + h_1^2 \eta^2 R_x^{\text{AA}} + 2h_1^2 \eta \zeta R_x^{\text{AB}} + h_1^2 \zeta^2 R_x^{\text{BB}} + h_2^2 \eta^2 R_y^{\text{AA}} + 2h_2^2 \eta \zeta R_y^{\text{AB}} + h_2^2 \zeta^2 R_y^{\text{BB}} + h_3^2 \eta^2 R_z^{\text{AA}} \\ & + 2h_3^2 \eta \zeta R_z^{\text{AB}} + h_3^2 \zeta^2 R_z^{\text{BB}} + h_1 h_2 \eta^2 S_{xy}^{\text{AA}} + 2h_1 h_2 \eta \zeta S_{xy}^{\text{AB}} + h_1 h_2 \zeta^2 S_{xy}^{\text{BB}} + h_2 h_3 \eta^2 S_{yz}^{\text{AA}} \\ & + 2h_2 h_3 \eta \zeta S_{yz}^{\text{AB}} + h_2 h_3 \zeta^2 S_{yz}^{\text{BB}} + h_3 h_1 \eta^2 S_{zx}^{\text{AA}} + 2h_3 h_1 \eta \zeta S_{zx}^{\text{AB}} + h_3 h_1 \zeta^2 S_{zx}^{\text{BB}}. \end{aligned} \quad (6)$$

The new intensity components are defined as :

$$Q_x^{\text{AA}} = -2\pi \sum_l \sum_m \sum_n \left(\frac{c_A}{c_B} + \alpha_{lmn} \right) \langle x_{lmn}^{\text{AA}} \rangle \sin 2\pi h_1 l \cos 2\pi h_2 m \cos 2\pi h_3 n, \quad (7a)$$

$$R_x^{\text{AA}} = 4\pi^2 \sum_l \sum_m \sum_n \left(\frac{c_A}{c_B} + \alpha_{lmn} \right) \langle x_0^A x_{lmn}^A \rangle \cos 2\pi h_1 l \cos 2\pi h_2 m \cos 2\pi h_3 n, \quad (7b)$$

etc., for the rest of the components.

Now all terms defined by (7) are strictly periodic. The procedure followed from this point on is basically the same as in the Borie and Sparks method. The diffuse intensity is measured at a set of h_1, h_2, h_3 values, for which the components of (6), Q_x^{AA} , etc., have the same or opposite value and the resultant system of linear equations is solved for Q_x^{AA} , Q_x^{BB} , Q_y^{AA} , etc. The procedure is more laborious, since twenty-five

($h_1 h_2 h_3$) points are required now, or more if a least-squares solution is performed. However, the difference is not 5 over the Borie and Sparks method, as one might suspect by glancing at the separation equation (5) (five measurements are needed in this case for each h_1, h_2, h_3 point). Notice that, for the separation of I_{SRO} and Q_x at the point h_1, h_2, h_3 , R_x and S_{xy} must be known at *other* points as well. The minimum volume

necessary for R_x and S_{xy} is appreciably larger than that for I_{SRO} . For the method described here, each separation determines *all* 25 components, hence, the minimum volume required is only that required for I_{SRO} . The real difference in total number of points for this method versus that of Borie and Sparks is 2.5, as one can see from the number of components in equations (1) and (6). Two advantages of this new method may, however, well justify the extra effort and time required :

- 1) For the first time the individual atomic displacements can be obtained.
- 2) Even in cases where large errors render the displacement results meaningless (for instance, when η and ζ are almost constant), reliable values for I_{SRO} may still be obtained. This is shown to be the case in the error analysis to be presented below.

Program description. — This method was implemented in a package of FORTRAN programs, designed to run on a Digital Equipment Corporation PDP8-E 16K mini-computer, interfaced to a diffractometer and the associated electronics. The diffuse scattering analysis is performed in real time, as the measurements are taken and no operator intervention is required.

The program starts with an initial dialogue with the operator, in which various experimental parameters and terms like scattering factors are specified, as well as a number of reciprocal lattice points at which the intensity separation is to be carried out. Then the following procedure is repeated sequentially for each of these points.

