**Polarization ratio for X-rays – A survey by the Commission on Crystallographic Apparatus**

The Commission on Crystallographic Apparatus is conducting a survey of measured values of the polarization ratio for crystal-monochromated X-ray beams. This note summarizes the definition of this ratio, mentions techniques for its measurement, emphasizes that the objective of the survey is to establish the range of values observed in practice, and is an invitation to all interested people to participate.

The polarization factor in a typical X-ray diffraction experiment is

\[ P = \frac{1 + K \cos^2 2\theta}{1 + K}, \]

where \( K \) is the polarization ratio, the ratio of the beam power with \( \pi \) polarization to that with \( \sigma \) polarization. A fractional error in \( P \) will be directly reflected as a fractional error in the results. Thus it is important that \( P \) (or, equivalently, \( K \)) be accurately determined. For example, in an experiment using unmonochromated characteristic radiation, \( K \) is very nearly unity.

In the case of crystal monochromated radiation, the situation is more complicated. Consider for concreteness the case where the planes of diffraction for the monochromator and for the sample are parallel. There is apparently a common, tacit ‘argument’ which goes like this. ‘The highest possible integrated intensities are achieved with a crystal in mosaic form. Since monochromators are chosen to give the highest possible beam power, it is probable that the polarization ratio will be very close to that given by an ideally mosaic monochromator, \( \cos^2 2\theta_m \) in this geometry. In any case, the limits on \( K \) are probably \( \cos^2 2\theta_m \) and the value for an ideally perfect monochromator, \( \cos 2\theta_p \).’

It was realized independently by a number of workers that the above argument is specious (Jennings, 1968; de Wolff, 1968; Olekhnovich, 1969). The correct reasoning is more like this: Although appropriate monochromating materials are those which could give a large integrated intensity, it is usually advantageous to arrange the geometry so that desired rays of both polarizations are almost totally reflected. Under these conditions, which can be considered an extreme case of secondary extinction, initially unpolarized radiation will be monochromated to a high-power beam with polarization ratio approaching unity. On the basis of this
reasoning and measurements on typical setups, one can estimate that $K$ would differ from $\cos^2 2\theta_H$ by about 40% for LiF at Cu $K\alpha$, 12% for graphite at Cu $K\alpha$, 8% for LiF at Mo $K\alpha$ and 3% for graphite at Mo $K\alpha$. Such errors would be intolerable in many modern experiments.

Unfortunately the polarization ratio depends on the physical state of the monochromator, beam divergences, and other geometrical factors. In the case of a diffracted-beam monochromator the size of the receiving slit and focusing conditions at the sample would also come into play, making precision measurements difficult with this configuration. In the case that the sample intercepts only a portion of the beam, it may be necessary to study this limited portion of the beam. In any case, accurate results require that the $K$ value be measured for the actual apparatus used; the above values are only typical. Fortunately it is quite simple to achieve 3% accuracy in the measurement of $K$ ($\pm$1% in $P$). One merely determines the center of gravity of the beam in the axial and equatorial planes (so that the average solid angle intercepted by the detector is well defined) and measures amorphous scattering at 90° in the two planes. Higher accuracies can be achieved, but only with much greater difficulty.

In spite of all these considerations, many workers do not measure the polarization ratio for their apparatus but instead assume the value $\cos^2 2\theta_H$. Some workers also do not consider the above values to be typical. This situation perhaps arises because measured values of $K$ are not conspicuously published; they do, after all, apply only to a single apparatus. But it appears that it would be useful for it to be generally known what the range of expected values might be. With this end in mind, the Commission on Crystallographic Apparatus of the IUCr has authorized a survey of measured values of polarization ratios obtained for crystal monochromated characteristic radiation. The Commission would be interested in collating both values which have been obtained in connection with experiments which have already been carried out and values which are newly measured. Since the primary objective of this survey is to show the range of polarization ratios which may be encountered in practice, a project with instructions to the participants is not visualized. Rather the submission of measured values along with any concomitant information will be welcomed. However, as assistance to interested workers, appendices to this note can be supplied which (1) expand on the rationale for expecting polarization ratios near unity, (2) give more detail about the simple experimental method for determining $K$, and (3) suggest some of the types of information which would be useful to the Commission as measured values of $K$ are collated. Please send your values or requests for information to Dr L. D. Jennings, Army Materials and Mechanics Research Center, Materials Sciences Division, Watertown, Massachusetts 02172, USA.

References


Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.


First impressions of this book are that accumulated knowledge on point defects in crystals is no longer merely qualitative but is very detailed, precise and of enormous amount. This impression will be common for most readers.

The book consists of ten chapters, the first three of which are concerned with theories on defects with tightly and loosely bound electrons and on vibrational properties of defects respectively. They are well summarized and include up-to-date references. This part is a useful and easy-to-read textbook for researchers in this area. Actually, it must be an advantage that the theories of the three topics mentioned above are collected in one volume.

The next three short chapters are titled Defect Chemistry, Experimental Methods and Electrons in Covalent and Ionic Crystals respectively. This part is an intermezzo to the massive descriptions that follow. The maps of valence-electron charge density for Ge, GaAs and ZnSe should be attractive to readers.

In the last four chapters, a survey of defects in elemental crystals (silicon, germanium and diamond), III-V compounds, II-VI compounds and alkali halides is given. The structure deduced mainly from results of EPR and optical experiments is presented for individual defects. In the case of silicon, for example, a description is given for Group V donors, lithium and magnesium, sulphur, Group III acceptors, boron associates, carbon, vacancy, vacancy–germanium associate, vacancy–Group V donor associate, aluminium centres, interstitial oxygen, etc. These chapters are a sort of handbook of defects in these crystals; readers will understand the state of present knowledge as well and realize how strong is the driving force of investigations in this field.

A. Okazaki

Department of Physics

Kyushu University

Fukuoka 812

Japan