

Errata

QPDA – A User-Friendly, Interactive Program for Quantitative Phase and Crystal Size/Strain Analysis of Powder Diffraction Data

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Abstract

Recent developments in the Rietveld method for the analysis of powder diffraction data have seen the method evolve from its original purpose of crystal structure refinement to include the determination of phase abundance in polycrystalline mixtures and the estimation of crystal size and strain parameters. However, the Rietveld method is not easy to use and may deter many powder diffractionists, who are not interested in structure refinement *per se*, from using the method in its non-structural applications.

In order to overcome the difficulties in using the Rietveld method, a program, QPDA (for Quantitative Powder Diffraction Analysis), has been written that sets the condi-

tions necessary for a single or multi-phase refinement, runs the Rietveld program and extracts phase abundance and size/strain information from the refined parameters. The program comprises a user-friendly, default-driven system of subroutines, written initially in VAX Fortran, and operates from a database of inorganic materials frequently encountered in a wide range of minerals and materials science industries.

Equations (3) and (5) should be corrected to read as follows:

$$e_{\text{rms}} = \pi (U-U_i)^{0.5} / 720 (2\ln 2)^{0.5} \quad (3)$$

$$D = \lambda (180/\pi) / (\gamma - \gamma_i) \quad (5)$$

The following citation should be added to the reference list:

Donnay, J.D.H. & Le Page, Y. (1978). *Acta Crystallogr.* A34, 584.

International Report

A word from the editor . . .

Dr. Jaroslav Fiala has submitted a report on the meeting on Advanced Methods in X-Ray and Neutron Structure Analysis of Materials which was held in Prague, Czechoslovakia, last August. His historical introduction is very interesting. I think you will enjoy it. I did.

Helein D. Hitchcock, Editor

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