Short Communications

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On the definition and practical use of crystal-based azimuthal angles. Erratum. By D. SCHWARZENBACH, Institut de Cristallographie, University of Lausanne, BSP Dorigny, CH-1015 Lausanne, Switzerland, and H. D. FLACK, Laboratoire de Cristallographie, University of Geneva, 24 quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland

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Abstract

In the paper by Schwarzenbach & Flack [J. Appl. Cryst. (1989), 22, 601-605], the equation describing the transformation properties of the crystal-based azimuthal angle $\psi$ is incorrect. The correct formula is derived.

The argument in the section Unit-cell transformations on p. 603 of the paper is erroneous since $|\mathbf{q}_a \times \mathbf{q}_b| = |\sin \Delta \psi|$ and not $\sin \Delta \psi$. Similarly, equation (10) is wrong since $v_a^T \mathbf{G}_{\alpha} v_a = V_a^{-2} s^{-2} \sin^2 \Delta \psi$, $V_a = \mathbf{a}_a \cdot \mathbf{h}_a$. Moreover, $\mathbf{v}_a$ is proportional to $\mathbf{h}_a$, $\mathbf{v}_a = c \mathbf{h}_a$. The sign of $\sin \Delta \psi$ is $\text{sign}(|\mathbf{q}_a \times \mathbf{q}_b|) = \text{sign}(c) = \text{sign}(v_a^T \mathbf{h}_a)$. Equation (10) thus becomes

$$A^T \mathbf{v} = (\sin \Delta \psi, 0, \cos \Delta \psi)$$

$$s = \text{sign}(v_a^T \mathbf{h}_a) \{v_a^T \mathbf{G}_{\alpha} v_a\}^{1/2}, 0, (v_a^T \mathbf{G}_{\alpha} \mathbf{v}_a)$$

$$s^{-2} = (v_a^T \mathbf{G}_{\alpha} v_a)^2, (v_a^T \mathbf{G}_{\alpha} v_a)$$

Computer Programs


MRIAAU – a program for autoindexing multiphase polycrystals. By V. B. ZLOKAZOV, Joint Institute for Nuclear Research in Dubna, Laboratory of Computing Techniques and Automation, Head Post Office, PO Box 79, Moscow, USSR

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Abstract

A method and algorithm are described for solution of the autoindexing problem of multiphase polycrystals. A Fortran program, called MRIAAU, which implements the algorithm, runs on a PC and can solve the problem in some minutes (IBM PC with 80286 and higher).

1. Introduction

Autoindexing is the determination of the lattice parameters and Miller indices of reflections. In a multiphase polycrystalline sample this can be done on the basis of a set (incomplete) of experimentally observed diffraction reflection positions.

The method, described below, is universal, straightforward and uses the analytical technique of approximation, which allows the user to get an acceptable problem solution quickly even in complicated cases [the program run takes on average a few minutes on a PC like the Wang 250/16 (IBM compatible, with an 8 MHz coprocessor)].

Let a diffraction (neutron or X-ray) measurement produce a spectrum where (approximate) positions of intensity maxima give the set $R = \{r_j\}, j = 1, 2, \ldots, m$, of which some are dependent on one another. Each reflection position is formally given by the formula

$$r = f(P, I),$$

where $P$ is vector (1) and $I$ is a vector of three integer numbers from a set of groups of three $M_k$ (Miller indices), $k = 1, 2, \ldots, n$, for any unknown phase.

The problem is: $R$ being given and $n$ fixed, determine $P_k$ and $M_k$ for each $k$. This problem is difficult even for a monocrystal sample, $n = 1$ particularly for a powder sample, $n > 1$.

A natural algorithm which offers itself here is as follows. Let bounded vector sets $P_k$ and sets of three integer numbers $M_{jk}$ $k = 1, 2, \ldots, n; j = 1, \ldots, m$, be given such that $Q_k \subset \{P_k\}, \{N_{jk}\} \subset \{M_{jk}\}$, where $Q_k$ and $\{N_{jk}\}$ are true parameters of the lattice and Miller indices for the $k$th phase. For components of vectors $P_k$ the following relations are true:

$$p_{kl} \leq p_k \leq p_{kw}.$$