therefore cost between $5 and $20. Access to the computer system is by local telephone call, using the Telnet communications network in most cities in the US, and a toll-free '800' long-distance telephone call elsewhere.

Those wishing further information regarding access to the system are invited to contact the JCPDS or the CIS Operations manager (GWAM).

References


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Computer program for radial distribution analysis of X-ray, neutron and electron diffraction data. By Peter D’Antonio and John H. Konnert, Naval Research Laboratory, Washington, DC 20375, USA

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Abstract

A rapidly converging radial distribution least-squares program (RADILS) is available for the analysis of X-ray, neutron and electron diffraction data from liquid and amorphous materials. The program automatically generates a radial distribution function, G(r), essentially free from termination effects and determines the empirical background scale and shape, absolute scale factor, bulk density and coordination numbers, disorder parameters and interatomic distances for the first few highly ordered distances in the sample.

Introduction

Structural information is derived from the distribution of distances, G(r), in the sample, which is the Fourier sine transform of the interatomic interference intensity, s(s). The momentum transfer s equals 4π sin θ/λ, where λ is the wavelength and 2θ is the angle between the incident and diffracted beams.

To generate an accurate G(r) from a truncated set of total intensity data, I(s), a data reduction procedure must:
1. isolate s(s) from I(s), by determining the experimental background intensity B(s);
2. minimize errors due to termination and scaling of the intensity data.

Other procedures (Kaplow, Strong & Averbach, 1965; Warren, 1969; Leadbetter & Wright, 1972) have been developed to enhance the reliability of the radial distribution analysis. The radial distribution least-squares program (RADILS) described here, while concerned with the same criteria, is characterized by a unique treatment of termination effects (Konnert & Karle, 1972, 1973), wherein the contributions from the first few ordered distances in the sample are subtracted from s(s) to form s'(s), before the Fourier transform which generates G'(r) is performed. RADILS exhibits very rapid convergence due to the fact that G'(r) is expressed explicitly as a function of the total intensity, scattering factors [f(s)], and refinable parameters for the scale and shape of B(s), the scale factor (k), the bulk density (ρ0) and the coordination numbers (NAB), disorder parameters (lAB) and interatomic distances (rAB) for the first few ordered distances.

\[
G'(r) = 4\pi [\rho(r) - \rho_0] + \sum_{\text{inner region}} \sum_{\text{outer region}} \sum f^2(s) \sin sr dS.
\]

Minimize \[
\sum_{\text{inner region}} G'(r) + 4\pi \rho_0 \sum_{\text{outer region}} \sum w[G'(r)]^2. \quad (2)
\]

w fixes the relative weights of the two regions. Equation (1) is minimized as shown in (2), subject to the following constraints:
1. the inner region of \( G'(r) + 4\pi \rho_0 \) should be zero where distances are known not to exist. By minimizing termination effects which affect this region as well as the rest of \( G'(r) \), this region can be utilized as a sensitive measure of background error.
2. the outer region of \( G'(r) \) should show a uniform distribution of distances;
3. the scaling of the intensity data should be consistent with the bulk density and/or known coordination numbers;
4. \( B(s) \) should be a smoothly changing function whose shape is compatible with theory.

Coordination spheres with non-Gaussian distance distributions (for example, the first coordination sphere for liquid metals) are represented with the sum of several Gaussians. This is accomplished by assigning several \( AB \) pairs in (1) to a single coordination sphere. Optimal parameters for representing the non-Gaussian distribution are determined by solving for the eigenvectors and eigenvalues of the linearized least-squares problem and employing a parameter filtering scheme. It may be noted that the analysis of multi-component systems, where all peaks in the inner region of the radial distribution function are composite, may be handled in the same way.

This approach has several advantages.

1. Termination error is minimized because \( s' (s) \) is essentially terminated at the experimental data limit, \( s_{\text{max}} \). This is the case because the primary contributions beyond \( s_{\text{max}} \) are the first few ordered distances due to their low disorder parameters.

2. The structural parameters for the short distances can be determined by minimizing the spurious detail in the region of \( G'(r) \) where these distances contribute. The range over which \( G'(r) + 4 \pi r \rho_0 \) is required to be zero is extended to include the region involving the distances which are subtracted.

3. Errors in the structural parameters of the ordered distances arising from the variability of the scattering factors with \( s \), for X-rays and electrons are minimized, because the short distance contributions, with variable scattering factors, are subtracted before transformation.

\( G(r) \) is generated by reintroducing a Gaussian or summation of Gaussians description of the short distances without the associated termination effects. A provision for decomposing these Gaussians is provided.

**Program highlights**

RADILS is a single self-contained program which includes all the necessary subroutines, a plotting and an eigenvector-eigenvalue package. The user need only substitute a matrix-inversion call recognized by his computing facility. There are many options and choices of input and output which are controlled by program flags. The user has a choice among several background treatments utilizing either an overlapping exponential or a summation of Gaussians background function. The solution of the normal equations can be obtained by matrix inversion or the eigenvector-eigenvalue method for unstable matrices. A filtering scheme for matrix stability is also provided. The structural parameters may be constrained with linear constraint relations if necessary. An estimate of the effect of random errors on the intensity \( \sigma [s(s)] \) and the radial distribution function \( \sigma [G(r)] \) is calculated. This is particularly important when assessing the effect of structural ordering in the outer region of \( G(r) \).

**Program input**

1. Total intensity and standard deviation data in equal increments of \( s \), corrected for all systematic effects.
2. Scattering factors.
3. Initial estimates for the background, scale, bulk density and structural parameters.

**Program output**

1. Line printer and calcomp plots for
   (a) \( I(s) \) and \( B(s) \),
   (b) \( s i(s), s' (s), e [s s(s)] \),
   (c) \( G(r), G'(r), 4 \pi r \rho_0, \sigma [G(r)] \).
2. Parameter and error estimates for
   (a) \( B(s) \), scale and shape,
   (b) absolute scale factor,
   (c) bulk density,
   (d) interatomic distances, disorder parameters and combination numbers for the distances subtracted.

A tape of the program, a detailed write-up describing the program and its applications and sample input card decks are available. If a magnetic tape were supplied there would be no additional cost. RADILS has been tested and applied in several analyses (Konnert & Karle, 1972, 1973; Konnert, Karle & Ferguson, 1973; D'Antonio, Moore, Konnert & Karle, 1977).

**References**