PREFACE

With this first issue of a series of articles The Rigaku Corporation ntroduces a new crystallographic publication policy in Europe, which has already been practiced with great success in Japan. Crystallography, particularly its important branch structure research with the aid of diffraction methods, has become increasingly important in material science and its applications to industrial products. Although this method, which has been opened by Max von Laue, and first been applied to structure research by W. H. and W. L. Bragg, is more than seventy years old, its development in the last decade is still exciting.

It is one of the great advantages of diffraction methods that the samples under investigation need not necessarily be destroyed. Furthermore the use of diffraction data for the determination of ordered and disordered crystal structures is of outstanding importance for understanding physical and chemical properties of matter. In this sense structure research contributes to the development of new materials with specific properties wanted.

On the other hand it is well known, that the quantitative interpretation of diffraction measurements may be very difficult, if data other than lattice constants or percentages of crystalline phases are needed. Since applied crystallography is not as well represented as e.g. applied physics a publication of this kind may fill a gap, which does not exist in the big fields of science. For this reason there are many results available in literature which could well be applied to other problems in science or technology, but they aren'tbecause of the barrier which unfortunately exists, although it could easily be overcome.

The rapid development that has taken place in the last two decades has been greatly influenced by three important factors:

1. The increasing possibilities of computer technology have facilitated the determination of the so-called averaged structure (time and space average of atomic positions in one unit cell) of a crystal such, that simple structures with less than about 100 independent atoms in the unit may be solved by the computer, if the crystal has a centre of symmetry. In practice, the latter condition is fulfilled very frequently. Since data collection including determination of lattice constants is fully automized, a procedure which begins with mountimg the crystal after some routine investigations of its quality, and ends with a structure containing all data of interest is nowadays possible. The whole procedure may be routine work done by the computer alone.

2. The fact, that intense neutron sources became available for any scientist, has emphasized the complementary character of neutron diffraction, when compared with other diffraction methods. Magnetic structures and the position of light elements such as hydrogen could now easily be determined. The study of inelastic neutron scattering yielded much information of the dynamic behaviour of crystals, even in the temperature range of phase transformations. Since white radiation only is generated in modern high-flux reactors, new experimental techniques had to be developed, including monochromators, detectors etc., which in its turn influenced the X-ray techniques appreciably.

3. More recently a similar development takes place for the use of synchrotron radiation, which enables experiments with polychromatic X-rays. This source of radiation is again complementary to rotating anodes, which are commercially available,and represent a most intense source for characteristic radiation, such as silver Kα and molybdenum Kα.

It is not astonishing that the rapid development of experimental techniques has challenged theoreticians to find new methods for the evaluation of data, the application of which is not always easy. The increasing number of papers and articles forces authors to cut down their publications, such that they may not easily be understood by readers being not familiar with the subject. It is the aim of this publication to assist the community of scientists wherever they are operating – in scientific or industrial laboratories–, and help them understanding a wide field of exciting new methods including their application.

Prof. Dr. H. Jagodzinski

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Institut fhr Kristallographie und
Mineralogie der Universit@t Mhnchen