The entire set of h_1, h_2, h_3 values, at which the intensity components have the same absolute value as at the given point is first generated, taking into account the symmetry of each component (simple cubic, BCC or FCC). If the generating point lies on a high symmetry direction in reciprocal space, the intensity components may not be linearly independent; some may be required to be zero by symmetry, others to be equal among themselves. These relations are detected and are used later as constraints to the final solution.

The set of h_1, h_2, h_3 values is then converted to diffractometer settings. Those outside the angular limits of the apparatus are discarded.

The matrix of the linear system of equations like (6) is then constructed. For each h_1, h_2, h_3 the coefficients of the equation are calculated and stored in successive rows of a matrix. Simultaneously, the diffractometer is moved to the corresponding settings, the diffuse intensity is measured, corrected for geometrical factors and converted to Laue units.

When the matrix is thus filled, the linearly dependent components are first eliminated from the system and the remaining ones are obtained by a least-squares method, employing a Householder transformation with iterative optimization of the final solution [6].

The maximum number of equations (i.e., matrix rows) permitted by the program is 49. The minimum number required is obviously equal to or greater than the number of linearly independent intensity components which ranges from 4 to 25.

Error analysis. — For the method presented in the preceding section, an analytical procedure to obtain error estimates for the solutions, when errors are involved not only in the measured intensities, but also in the coefficients of the matrix of the linear system, would be next to impossible. Therefore, a simpler approach was taken. Diffuse intensities were simulated in a volume of reciprocal space, using reasonable experimental parameters for three representative binary alloys. Various errors were then introduced to these simulated intensities and the analysis was carried out. Thus, the effects of these errors on the final solution were established in each case.

Three binary alloys were chosen for analysis :

- 1) Cu_3Au , as being a typical ordering alloy, reliably analyzed by the Borie and Sparks method [7]. Data for the intensity simulation were taken from ref. [7]. In particular, α 's and displacement coefficients were taken from the results in this publication at 420 °C to simulate intensity.

- 2) Ni_3Fe , an alloy with very large variations in the scattering factor ratios and very weak SRO scattering. SRO parameters were taken from Lefebvre [8]. Displacement coefficients were not available, so they were set approximately the same as in (1).

- 3) Al-5 at % Cu, a typical clustering alloy, very difficult to analyze by the Borie and Sparks method, since the SRO intensity is concentrated in the same regions of reciprocal space as the displacement intensity and the size terms are larger (see ref. [3]). Data are not available for this alloy, so simple spherical clusters were considered. The SRO coefficients, starting at a value of 0.7 for the nearest neighbors, were made to fall off with the square of the interatomic vector. The displacement coefficients were again chosen to be about equal to those in (1).

Scattering factors for all cases were taken from the International Tables of Crystallography [9]. For the $\sin \theta/\lambda$ range (0.1-0.5 \AA^{-1}) in which diffuse intensities were simulated in all three cases, the scattering factor ratios were found to vary $\sim 15\%$ for Cu_3Au , $\sim 20\%$ for Al-5 % Cu and by almost a factor of 2 for Ni_3Fe .

The simulated intensities were in each case separated along $[h00]$ (from 0 to $[100]$), $[hh0]$ (from 0 to $[0.5, 0.5, 0]$) and $[hhh]$ (from 0 to 0.4, 0.4, 0.4). A variety of possible errors of reasonable magnitude were examined. They are listed below (and the way they were introduced is indicated).

- 1) *Roundoff errors in the computer.* — The data were analyzed using exactly the same parameters as in the simulation. These results are represented by filled circles in figures 1, 2 and 3.

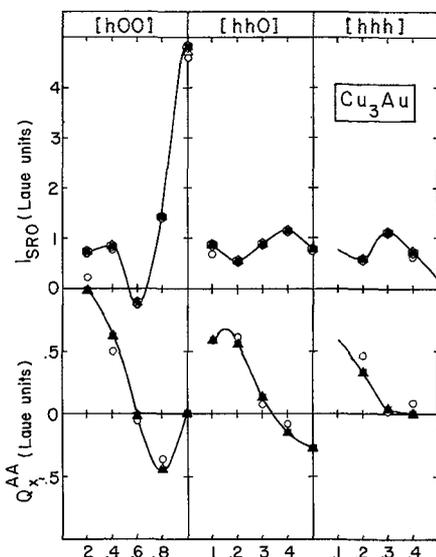


FIG. 1. — Results of the error analysis for Cu_3Au . — Given. (●) Roundoff errors introduced. (○) Statistical errors introduced. (△) Surface roughness errors introduced. (◊) Scattering factor errors introduced. (◻) Compton scattering errors introduced. Composition and background errors not shown.

