could be at least misleading. Two examples: (i) it would be helpful if it were specified that the given form of the third-rank piezoelectric tensor for the point group 2 (and m) refers to a special orientation of the twofold axis (and the plane m), and how the form of the tensor can change for different orientations; (ii) there is only one listed entry for the elasticity fourth-rank tensor for the tetragonal system while one has to distinguish between two tensor forms: one for the point groups $4mm$, $\bar{4}m2$, 422, $4/mmm$, and the other for the point groups 4, $\bar{4}$, $4/m$.

I would add that it is a pity that in the present third edition the author has not used the opportunity to update the presentation of *IT*A (Chapter 3) in accordance with the new fifth edition of the tables or to improve the quality of some of the figures (*e.g.* Fig. 2.1).

Leaving these defects aside, I believe that the book will be useful both to graduate students in physics, chemistry and engineering who have an interest in structural crystallography and to experts seeking a review of numerical methods and implementation strategies. A great advantage of the book is that it is written in a style that makes it accessible also to material scientists whose background does not include structural crystallography. The main messages are clearly stated and not buried beneath technical details.

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Crystal structure determination. Second edition. By Werner Massa. Pp. xi + 210. Translated into English by Robert O. Gould. Berlin: Springer, 2004. Price EUR 44.95, USD 49.95. ISBN 3-540-20644-2.

This textbook, *Crystal structure determination*, is a translation by Robert O. Gould based on the third German edition of *Kristallstrukturbestimmung* by Werner Massa of the University of Marburg, Germany, published in 2002. This new edition in English has been updated from previous editions, particularly in the chapter on experimental methods. It is an excellent teaching text, highly recommended, particularly for those interested in the general principles of this experimental technique and its application to small-molecule crystallography (although the general principles described here are similar for all sizes of molecules). The chapters are short and to the point (179 pages, plus a worked example). The translation is excellent and I understand that the translator worked with the author in order to clarify certain portions of the text. Different students have different needs for the amounts of mathematics used in a textbook of this kind. I recommend they try this text as it contains a medium amount of mathematics.

Initially, we are introduced to crystals and crystal lattices. It seems that not enough emphasis is given to examining the symmetry of the crystal when determining which crystal system it belongs to, although the problem of β near 90° in a monoclinic crystal (which could be mistaken for orthorhombic) is discussed. The descriptions of centered, hexagonal, trigonal, rhombohedral and reduced unit cells, however, are excellent. Then the geometry of X-ray diffraction is described. The reason the characteristic spectral lines are obtained plus a background of white radiation is explained, as is how to select and collimate one component only (usually $K\alpha$). Diffraction is then described, starting with a one-dimensional lattice and proceeding to the Laue equations and the indexing of lattice planes, and finally presenting the Bragg equation and how to calculate scattering angles of diffracted beams if the unit-cell dimensions are known. Then follows a description of the reciprocal lattice that the student should find very helpful. I found this chapter particularly clear. In the chapter on structure factors, I particularly liked the description of what happens to the diffraction pattern as more and more atoms are added to the unit cell.

In the chapter on symmetry, the essentials are described clearly with some fine figures to illustrate each topic. Interestingly (and successfully), the author starts with space groups and then proceeds to Bravais lattices and crystal classes (although the two latter were also mentioned earlier in Chapter 2). I thought the section on space-group determination was very helpful, but the section on group–subgroup relationships was somewhat hard to follow and could have been expanded, for example, by a more comprehensive figure.

The newly expanded chapter on experimental methods will be of great use to students. Some useful recipes for crystallizing small molecules are given. Advice on crystal size, choice of radiation and what to do if the crystal is unstable is given for small molecules only. The various useful film methods are described – again I would have liked more information in the figure captions. There is a good section on reflection profiles and scan types (as seen with the four-circle diffractometer). This involves a discussion of mosaic structure and which portion of reciprocal space needs to be measured (thereby teaching again about symmetry). While nothing is written about the crystallization of macromolecules, the section on area detectors (used now also for small molecules) is highly recommended for all crystallographers. Charge-coupled-device (CCD) systems and image plates are nicely described. The photographs of diffraction and equipment are good. Neutron diffraction is also touched on. There is an excellent treatment of accuracy and estimated standard deviations and absorption coefficients.

The chapter on structure determination begins with the Patterson function. The extension to macromolecules is briefly mentioned, including the multiple isomorphous replacement (MIR) and multi-wavelength anomalous dispersion (MAD) methods. Again the diagrams need more explanation. It is nice to see Harker–Kasper inequalities (Section 8.3.1) and the Sayre equation (Section 8.3.3) given prominence. Then follows the work of Karle and Hauptman for which the 1985 Nobel Prize was awarded. I am not sure that the left side of Fig. 8.4*b* is correct. There is a good description of strategies of phase determination. The author gives information on the programs available and also describes what all the terms derived in these programs are. So there is a good mixture of theory and practice in this chapter, which should help students.

In the chapter on structure refinement, it is stressed that there are errors in both the model and the data and this is an excellent fact to stress. It is pointed out how important the advances in computing power have been for X-ray crystallographic research, especially structure refinement. Problems with hydrogen atoms (bond lengths, isotropic refinement only) are also touched on. The refinement of rigid groups is described, as is Rietveld refinement of powder diffraction data.

