

A Gauss–Seidel Least-Squares Refinement Procedure with Rigid-Group and Parameter Restraint Capabilities

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Abstract

A fast Gauss–Seidel least-squares procedure (FGLS) has been developed for crystallographic refinement of atom parameters in large asymmetric units. The procedure combines the minimum matrix requirements and the rapid convergence of the Gauss–Seidel algorithm with rigid-group constraint and subsidiary parameter elastic restraint capabilities. As the procedure is essentially block diagonal, considerable computational efficiency is achieved by determining contributions from one atom to all reflections at a time, instead of the usual practice of determining the contributions from all atoms to each reflection in turn. Application of the method to a 1104-atom protein at 2.5 Å resolution is described.

Introduction

Until recently, use of structure factor least-squares (SFLS) methods in the refinement of macromolecular structures has been limited by the prohibitive computing effort required. Watenpaugh, Sieker, Herriott & Jensen (1973) successfully refined a 558-atom model of rubredoxin by adjusting individual-atom coordinates and thermal parameters, but at substantial cost (Watenpaugh, 1973). The magnitude of the problem required the partitioning of the normal equations matrix into ten blocks along the diagonal, each block containing over 200 parameters. The conventional, and much less costly, individual-atom block-diagonal method was found inapplicable, since the low resolution caused neighboring atoms to be strongly correlated.

Konnert (1976) improved the conventional block-diagonal approximation to the full normal matrix by including all off-diagonal matrix elements relating parameter pairs for which he had assigned a subsidiary (elastic) restraining condition (Waser, 1963). By incorporating distance restraints between atoms in the system of observational equations, it was possible to

retain chemically reasonable stereochemistry even while using a limited subset of the reflection data. Konnert (1976) demonstrated the convergence properties of the method in the refinement of the 2436 atomic positional parameters of carp calcium-binding protein with respect to only 1370 reflection data plus 2030 distance restraints.

Certain molecular fragments, *e.g.* various peptide and side-chain units, may have geometries which are well established and should be maintained, at least in the initial refinement. The imposition of these rigid-body constraints is described by Scheringer (1963) as having the advantages of improving the radius and rate of convergence, allowing the use of model groups known to greater accuracy than can be determined from the data, and, in the case of the usual full-matrix refinement, substantially reducing the cost. Sussman, Holbrook, Church & Kim (1977) incorporated rigid-group constraints into the conditional SFLS method (Waser, 1963), and described a successful refinement of yeast phenylalanine tRNA by initially subdividing the 1652-atom model into 132 constrained (rigid) groups linked together by subsidiary (elastic) distance restraints. This reduced the number of variable positional parameters to 888 rather than the 4956 required for the individual atoms.

To reduce the effort of constructing the matrix, the procedures of Konnert (1976) and Sussman *et al.* (1977) utilize the 'sparse' matrix, evaluating only those matrix elements involving parameters of the same atom (constrained group) or between atoms (groups) having at least one restraint in common. All other elements are assumed to be small and are set to zero. If the conjugate gradient method (Hestenes & Stiefel, 1952) of solving linear equations is used, only the non-zero matrix elements need be stored with a substantial saving in the memory requirements.

An alternative procedure, initially developed for large non-protein structures (Hoard & Nordman, 1974), is the fast Gauss–Seidel least-squares (FGLS) routine. The basic approach of the Gauss–Seidel method, as used in the present procedure, is to form and solve the normal equations of a structural unit, *e.g.* an atom or a rigid group, and utilize these new

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estimates of the unit parameters to update the calculated structure factors before forming the equations for the next structural unit. Thus all remaining units are cognizant of the shifts applied to the parameters of units treated earlier in the refinement sequence. This method, first proposed for individual-atom refinement by V. Schomaker and J. Waser (Sparks, 1961), is stated by Sparks (1961) to be the most rapidly convergent of the various block least-squares refinement techniques he compared. The contributions from subsidiary conditions are accommodated readily into the derivative matrix and vector to make this a conditional SFLS method. The computational efficiency of the procedure can be optimized by noting the sequential manner in which the atoms are treated. Ahmed & Cruickshank (1953) described a procedure for calculating structure factor contributions for all reflections from each atom at a time, which was considerably faster than the conventional procedure of calculating contributions from all atoms to each reflection. Extending the procedure to the least-squares process was considered by Cruickshank, Pilling, Bujosa, Lovell & Truter (1961), but was not implemented owing to the limitations imposed, at that time, by computer unreliability and lack of sufficient memory storage.

