for these motions the centre of gravity of the atoms in the unit cell is not at rest and a matrix **G** which resolves the vibration coordinates into internal and external ones, cannot be constructed. Therefore the mass dependency of the matrices **L**, $\mathbf{L}^{-1}$ and **U** vanishes.

6. Discussion

To sum up: it is the long-wave optic modes of a crystal which cause a strong mass dependence of the atomic mean-square amplitudes. The smaller the value of q the more pronounced the mass dependence will be. According to equation (1) the vibration tensors $\mathbf{U}_r$ are calculated from the inverse dynamical matrices of all wave vectors **q** of the crystal. Since the long waves with small q are less frequent than the short waves with large q, the long waves do not govern the vibration tensors $\mathbf{U}_r$ but still have an impact upon them. Thus the mass dependency, which is expressed by equation (9) for $q=0$, is greatly weakened but not fully eliminated in the vibration tensors $\mathbf{U}_r$. This result is in full agreement with the observations made on actual structures. Generally, for a given structure, we find the smaller amplitudes for the heavy atoms and the larger amplitudes for the light atoms. Exceptions to this behaviour were observed; however, they remain the rare cases. A detailed statistics, gained from many structures, would certainly be interesting.

Two predictions can be made from the treatment given in this paper:

(1) Given a fixed mass ratio of two atoms in the unit cell then, the fewer the atoms in the unit cell the greater the tendency for the heavy (light) atom to have the smaller (larger) amplitude. Thus, one will primarily observe that a heavy (light) atom has a relatively large (small) amplitude when the unit cell is large.

(2) Given a fixed number of atoms in the unit cell the bigger the difference between the masses the greater the tendency for the heavy (light) atom to have the smaller (larger) amplitude.

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A Simplified Procedure for Orientation of Single Crystals of Any Structure

BY B. KRAHL-URBAN, R. BUTZ AND E. PREUSS

*Institut für Technische Physik der Kernforschungsanlage Jülich, D*517 *Jülich, Postfach* 365, *Germany (BRD)*

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Single crystals with any type of crystal structure can be set up in any desired orientation by a simple and time-saving method of comparing the Laue pattern of the single crystal with a computed and plotted Laue pattern. For this orientation procedure a special goniometer polishing jig has been developed. As examples, both the determination of an unknown direction and the preparation of a specified crystal plane of a hexagonal structure are demonstrated.

Introduction

In the field of solid-state and surface physics many physical properties depend on the orientation of single crystals (see *e.g.* Butz, Erley & Wagner, 1971; Krahl-Urban & Wagner, 1972). As long as such investigations are restricted to the main directions (*e.g.* [100], [110], and [111]) of cubic crystals, it will be easy to recognize

such directions on Laue patterns because of their symmetries. A more difficult and time-consuming task, even in the case of a cubic structure, is the determination of an unknown specimen orientation or the preparation of a sample with high Miller indices. Computation time and work will noticably increase if these two jobs have to be done on single crystals with hexagonal structure.

Laue method

The determination of an unknown crystal orientation is normally carried out by the Laue method (*e.g.* Glocker, 1971). A stereographic projection is produced from the Laue pattern and one zone is revolved onto the periphery by the aid of a Wulff net. By this method, a low-indexed direction of the crystal is brought into the centre of the stereographic projection. One then tries to identify this low-indexed direction by means of comparison with properly designed stereographic figures or patterns from literature (*e.g.* Schiebold & Sachs, 1962). Having performed this successfully it will be possible to index the revolved stereographic projection and to compute the angles of the unknown direction in relation to the main directions of the crystal. The determination of the Miller indices of the unknown direction on the basis of these angles requires a longer computation. Considerable time is needed for the completion of the stereographic projection and its revolution.