In a chapter entitled *Additional topics*, the author tackles disorder in crystals. This was most interesting to me. He describes how to refine such a model with disorder, *e.g.* orientational disorder, and also the problem of dynamic and static disorder. He also mentions the crystal defects that occur on increasing the temperature, together with one- and two-dimensional disorder, modu-

lated structures and quasicrystals. There is also a description of anomalous dispersion and chiral and polar space groups. An excellent example of the structure of a compound with possible inversion twinning is given. Extinction is well described, and the Renninger and $\lambda/2$ effects and thermal diffuse scattering are mentioned.

There is also an excellent chapter on *Errors and pitfalls* that all crystallographers should read. The author provides an interesting example from the literature of a structure with some incorrect atom types and shows how this problem was identified and rectified. There is a nice section with a clear example on the various possible types of twinning and how to analyze them. This subject is becoming more important especially for precious proteins where twinned crystals may be all one can obtain. There is also a table (11.1) showing a possible cause of incorrect space-group choices giving the cause of the problem (space groups that differ only in the presence or absence of a center of symmetry so that the condition for reflections is the same). There are also some hints on what may be wrong if anisotropic displacement parameters are poor.

The chapter on *Interpretation and presentation of results* covers the meaning of x, y, z and the use of drawing programs and stereo. Deformation density with X–X and X–N maps is also mentioned. *Crystallographic databases* describes how to use these and, importantly, how to put your structures in them or ensure that they are there. The ICSD (Inorganic Crystal Structure Database), CSD (Cambridge Structural Database), CRYST-MET (Metals Crystallographic Data File) and *Structure Reports* are described. The use of crystallographic information files (CIFs) and how to use the Internet to find crystal structures is also described.

The ending of the book is superb for the crystallographic experimentalist. In the outline of a crystal structure determination, the author tells the reader where to find information on each step within the book. There is also a nice list of questions at the end to ensure that the data collection and analysis were done properly. Finally, there is a worked example of a structure determination. This is a nice example of a small-molecule structure. It goes into experimental details as well as structure determination and refinement. Both Patterson and direct methods are used for structure determination.

My criticisms are minor. The main one is that the author has not paid sufficient attention to the captions for figures. This is something most of us are guilty of. It would be helpful to have a more complete description of what the figure shows and all the symbols used should be described in the caption. There is probably not enough written on structure solution but the example at the end may help clarify that. Also some terms in the text are not adequately described – maybe a glossary would help. For example, in Fig. 3.5, what is 2π?

This book is an excellent blend of theoretical and experimental information and will help students and teachers alike. The student can browse through several such texts and find the one that best satisfies his or her needs with respect to explanation and the use of mathematical and physical concepts. I suspect this book, with its outstanding blend of theory and experiment, will be ideal for many such students.

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Light is a messenger – the life and science of William Lawrence Bragg. By G. K. Hunter. Pp. xxi + 301. Oxford: Oxford University Press, 2004. Price Hardback GBP 35.00. ISBN 0-19-852921-X.

Little did I think when I chose W. L. Bragg's *Electricity* as a school prize 60 years ago that I would have the great privilege of being a member of Bragg's research team during his last appointment, as Resident Professor at the Royal Institution (the RI) and Director of the Davy Faraday Research Laboratory in London. By that time, he was recognized internationally as the Father of X-ray crystallography; what my colleagues and I encountered was a quintessentially courteous English gentleman whose relationship with us was more like a father figure than our 'boss'. Because the Resident Professor has an apartment on the RI premises, we saw a great deal of him and his wife and other family members and felt like members of an extended family, notably being invited to his daughter's wedding. Knowing him towards the end of his professional life, it seemed that he could hardly have had a more successful career – starting with the discovery of 'Bragg's law' and the derivation of the structure of sodium chloride, for which he became (and remains) the youngest person to receive a Nobel Prize, uniquely shared with his father; then to unravel the complexities of mineral structures, and of metals and alloys; and finally to have made crucial contributions in the applications of crystallography to molecular biology. What could have been more satisfying?

But, as Graeme Hunter explains in this excellent and warm-hearted biography, Bragg's life had not been anything like as straightforward as it seemed. Born in Adelaide, one of the two sons of William Henry Bragg, he was a precocious boy whose intellectual brightness led him to be lonely at school, taught in classes with older boys with whom he had little in common. He went on to study physics and mathematics in his father's department at the University of Adelaide, indeed working part of the time in his father's office – a rather odd misjudgement by his father.

When the family came to England on his father's appointment to the University of Leeds, Bragg went to Cambridge, took a second degree, and was in line for a college fellowship when he thought of a simple explanation for the geometrical relationship between a crystal and its X-ray diffraction pattern. I remember Bragg saying that nobody had a bright idea all by himself – he must have come closer than most people to doing so, but he acknowledged the value of Schuster's optics lectures in developing the idea of what became Bragg's law. The law was confirmed and the first crystal structures elucidated in collaboration with his father, who had better apparatus in Leeds. Sadly, the joint work and its recognition created lasting problems between father and son; both rather reserved men, they had difficulty in discussing the matter, and the younger inwardly resented the way in which outsiders tended to give too much credit to his father.

Bragg's career was interrupted by the First World War, in which he served with distinction, developing sound-ranging methods for locating enemy guns. Shortly after returning to Cambridge, he was appointed in 1919 to the Chair of Physics at Manchester in succession to Rutherford, at the age of 29. In Hunter's words, 'his new job quickly degenerated into a fiasco'. He had had no experience of lecturing, he had no administrative experience, and he found himself surrounded by older subordinates and confronted by tough students, many of them ex-servicemen. But he gradually learned the ropes and started a research programme, very largely carried through by his own hands, sometimes on his own and