The basic principles involved in the FGLS procedure are described in this paper. The topics reviewed are implementation of the Gauss-Seidel procedure, optimization of the reflection processing and storage requirements, and incorporation of subsidiary restraints and rigid-body constraints into the general method.

Implementation of the Gauss-Seidel method in SFLS refinement

In principle, the structure factor and derivative contributions to the normal equations can be obtained by making the major processing loop range either over the reflections (all atoms would contribute to the 'active' reflection) or over the atoms (all reflections would be treated for the 'active' unique atom). The latter scheme can be made computationally much faster than the former, but has significantly greater requirements for storage, either core memory or auxiliary store. The latter scheme does not lend itself to the formation of the full normal matrix, nor to a block containing more than the parameters for one unique atom (unless the atom is contributing to the block as a member of a rigid group with the parameters in the matrix and vector corresponding to that group), since the derivatives for an atom are known only when that atom is 'active'. For a block-diagonal or Gauss-Seidel block refinement, the scheme is ideal.

The Gauss-Seidel algorithm is an iterative method of solving systems of linear and non-linear equations by

solving the equations in a sequential fashion while using the latest estimate of each unknown (Carnahan, Luther & Wilkes, 1969). This method may be shown to converge for any positive definite matrix. The process may be converted into a block process (Rollett, 1965) by solving for the new estimates of a set of parameters corresponding to a block of equations, usually by direct solution of the small set of simultaneous equations for the block. As for most methods of solving simultaneous equations, shift ('fudge' or damping) factors may be used to ensure convergence. Although these shift factors are less than 1.0 for most methods, the optimal value for the Gauss-Seidel procedure is generally greater than unity (Rollett, 1965). Sparks (1961) found optimal convergence with a shift factor of 1.53.

A simplified flow diagram of the FGLS procedure is outlined in Fig. 1. The outermost loop is over the atoms, where the pointers IAT1 and IAT2 indicate the first and last atoms, respectively, to be refined in the list of unique atoms. The processing within the atom loop begins with the calculation and accumulation of the structure factor and derivative contributions of atom i to all reflections, then the parameter shifts are determined, displayed and applied, and finally the structure factors are updated to reflect the applied shifts. This process is repeated until the last atom in the list has been refined. A new overall scale factor is computed to complete the cycle. In actual practice, the overall scale factor may be updated as desired within the cycle.

Optimization of reflection processing and storage

To make the processing efficient within the atom loop, it is important to treat the reflection data in an ordered sequence with respect to their Miller indices (Ahmed & Cruickshank, 1953; Burnett & Nordman, 1974). A program flowchart based on the procedures used in the FGLS program is given in Fig. 2. This diagram assumes that the reflections have been sorted in ascending order of hkl with h varying slowest and l varying fastest. Within the atom loop, the structure factor and derivative contributions from atom i and

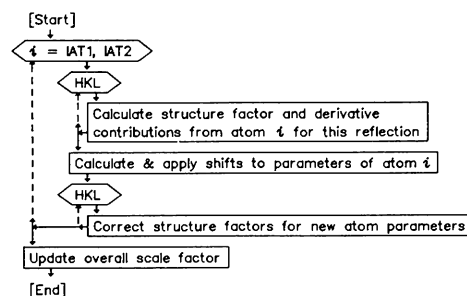


Fig. 1. Basic flow diagram for Gauss-Seidel least-squares refinement.

symmetry-related atoms are computed for each reflection in turn while using the reflection indices h , k and l as the loop indices. The values of the index limits and the reflection-present flag, IS, for each reflection within those limits are obtained from the array ISTAB in a sequential manner. If IS is minus one, the reflection is not in the data, and processing moves to the next reflection. Otherwise, the reflection pointer is incremented, and the structure factor and derivative contributions are calculated and accumulated. The partial contributions to A_c and B_c are stored in the arrays AP and BP, respectively. After all reflections have been processed the parameter shifts for atom i are determined and displayed. Subsidiary conditions such as bond-length or thermal-parameter restraints may be included at this stage in the derivative matrix and vector for the shift determination (Waser, 1963). If the shifts are to be applied, the atom parameters are adjusted and the structure factors updated by subtracting out the old contributions AP and BP and adding in the new. After the atom loop has been completed, a new overall scale factor is calculated if shifts have been applied.

