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A simple protocol for determining the zone axis direction from selected-area electron diffraction spot patterns of cubic materials. Addendum. Comprehensive tables for pattern reindexing

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A set of 45 reindexing tables has been calculated for the 15 most common zone axis diffraction patterns of cubic lattices (*P*, *I* and *F* types). These tables cover all possible alternative lattice orientations, providing a systematic and efficient method of reindexing *hkl* reflections. They complement and extend the *Atlas of Zone Axis Spot Patterns for Cubic Lattices* (Weirich, 2024) and the table of standard settings provided by Weirich [*J. Appl. Cryst.* (2024), **57**, 1263–1269].

1. Introduction

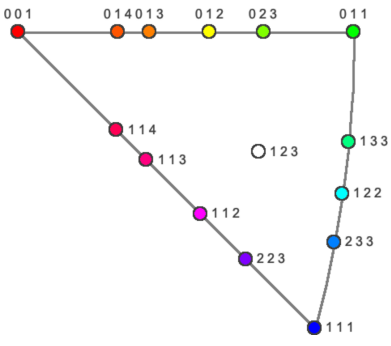
In a previous article (Weirich, 2024*a*), a protocol for identifying lattice directions for the 15 most common cubic zone axis electron diffraction patterns was introduced. This was accomplished using the R_n ratio method, which utilized the three shortest reciprocal-lattice vectors and the angles between them. As the *Atlas of Zone Axis Spot Patterns for Cubic Lattices* (Weirich, 2024*b*) and the table in the recent work only provide one standard orientation as solution, there may be limitations for practical applications if a different orientation is required. To address this issue, tables were compiled for the 15 above-mentioned orientations, which list all alternative orientations together with the Laue indices for the three base vectors.

2. Method

The *hkl* Laue indices of the three basis vectors for the alternative orientations of the 15 zone axis directions shown in Fig. 1 were calculated by means of the 48 inverse matrices M^{-1} (see supplementary material, pp. 3–8) of the point symmetry operations for the cubic crystal system (Wondratschek & Aroyo, 2016; Borchardt-Ott & Sowa, 2018) using equation (1):

$$h'k'l' = hkl\ M^{-1}. \qquad (1)$$

Each row in the obtained lists (see supplementary material, pp. 9–50) contains the alternative zone axis direction [*uvw*], the Laue indices of the three base vectors *A*, *B* and *C*, and the reference to the matrix equation used for the calculation. As two symmetry operations always yield the same orientation for the [001] and [011] zone axes, these tables have been shortened accordingly to improve readability.



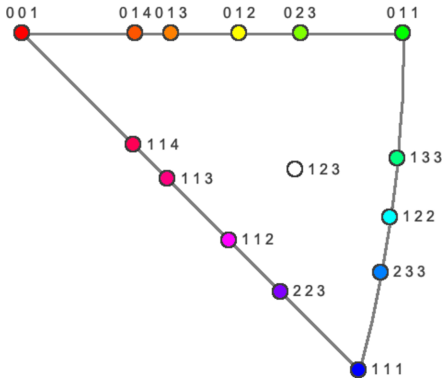


Figure 1
The 15 (standard) zone axis directions covered by the earlier paper (Weirich, 2024*a*) and the *Atlas of Zone Axis Spot Patterns for Cubic Lattices* (Weirich, 2024*b*) are shown within the standard stereographic triangle of the cubic system. All alternative orientations and corresponding *hkl* Laue indices for their pattern base vectors have been calculated for the cubic *P*, *I* and *F* lattices and compiled in tables (see supplementary material, pp. 9–50.

3. Example

Fig. 2 illustrates the procedure for reindexing and shows the six possible variants for indexing a [111] face-centered cubic (f.c.c.) lattice. The pattern labeled M1 corresponds to standard indexing (Weirich, 2024*a*; Weirich, 2024*b*), with $A = 20\bar{2}$ (pointing to north), $B = 02\bar{2}$ and $C = 2\bar{2}0$ (see Table 9 on p. 14 of the supplementary material). For tracking the movement of the initial indices during reindexing, the diffraction spots *A* and *B* have been marked with a star. Note that the corresponding matrix equation (M1 on p. 3 of the supplementary material) is the identity matrix, which does not change the *hkl* indices and refers therefore always to the initial (standard) indices before the transformation. An alternative setting for the same [111] zone axis can now be obtained by searching the table for all entries with the same indices and replacing the initial indices of *A*, *B* and *C* of the standard setting with those from the corresponding row. The other five patterns in Fig. 2 were obtained in this way, with the condition that the spots relating to *A* were plotted so that they always point towards north. The matrix equations used to calculate the *hkl* Laue