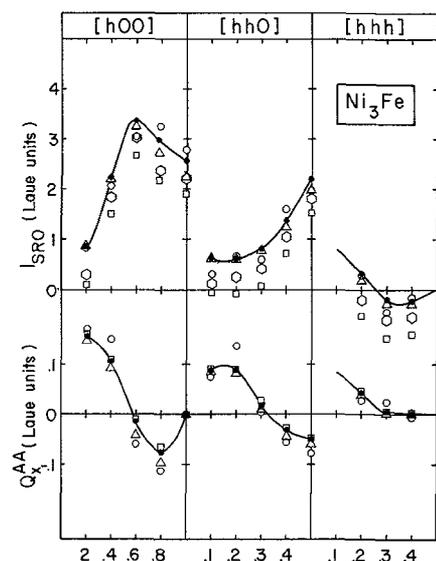


FIG. 2. — Same as figure 1, for Ni_3Fe .

2) *Random statistical errors.* — In all cases shown, the synthesized data had approximately 1 000–8 000 counts at minima and maxima of the diffuse intensity respectively. Some other cases not shown, were tried with lower (200–2 000 counts) or higher (5 000–50 000 counts). A random error, obeying the Poisson distribution was added to or subtracted from the simulated intensities and the analysis was carried out with the perturbed data. Results are represented by open circles.

3) *Errors in determining the influence of surface roughness.* — The data were analyzed adding a 10% correction at low 2θ , dropping off to no error at $50^\circ 2\theta$ and higher. Results are indicated by triangles.

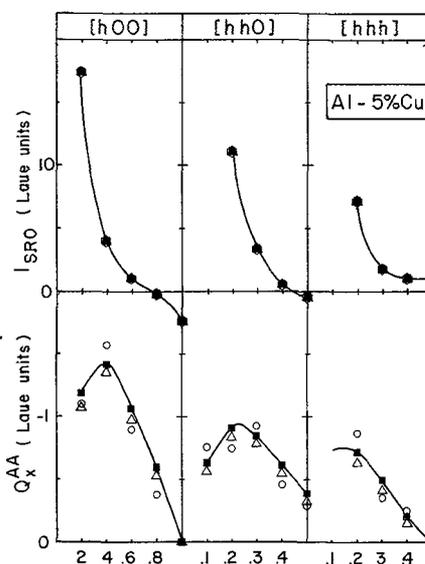


FIG. 3. — Same as figure 1, for Al-5% Cu.

4) *Composition errors.* — It is known *a priori* that composition errors have only a multiplicative effect on the results, due to an error in the normalization of the measured intensity by $c_A c_B$.

5) *Scattering factor errors.* — The analysis was carried out adding an error in the Debye-Waller factor of 0.1 \AA^2 for the first constituent of each alloy except in the case of Al-5% Cu, where B_{Cu} was perturbed. For Cu_3Au errors of 0.2 and 0.3 \AA^2 in B_{Au} were also tested. Results are shown by hexagons.

6) *Compton scattering errors.* — Compton scattering of the first constituent in each case was increased by 5 eu/atom ($\approx 30\%$ error at $\sin \theta/\lambda = 0.2$) at low angles, the error dropping to zero at high angles. Results indicated by squares.

7) *Background errors.* — An error of 100 counts was added in the analysis—almost a 100% error in typical cases.

In all figures, the exact synthesized intensity component is indicated by a solid line.

In the following, the effects of these errors are examined for two intensity components, I_{SRO} and Q_x^{AA} . Unfortunately, the solution was very unstable for R and S terms, the results varying by a factor of 10 from the exact values when the above mentioned errors are included.

The results for Cu_3Au are shown in figure 1. Figure 2 shows the results for Ni_3Fe and figure 3 for Al-5% Cu.

1) *Roundoff errors.* — In all cases, the errors in I_{SRO} were less than 0.1% and less than 1% in Q_x^{AA} .

2) *Statistical errors.* — These were always small for I_{SRO} . The term Q_x^{AA} was more sensitive, as expected. In some cases examined, where the included statistical error was larger, the errors in I_{SRO} and Q_x^{AA} increased proportionately.