The array ISTAB has been devised to facilitate the efficient processing and storage of reflection data. An ISTAB structure consistent with the hkl looping of Fig. 2 is

$$\text{HMIN, HMAX, (KMIN, KMAX, (LMIN, LMAX, (IS))), ISFLAG,}$$

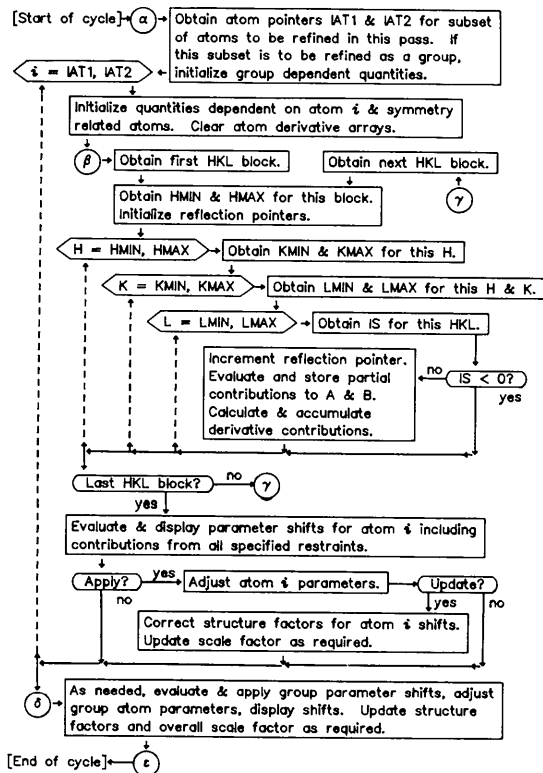


Fig. 2. Flow diagram for the FGLS routine.

where each parenthetical expression must be evaluated for the ranges of the indices whose minimum and maximum values precede the expression. Thus, for a given h and k , there would be values of IS for LMIN, LMIN + 1, ..., LMAX. If a reflection is present, IS equals $1000 (\sin \theta/\lambda)^2$ and is used as a pointer into the scattering-factor table for the atom. Reflection data, such as F_o , A_c , AP, etc., are stored in separate linear arrays in an order defined by the appearance of their h, k, l in the ISTAB array. Although the dimension of the ISTAB array must be somewhat larger than the number of reflections in core memory, the other data array dimensions need not exceed that number. If the reflection data are more numerous than is possible or economical to hold in core memory, the data may be subdivided into manageable blocks, each with its own ISTAB array, to be input at γ concurrent with the data block. The ISFLAG is a flag to indicate the end of the reflection blocks to be processed.

Optimization of the calculations of the structure factor and derivative contributions for atom i is dependent on the nature of the atom and the space-group symmetry. As discussed by Ahmed & Cruickshank (1953) for structure factor calculations, if the atom is assumed to have isotropic thermal behavior, it may be possible to factor out the depen-

dence of the structure factor on an index, say l . This index should be used as the innermost loop since tables of $\cos 2\pi lz_l$ and $\sin 2\pi lz_l$ (for all l) may be prepared. If no index may be factored out, or if the atom is assumed to have anisotropic thermal behavior, the method of Burnett & Nordman (1974) would be appropriate. They accumulate the trigonometric arguments by integer addition and use these arguments, modulo the period of the stored trigonometric table, as subscripts into that table. The arguments for the anisotropic thermal-factor expression may be accumulated in a similar fashion. In any case, any expression should be evaluated outside of loops within which the expression does not vary.

Parameter restraints and rigid-body constraints in FGLS

Waser (1963) recommended treating the desired subsidiary conditions as additional observational equations. If distances between certain pairs of atoms are to be restrained, for example, the function to be minimized is

$$Q_2 = Q_1 + \sum_q w_q (d'_q - d_q)^2, \quad (1)$$

where

$$Q_1 = \sum_h w_h (|F_{o,h}| - G|F_{c,h}|)^2 \quad (2)$$

and the second term is the sum over the q subsidiary distance restraints of the weighted squares of the distance residuals. The d'_q is the assumed 'ideal' distance between a specified pair of atoms (this may correspond to a bond length, bond angle or a minimum distance between non-bonded atoms) and d_q is the distance calculated from the model. The w_q is the weight to be assigned to the particular equation and is given by Pawley (1972) as

$$w_q = Q_1 / [\sigma_q^2 (M - N)], \quad (3)$$

where σ_q is the standard deviation assigned to the q th restraint, M is the number of structure factor observations included in Q_1 , and N is the number of parameters varied in the block. Consistent with the Gauss-Seidel algorithm, restraints to parameters already refined in the cycle are given more weight than those to parameters as yet unrefined in the cycle.

