data require that reflections originate from a single crystal. However, if the material under study is polycrystalline, an X-ray beam may illuminate many crystallites. The resulting reflections will originate from different crystallites and may be difficult to sort. The computer code described here sorts such reflections according to their crystallite of origin. We have used this code to successfully sort over 100 reflections resulting from a polycrystalline film.

Method of solution: Two pairs of reflections can originate from the same crystallite only if they can be formed from the same orientation matrix, U (Busing & Levy, 1967). This U must be a proper unitary matrix that gives the wave-vector difference $\mathbf{K}$ in terms of a reciprocal-lattice vector $\mathbf{G}$ as follows:

$$\mathbf{K} = U\mathbf{G}.$$

If a set of measured wave vectors $\mathbf{K}_1$, $\mathbf{K}_2$, $\mathbf{K}_3$, . . . originates from the same crystallite, they must be associated with a set of allowed reciprocal-lattice vectors, $\mathbf{G}_1$, $\mathbf{G}_2$, $\mathbf{G}_3$, . . . such that

$$\mathbf{G}_i \cdot \mathbf{G}_j = \mathbf{K}_i \cdot \mathbf{K}_j$$

for any pair i, j. In theory, this condition does not ensure that the reflections originate from the same crystallite. Two crystals oriented at the same angle as two reciprocal-lattice vectors will produce two sets of reflections satisfying this condition. In practice, however, such coincidences are rare and they have not been encountered in the test data.

The reflections are grouped together such that the angle between every pair $\mathbf{K}_i, \mathbf{K}_j$ agrees with the angle between the corresponding $\mathbf{G}_i, \mathbf{G}_j$ to within some tolerance, supplied by the user. The reciprocal vectors $|\mathbf{G}|$ are assigned to each reflection from those allowed, given the length $|\mathbf{K}|$. The different allowable $|\mathbf{G}|$ assignments are searched so that the number of reflections in a grouping is maximized.

Software and hardware environments: The coding is titled *SORTREF* and can be run on any computer that can compile the source C code. It only requires access to the standard C libraries, so no special software interface is required. The user provides a file in which each line contains the four-circle diffraction angles, 2θ, ω, χ and φ (Busing & Levy, 1967). The program creates a file containing the same data but grouped according to crystallite. *SORTREF* has been successfully run on an IBM RS6000, a Sun SPARCstation and a DEC MicroVAX, typically taking less than 1 min to sort over 100 reflections.

Program specification: This algorithm assumes that the user has supplied reciprocal-lattice vectors accurate to within ±10%. It also expects the reflections to have been refined, although those of weak intensity may be rejected if desired. The code currently cannot recognize reflections with $|\mathbf{K}|^2/b^2 > 36$, where b is a user-supplied length scale.

Availability and documentation: The source C code, as well as documentation and sample input, are available by ftp from lassp.cornell.edu. At the user-name prompt, login as 'anonymous'; the files are in the directory /pub/sadd.

Keywords: Crystalline, sort, X-ray reflections, polycrystalline.

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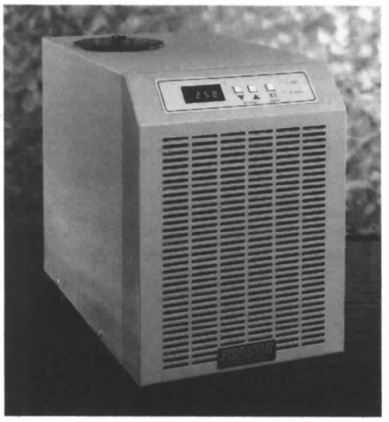

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