Computer programs

To reduce this enormous amount of computation work and time Preuss (1972) has prepared two computer programs in Fortran IV. The first computer program is a plot program delivering Laue figures for a specified direction. For this purpose, it is necessary to feed the computer with the Miller indices of the desired crystal direction, the lattice constants, the crystal angles, the scale of the figure and the maximum Miller index of the reflexions (≤ 15) to be plotted. With this computer program a catalogue of Laue figures has been established (Preuss, Krahl-Urban & Butz, 1973). The catalogue contains Laue figures for back reflexion and transmission of the commonly used orientations and crystal structures. By the second computer program the direction of a specimen can be calculated, if the coordinates of three reflexions are known on a Laue pattern with reference to the centre of the photograph, and if their indices and the distance between film and crystal are known. Moreover, the lattice constants and the crystal angles have to be inserted into the program.

In the following a simplified and time-saving procedure for the orientation of crystals with any type of crystal structure is described. By this procedure the Laue pattern of the single crystal to be oriented is compared with the Laue figures plotted by the first computer program. This simplified method for determining an unknown orientation and for preparing a specified crystal plane with high indices will be explained by means of two examples with hexagonal structure.

Determination of an unknown direction

For the purpose of determining an unknown direction it is useful to produce with the plot program a catalogue of Laue figures for the main directions of the single crystal to be oriented. After this a Laue pattern (Fig. 1) has to be taken from the sample. For this purpose the specimen is mounted on a goniometer. In the present case, a hexagonal rhenium crystal was used. For the orientation of this sample with the second computer program, the coordinates x,y relative to the centre of the pattern and the indices of three reflexions have to be known. The simplest and safest method is to identify one of the stronger reflexions on the Laue pattern. In the present case reflexion A in Fig. 1 is the most appropriate one to be used. In order to recognize this reflexion in the pre-established catalogue of Laue figures the sample is tilted on the goniometer in such a direction that this reflexion is transferred to the centre of a second Laue pattern. Fig. 3 shows the Laue pattern of the tilted sample. A twofold symmetry can be observed. By comparing the Laue figure (Fig. 4) of the [100]* direction of rhenium from the model Laue figures with the Laue pattern (Fig. 3) it is possible to identify the reflexion A as 100. This is a main direction vertical to the c axis. The comparison of the Laue pattern with the plotted Laue figure can be simplified in difficult cases by projecting the Laue pattern onto the computer diagram and bringing the patterns into coincidence. In the present case, the coordinates x,y of the reflexions A, B and C (see Figs. 1, 3 and 4) and the distance between film and specimen were fed into the computer. With these data the computer calculated the direction to be determined as the [484, 124, 9] direction. This direction deviates from the [410] direction by 0·55 degrees. To check the calculated direction the corresponding Laue figure (Fig. 2) was plotted. By comparing Fig. 1 with Fig. 2 the identity of the directions can be easily recognized. Table 1 shows a comparison of the Laue method with the simplified method. In the procedure outlined above the time-consuming stages 3 and 4 of the revolution method (Table 1) are replaced by simple experimental operations. By the procedure described here the Miller indices of the direction to be oriented are given by the second computer program.

Preparation of a sample with a predefined orientation

The preparation of a sample in any desired orientation is illustrated by the example of a rhenium single crystal. The (312) plane should become the surface of this

* The use of three Miller indices hkl for hexagonal crystal lattices is equivalent to the other type of characterization by four Miller indices $hkil$. The index i is linked with h and k by the correlation $i=-(h+k)$.