When the internal geometry of a group of atoms is to be strictly maintained as suggested by Scheringer (1963), we have a constrained or 'rigid' group. The location and orientation of this rigid group within the unit cell may be specified by six parameters (three translational and three rotational). The fractional coordinates, x_p , of atom i in the group j may be related to its coordinates, X_p , in a convenient Cartesian reference frame by the expression

$$x_i = t_j + \mathbf{UR}_j \mathbf{X}_i, \quad (4)$$

where t_j is the translation vector in fractional coordinates of the origin of the group relative to the unit-cell origin, \mathbf{U} is the transformation matrix from the Cartesian to the fractional crystallographic coordinates and

$$\mathbf{R}_j = \begin{pmatrix} \cos \varphi \cos \rho - \sin \varphi \sin \theta \sin \rho & -\sin \theta \cos \theta & \cos \varphi \sin \rho + \sin \varphi \sin \theta \cos \rho \\ \sin \varphi \cos \rho + \cos \varphi \sin \theta \sin \rho & \cos \varphi \cos \theta & \sin \varphi \sin \rho - \cos \varphi \sin \theta \cos \rho \\ -\cos \theta \sin \rho & \sin \theta & \cos \theta \cos \rho \end{pmatrix} \quad (5)$$

is the rotation matrix (Doedens, 1970) corresponding to successive rotations of the group, first by the angle φ about the Cartesian Z axis, next by θ about the new Cartesian X axis, and finally by ρ about the new Cartesian Y axis. Once a \mathbf{U} matrix appropriate to the crystal system has been chosen, the x_i may be expressed in terms of the X_i by (4) and *vice versa*.

The quantity Q_2 in (1) is to be minimized with respect to the parameters of group j . The derivatives of F_c with respect to the group parameters are obtained from the individual-atom derivatives by application of the chain rule (Doedens, 1970).

(1) For the group translation

$$\frac{\partial F_c}{\partial t_{jk}} = \sum_i \frac{\partial F_c}{\partial x_{ik}} \quad (k = 1, 2, 3). \quad (6)$$

(2) For the group rotation

$$\frac{\partial F_c}{\partial \varphi_j} = \sum_i \sum_k \frac{\partial F_c}{\partial x_{ik}} \frac{\partial x_{ik}}{\partial \varphi_j} \quad (k = 1, 2, 3), \quad (7)$$

and similarly for θ_j and ρ_j .

(3) For the group overall isotropic thermal factor, BG_j

$$\frac{\partial F_c}{\partial BG_j} = \sum_i \frac{\partial F_c}{\partial B_i}, \quad (8)$$

where the summation of i ranges over all atoms in the group j . As formulated in (5), a singular matrix of normal equations will result if θ is near 90 or 270°. To reduce the chance of this difficulty, the FGLS procedure utilizes a revised form of (4) given by the expression

$$x_i = t_j + \mathbf{UR}_j \mathbf{R}_0 \mathbf{X}_i, \quad (9)$$

where \mathbf{R}_0 has the same form as (5) with the angles $\varphi_0 = \theta_0 = \rho_0 = 0$. Thus, \mathbf{R}_0 is the identity matrix and the derivatives with respect to the 'group' angles φ_0 , θ_0 and ρ_0 are orthogonal to each other. After the shifts have been determined for these angles, the product $\mathbf{R}_j \mathbf{R}_0$ is formed and the new values of φ , θ and ρ can be obtained by inspection of (5). The evaluation of the angular shifts with respect to the matrix \mathbf{R}_0 permits the group to be oriented as desired in the Cartesian reference frame for analysis of group motion or restriction of angular parameters for linear groups.

Although incorporated in the working program, the rigid-group option is not explicitly shown in Fig. 2. In this mode the Gauss-Seidel updating of structure factors for each atom in turn must be suspended until

all atom shifts within the group have been determined. At α in Fig. 2 the atom list pointers IAT1 and IAT2 are set to indicate the first and last atoms which constitute the group. The group orientation angles and translation vectors are obtained, and the group derivative arrays are cleared. At β within the atom loop, the Cartesian coordinates X_i are calculated from the fractional crystal coordinates x_i by the inverse of (9), and the factors required to convert the individual-atom derivatives to group derivatives are calculated. Within the reflection loop, the normal equations corresponding to the individual atom as well as the rigid body are formed. This allows the 'free' shifts of atom i to be calculated and displayed to assist in the detection of false atoms or conformational distortions. At δ the loop over all atoms in the group is complete, and group

shifts may be calculated and applied. If any shifts were applied, the structure factors are updated. At ϵ the processing of group j is complete and program flow jumps back to α to process group $j + 1$, if necessary.