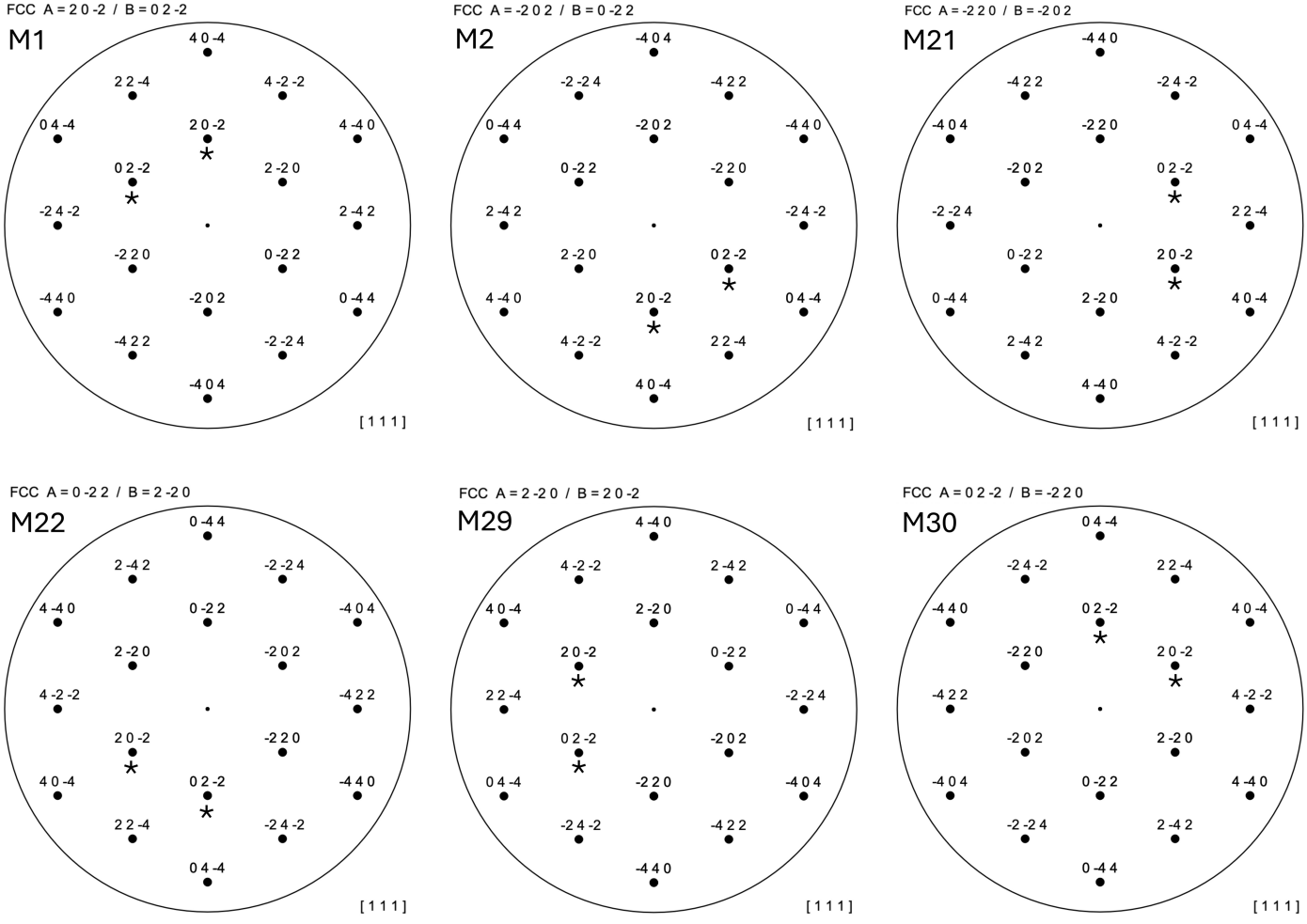


Figure 2
The six possible variants for indexing a [111] f.c.c. lattice are obtained from Table 9 on p. 14 of the supplementary material. The corresponding matrix equation *M* (see supplementary material, pp. 3–8) to obtain the indices in the reindexed pattern is shown in the top-left corner of each pattern. For comparison, each pattern has been drawn so that the reciprocal lattice vector *A* points to the north, and the spot indices *A* and *B* of the standard setting are labeled with stars.

indices for a reindexed pattern are shown in the top-left corner of each pattern.

4. Summary

A comprehensive set of 45 tables for reindexing the 15 most common zone axis diffraction patterns of cubic lattices have been calculated for the *P*, *I* and *F* Bravais lattices by means of the inverse matrices of the point symmetry operations for the cubic crystal system. This new set of tables is a valuable supplementary resource to the *Atlas of Zone Axis Spot Patterns for Cubic Lattices* (Weirich, 2024*b*) and the table presented by Weirich (2024*a*), since they facilitate the reindexing of the *hkl* indices of standard patterns in a streamlined manner.

Conflict of interest

The author declares no conflicts of interest.

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