

Orientation of single crystals by back-reflection Laue pattern simulation. By C. Marín & E. Diéguez. Singapore: World Scientific Publishing, 1999. Pp. xii + 164 + 3½" floppy disk. USD 38, GBP 27. ISBN 981-02-2871-6.

The accurate orientation of crystals has been an important activity ever since Max von Laue and his team (W. Friedrich and P. Knipping) first shone X-rays on to copper sulfate and zinc blende crystals in 1912. The back-reflection technique is essentially the same today as it was ninety years ago. What has changed is the massive increase of computer power, which we enjoy with our desktop computers in the laboratory or at home.

The preface has been written by Professor J. L. Amorós, of the same department as the authors: Department of Physics of Materials, Universidad Autónoma de Madrid. There are two introductory chapters on X-ray diffraction and the back-reflection Laue technique. Two further chapters deal with the development of computational procedures and software. The final chapter compares experimental Laue patterns with simulations, in all seven crystal systems, which is followed by some useful appendices, references and a subject index. (The

index could, however, be improved by including more keywords relevant to the computer program, such as 'detection level' and 'saturation level'.)

The book is written from the perspective of a laboratory source of X rays [in particular, lengthy exposures (2–3 h) of molybdenum radiation of less than 20 kV], but I think that users of synchrotron radiation would also find it useful. There are worked examples of indexing Laue patterns for crystals of GaSb (cubic), KH_2PO_4 (tetragonal), KTiOPO_4 (orthorhombic), $(\text{CH}_2\text{NH}_2\text{COOH})_3\text{H}_2\text{SO}_4$ (TGS) (monoclinic), ZnO (hexagonal), LiNbO_3 (rhombohedral), and $\text{Na}_2\text{W}_4\text{O}_{13}$ (triclinic). In each case, a Laue photograph of unknown orientation is presented, three or four important Laue spots are chosen, their (x, y) coordinates are measured and the crystal-to-film distance noted. These data are put into the algorithm and various solutions are obtained. A simulated Laue photograph can also be displayed. Combinations of angles are given to orient the crystal, so that X-rays become incident along a chosen symmetry axis; examples of Laue photographs and their computer simulations in these settings are given. I tried simulating Laue photographs of my favourite substance, diamond, but I was only partially successful: for some

unknown reason, I could not get any of the even reflections to display.

It is a pity that there are some typographical errors and that the English is far from perfect, but, in most cases, it is understandable. I found the text (point size) and many of the diagrams uncomfortably small. With imperfect eyesight, I had to use a hand lens in addition to my reading glasses in order to read the finer lettering in the figures. The page size would benefit from being twice the area.

The real test is whether I should recommend this book and software to my students. The younger generation would obviously take to the computer program more readily than myself, but I think they too would be frustrated by the inability to correct mistakes easily. If one incorrectly types the coordinates of the 29th atom in the unit cell, there is no obvious way of avoiding having to type in the whole lot again. To be able to simulate Laue patterns quickly is a real asset and I learnt much by making small adjustments to the various parameters. Therefore, with several misgivings, I would recommend this book.

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