Application to protein structure refinement

In order to evaluate the performance of the program, and to explore the effect of varying the softness of distance restraints, a moderate-resolution structure refinement of the semiquinone form of *Clostridium MP* flavodoxin (Smith, Burnett, Darling & Ludwig, 1977) was carried out.

The starting model consisted of 1003 atoms which had been fitted to the density of the isomorphous-replacement map by real-space refinement (Diamond, 1971). The remaining 101 atoms, in the 1104-atom protein molecule, were not observed in the map density, but were positioned consistent with the amino acid sequence information and standard stereochemical considerations. These 101 atoms were assigned zero occupancy, so that they could be carried along in the group refinement of the rest of the protein, without exerting any direct influence on the calculated structure factors. Approximate local stereochemistry was imposed on the model (Levitt, 1974) prior to the least-squares refinement.

4660 reflections with $I > 2\sigma(I)$ within the resolution limits 2.5 to 5.0 Å were used in the refinement. Although data to 1.8 Å have been collected (Smith *et al.*, 1977) the 2.5 Å limit was chosen to save calculation time, and also to enhance the significance of the restraints being tested.

Groups of atoms in chemically known geometry were treated as rigid. These included short side chains, three (*e.g.* Met) or four (Arg, Glu *etc.*) atoms at the ends of flexible side chains, and the planar groups in Phe, Trp, *etc.* The peptide O=C-N groups were taken as rigid. Elastic restraints were applied to all pairs of nearest- and second-nearest-neighbor atoms not within the same rigid group. Thermal B restraints were applied between all nearest-neighbor atoms, including pairs wholly within the same rigid group. The thermal restraints were applied only when the difference between two neighboring B values exceeded a threshold value of 3.0 Å².

An auxiliary program identifies the rigid groups and generates the restraint information for each restrained atom pair in the polypeptide chain. This restraint information includes 'ideal' interatomic distances and nominal σ values, *i.e.* elastic constants, assigned to the distance constraints. Threshold values, ΔB , and σ values for thermal-parameter restraints are also included.

A rescaling of the restraint σ values is generally done before each refinement cycle. Since the refinement proceeds from one atom (or rigid group) to the next, it is advantageous to allow more softness in *forward* restraints, that is, in restraints from the active atom to atoms not yet refined, than in backward restraints. It is important that distance σ 's be chosen sufficiently high in the beginning of the refinement, since undue insistence on maintaining ideal bond lengths will slow down the refinement of a misplaced chain segment.

The progress of four cycles of refinement is shown in Table 1. The shift factors were chosen as 1.2 for both coordinates and thermal parameters. An analysis of parameter shifts in successive cycles indicated that a somewhat higher value would have been optimal, in qualitative agreement with Sparks's (1961) finding.

Reflection weights were taken as $w = (1 + cF_o^2)^{-1}$ with c chosen so as to downweight the terms in (2) containing the upper quintile of F_o values by an average w of about 0.25. This gave a nearly even distribution of $\langle w(\Delta F)^2 \rangle$ as a function of F_o^2 .

Restrainted refinement at low resolution necessarily involves a balance between structure factor agreement and adherence to ideal stereochemistry. This balance is controlled by the choice of the standard deviations σ_q assigned to the restraints [equation (3)]. The σ_q values used for nearest-neighbor distance restraints are given in columns 2 and 3 of Table 1. Second-nearest-neighbor distance σ 's were taken as 1.2 times as large, thermal B restraint σ 's as 6.0 Å² with a threshold ΔB of 3.0 Å².

The actual deviation from ideal bond lengths is shown in column 4, and the reciprocal-space measures of agreement in the last two columns. As shown in columns 5 and 6, the refinement has essentially converged in three cycles.

The computing time was 9 min per refinement cycle on an Amdahl 470/V6 computer, or 1.1×10^{-4} s per atom-reflection. These values include structure factor

Table 1. *Refinement statistics*

Cycle	Bond restraint σ (Å)		Bond length	Average atom shift (Å)		Relative $\Sigma w(\Delta F)^2$	R
	forward	back	r.m.s. ($d - d'$) (Å)	cycle	cumulative		
0	—	—	0.012	—	—	309	0.350
1	0.8	0.40–0.13	0.090	0.241	0.241	179	0.265
2	0.40–0.13	0.13–0.05	0.070	0.096	0.251	152	0.245
3	0.13–0.05	0.05–0.03	0.051	0.056	0.251	152	0.244
4	0.03	0.03	0.037	0.042	0.248	156	0.247

updating, an integral part of the refinement cycle. Structure factor computation alone requires 2.1×10^{-5} s per atom-reflection.