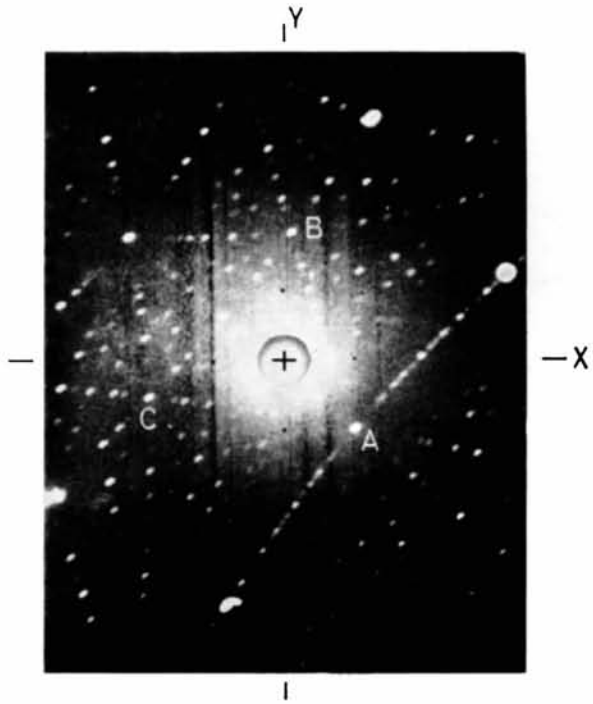

Fig. 1. Laue pattern of an unknown direction of rhenium.

Fig. 2. Plotted Laue figure of the [484, 124, 9] direction of rhenium.

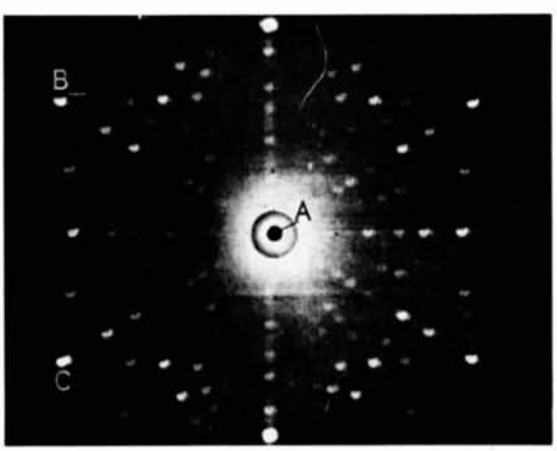

Fig. 3. Laue pattern of the strong reflexion *A* {[100] direction of rhenium}.

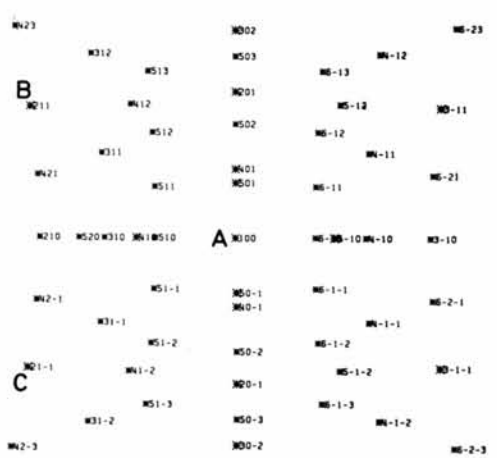

Fig. 4. Plotted Laue figure of the [100] direction of rhenium.

[*To face p.* 88

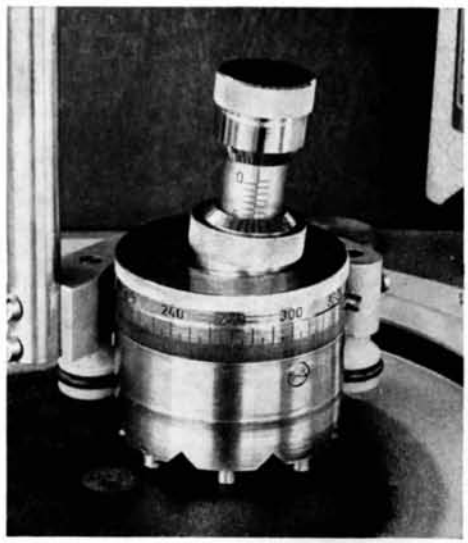

Fig. 5. Goniometer polishing jig.