3) *Surface roughness errors.* — These were negligible in all cases.

4) *Scattering factor errors.* — I_{SRO} was severely affected in the case of Ni_3Fe . In the other two cases the effects were small. However, Q_x^{AA} proved most sensitive, even to small errors. The effect was always multiplicative. Q_x^{AA} was multiplied by a constant factor, independent of $h_1 h_2 h_3$. For Cu_3Au and for an error in B_{Au} of 0.3, 0.2 and 0.1 \AA^2 (out of 0.6 \AA^2), Q_x^{AA} was larger by factors of 3, 2 and 50 % respectively. For Ni_3Fe 0.1 \AA^2 error in B_{Ni} caused Q_x^{AA} to double. For Al-5 % Cu, the same error in B_{Cu} caused Q_x^{AA} to be halved.

5) *Compton scattering errors.* — There were negligible effects in the cases of Cu_3Au and Al-5 % Cu, and only a small effect in Q_x^{AA} for Ni_3Fe . In the latter case, however, I_{SRO} was seriously perturbed, being reduced by a constant amount of ~ 0.6 eu/atom.

6) *Background errors.* — In all cases, they were negligible (< 0.5 %).

Thus the most severe errors seem to be associated with errors in scattering factors and these affect only the Q terms. On the positive side is the fact that, at least, the errors are multiplicative. Although the actual displacement values may be greatly in error, the directions of the displacements will be correct and the magnitudes will be in the correct proportions.

A pleasant surprise was the success of the method in the case of Al-5 % Cu. Clustering systems have always been very difficult to analyze quantitatively, and the results demonstrated above show considerable promise.

Systems like Ni_3Fe which are difficult to analyze by the Borie-Sparks method because of the large variation in scattering factor over the minimum required volume of measurement in reciprocal space are still a problem with this method.

Compared to the Borie and Sparks method and the errors associated with it [3], it seems that the errors of the method presented here are not worse than those of the Borie and Sparks method and, of course, the errors associated with the scattering factor ratio variation are eliminated altogether.

In order to have an indication as to the propagation of errors through the Fourier inversion to the final SRO and displacement coefficients, a full volume analysis was performed on the simulated data for Cu_3Au for two cases.

1) Only statistical errors were included.

2) The following errors were all included : Statistical error, surface roughness error of + 20 % at low 2θ , dropping to 0 at $50^\circ 2\theta$ and above, Compton errors for Au of 3 eu/atom (about 30 %) at low angles, decaying to 0 at high angles and finally, B_{Au} was perturbed by 0.05 \AA^2 .

The results are shown in table I for a_{lmn} and $\langle x_{lmn}^{\text{AuAu}} \rangle$. They are highly satisfactory in both cases.

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TABLE I

Effects of errors in simulated data on Fourier coefficients

lmn	α_{lmn} in simulation	Only statistical error introduced prior to analysis	Total error introduced prior to analysis	$\langle x_{lmn}^{\text{AuAu}} \rangle$ in simulation	Only statistical error introduced prior to analysis	Total error introduced prior to analysis
000	1	1.003	0.967 4			
110	- 0.093	- 0.091 6	- 0.088 7	- 0.006 6	- 0.006 24	- 0.006 73
200	0.140 7	0.139 2	0.133 0	0.034	0.034 7	0.040 88
211	0.035 4	0.034 4	0.035 5	0.009 3	0.007 7	0.010 1
220	0.050 3	0.051 8	0.048 5	0.009 3	0.007 5	0.008 6
310	- 0.099 1	- 0.100 5	- 0.098 2	- 0.002 4	- 0.002 94	- 0.004 85
222	0.018 2	0.018 9	0.017 1	0.001 6	0.003	0.002 1
321	- 0.005 9	- 0.008 1	- 0.007 8	0.003 4	0.004 4	0.005 0
400	0.75 2	0.072 0	0.068 6	0.009 5	0.007 3	0.011 7
411	0.017 2	0.017 7	0.016 0	0.007 9	0.008 6	0.009 4
330	- 0.018 9	- 0.014 5	- 0.015 9	- 0.000 8	- 0.001 4	- 0.000 8
420	0.037 5	0.033 5	0.034 7			
332	0.001 2	0.002 3	0.002 5			

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