The completion of the model of the protein molecule and associated solvent, and the extension of the refinement to 1.8 Å resolution will be discussed in a separate publication.

The program is written in Fortran and includes documentation and patches for most common space groups. It is available from either author. Included in the package are programs for generating the reflection and ISTAB files, blocked as needed, and a program for automatic generation of parameter restraint files for polypeptides.

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References

- AHMED, F. R. & CRUICKSHANK, D. W. J. (1953). *Acta Cryst.* **6**, 765–769.
- BURNETT, R. M. & NORDMAN, C. E. (1974). *J. Appl. Cryst.* **7**, 625–627.
- CARNAHAN, B., LUTHER, H. A. & WILKES, J. O. (1969). *Applied Numerical Methods*. New York: John Wiley.
- CRUICKSHANK, D. W. J., PILLING, D. E., BUJOSA, A., LOVELL, F. M. & TRUTER, M. R. (1961). *Computational Methods and the Phase Problem in X-ray Crystallography*, pp. 32–78. New York: Pergamon Press.
- DIAMOND, R. (1971). *Acta Cryst.* **A27**, 436–452.
- DOEDENS, R. (1970). *Crystallographic Computing*, pp. 198–200. Copenhagen: Munksgaard.
- HESTENES, M. R. & STIEFEL, E. (1952). *J. Res. Natl Bur. Stand.* **49**, 409–436.
- HOARD, L. G. & NORDMAN, C. E. (1974). *Am. Crystallogr. Assoc. Abstr. Ser. 2*, Vol. 2, p. 248.
- KONNERT, J. H. (1976). *Acta Cryst.* **A32**, 614–617.
- LEVITT, M. (1974). *J. Mol. Biol.* **82**, 393–420.
- PAWLEY, G. S. (1972). *Adv. Struct. Res. Diffr. Methods*, **4**, 1–64.
- ROLLETT, J. S. (1965). *Computing Methods in Crystallography*, pp. 75–76. Oxford: Pergamon Press.
- SCHERINGER, C. (1963). *Acta Cryst.* **16**, 546–550.
- SMITH, W. W., BURNETT, R. M., DARLING, G. D. & LUDWIG, M. L. (1977). *J. Mol. Biol.* **117**, 195–225.
- SPARKS, R. A. (1961). *Computational Methods and the Phase Problem in X-ray Crystallography*, pp. 170–187. New York: Pergamon Press.
- SUSSMAN, J. L., HOLBROOK, S. R., CHURCH, G. M. & KIM, S. H. (1977). *Acta Cryst.* **A33**, 800–804.
- WASER, J. (1963). *Acta Cryst.* **16**, 1091–1094.
- WATENPAUGH, K. D. (1973). *Computational Needs and Resources in Crystallography*, pp. 37–46. Washington, DC: National Academy of Sciences.
- WATENPAUGH, K. D., SIEKER, L. C., HERRIOTT, J. R. & JENSEN, L. H. (1973). *Acta Cryst.* **B29**, 943–956.

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Short-range ordering in $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$. By H. BRIGITTE KRAUSE, *Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA* and J. M. COWLEY and JOHN WHEATLEY, *Arizona State University, Tempe, Arizona 85281, USA*

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Abstract

High-resolution electron-microscope images in conjunction with selected-area electron diffraction were used to investigate the short-range order in $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$. Intensity fluctuations of the [110] image indicated ordered domains extending over about 20 to 50 Å. Decomposition phases were observed.

atoms are generally believed to occupy the *A* metal positions while the Mg and Nb atoms are assumed to be distributed in the *B* metal positions. The questions of whether or not ordering of the *B* atoms takes place has previously been investigated with no conclusive results (Krause & Gibbon, 1971): X-ray powder measurements showed no superlattice reflections while selected-area electron diffraction yielded diffuse superlattice points in the body-centered position of the reciprocal unit cell. These results suggested either short-range ordering of the Mg and Nb atoms or slight distortions of the cubic unit cell associated with ferroelectric behavior. Electron microscopy imaging methods have now been used to distinguish between these possibilities.

$\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ crystallizes in the cubic perovskite structure with a lattice constant of 4.04 Å (Ismailzade, 1961). The Pb

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