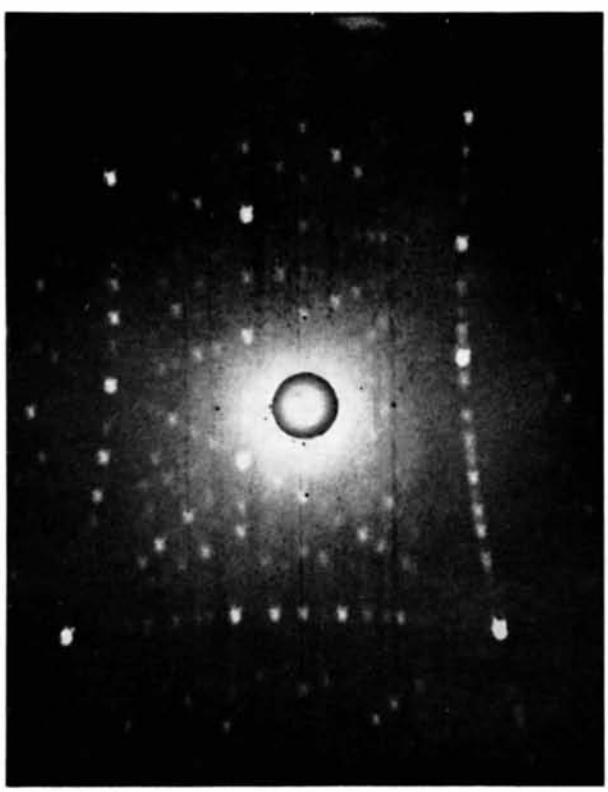

Fig. 6. Laue pattern of the [312] direction of rhenium.

Fig. 7. Plotted Laue figure of the [312] direction of rhenium.

Table 1. *Comparison of the Laue method with the simplified method for determination of an unknown direction*

Stage	Laue Method	Simplified Method
1	Catalogue of stereographic figures	Laue figures
2	Collection of a Laue pattern	
3	Drawing a stereographic projection	Tilting the goniometer on a strong reflexion
4	Revolution of the stereographic projection	Collection of a Laue pattern
5	Comparison with model figures	
6	Calculation of the unknown direction (angles only)	(Miller indices and angles)

specimen. The 312 reflexion can be identified on the upper left-hand side of the plotted Laue figure of the [100] direction. Thus, it will be possible to identify the 312 reflexion on a Laue pattern of the rhenium single crystal used, which has the [100] direction parallel to its axis. The single crystal is now tilted on the goniometer so that the 312 reflexion will move into the centre of the next Laue pattern. Now a slice is cut off from the pre-oriented single crystal by spark erosion and fixed onto a special goniometer polishing jig designed by Butz, Krahl-Urban & Mench (1973). This goniometer polishing jig (Fig. 5) permits one to carry out all operations such as plane etching by means of a spark-erosion machine, tilting the sample exactly in the desired direction, recording Laue patterns and polishing in the tilted orientation on any horizontally running polishing machine (Butz & Krahl-Urban, 1973) without detaching the sample. A Laue pattern is now prepared from the rhenium sample on the goniometer polishing jig. This Laue pattern is compared with the Laue figure plotted for the [312] direction. If necessary, the goniometer polishing jig is readjusted so that the Laue pattern and the plotted figure of the [312] direction will be identical. Fig. 6 shows the Laue pattern of the oriented rhenium specimen with the [312] direction and Fig. 7 the corresponding plotted Laue figure.

Following this procedure, it is possible to prepare single-crystal specimens in a pre-defined orientation with a deviation of less than $\pm 15'$. Table 2 gives a summary of the individual stages for the preparation of an oriented sample with reference to the present example. The time-consuming stages 4, 5 and 8 of the Laue method are replaced by experimental operations in the simplified method.

Table 2. *Comparison of the Laue method with the simplified method for preparation of a sample with a predefined direction*

Stage	Laue Method	Simplified Method
1	Catalogue of stereographic figures	Laue figures
2	Collection of a Laue pattern	
3	Identification of the predefined direction in catalogue	
4	Drawing a stereographic projection	Tilting the goniometer in predefined direction
5	Revolution of the stereographic projection	Collection of a Laue pattern
6	Measuring the tilting angles and tilting the goniometer	Comparison with model figure of predefined direction
7	Collection of a Laue pattern	
8	Drawing a stereographic projection	
9	Comparison of the stereographic projections	

Summary

The determination of an unknown orientation of a single crystal and the preparation of any specified crystal plane has been shown by using the simplified methods. Considerable time is saved in comparison with the conventional methods. The required time is dependent on the difficulty of the job.

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