

16.X-01 SEMICONDUCTOR-CONDUCTOR TRANSFORMATION IN GaAs AS A PRESSURE-FIXED POINT. By S. Akimoto, Institute for Solid State Physics, University of Tokyo, Minato-ku, Tokyo, Japan.

As an official activity of the Commission on Crystallographic Studies at Controlled Pressures and Temperatures, the extension of the study of transformations at specific pressures to the higher pressure region was undertaken. The target was focused to the semiconductor-conductor transformation in GaAs which occurs in the region 180-193 kbar according to previous investigations. This is a direct extension of the former report on the transformation pressure in ZnS by Block at the Warsaw meeting (1978).

A high-purity, non-doped crystal of GaAs was distributed to more than ten laboratories as a standard sample. In the participating laboratories, the transformation was detected by X-ray diffraction, electrical resistance as well as visual observation, and the transformation pressure was determined based on the compression of NaCl and the shift of the ruby R_1 fluorescence line. Both the diamond-anvil cell and the multi-anvil type high-pressure apparatus were used for the present round-robin study. The most probable value of the semiconductor-conductor transformation pressure in GaAs is reported based on the data presented by the participating laboratories. The correlation of the transformation pressure obtained by the different methods and by the different high-pressure apparatus is also shown.

16.X-02 A COMPARATIVE STUDY OF THE CHARACTERISTICS OF X-RAY FILMS. By S.C. Dawson, O.S. Mills and M. Elder, Department of Chemistry, University of Manchester, Manchester, M13 9PL, and Science Research Council, Daresbury Laboratory, Warrington, WA4 4AD, U.K.

X-ray film characteristics, last surveyed by Morimoto and Uyeda (Acta Cryst. 16, 1107, 1963), have been reinvestigated using 23 available X-ray films. The properties which have been measured include thickness and silver content, speed, granularity at four different optical densities, background fog level, film factor, and linearity and uniformity of response. The X-ray measurements were made using Ni-filtered Cu fluorescent radiation, exposing packs of two films to record rows of spots of regularly stepped intensity. All the films were processed using standard chemicals for comparison purposes, and where the manufacturers issued specific recommendations for chemicals additional films were processed using these materials. Digitised density data were obtained with an Optronics drum scanner and checked with a Joyce-Loebl machine. The effect of ageing has also been assessed. The 23 films exhibited relative speeds ranging from about 1.4 to 0.1 compared with the now unavailable Ilford Industrial G at 1.0.

16.X-03 COMPARISON BETWEEN FILM AND DIFFRACTOMETER DATA. By Oliver Lindqvist and Astrid Magnusson, Department of Inorganic Chemistry, Chalmers University of Technology and the University of Göteborg, S-41296 Göteborg, Sweden

The IUCr Microdensitometer project, Part I: Inter-Experimental Agreement (J. Appl. Cryst. (1980) 13, 318-337) compared the precision of film intensity measurements performed at fifteen different laboratories. The aim of the second part of the project is to obtain an estimate of the accuracy of microdensitometer intensity data. The study comprises two parts:

1) Collection of three-dimensional data on precession films and with a four-circle diffractometer from the smaller of the sodium tartrate dihydrate crystals used in Part I of the project. Comparison of the refined structural parameters and evaluation of the relevance of the standard deviations of these parameters with respect to different estimates of $\sigma(I)$ for film data. The previous diffractometer study (Ambady, G.K. & Kartha, G. Acta Cryst. (1968) B24, 71-83) will also be included.

2) Refinement of the ab projection of the sodium tartrate dihydrate based on each of the fifteen hk0 data sets submitted by the participants in the microdensitometer project. Analysis of the parametric spread with respect to the standard deviations in parameters obtained for different intensity weighting systems, i.e. based on the $\sigma(I)$ values supplied by the participants and on artificial weights.

16.X-04 PROTEIN CRYSTAL OSCILLATION FILM DATA PROCESSING: A COMPARATIVE STUDY. J.R. Helliwell, A. Achari, A.C. Bloomer, P.E. Bourne, P. Carr, G.A. Clegg, R. Cooper, M. Elder, T.J. Greenhough, B. Shaanan, J.M.A. Smith, D.I. Stuart, E.A. Stura, R. Todd, K.S. Wilson, A.J. Wonacott, P.A. Machin.

On behalf of the UK Collaborative Computational Project for Protein Crystallography SRC, Daresbury Laboratory, Warrington WA4 4AD, England.

A project has been instigated to evaluate the relative performance of different microdensitometers and protein crystal oscillation film data processing packages used in the U.K. The single crystal oscillation data set chosen for study was from a horse spleen apoferritin crystal, space group F432 (cubic with $a = 184.0 \text{ \AA}$, with X-ray data collected on a conventional source at Cu K α wavelength (1.5418 Å). The particular advantages of this crystal space group system were that only 15° total rotation angle was needed for a complete data set (neglecting a blind region) with four equivalent reflections which could be collected from a single crystal before serious radiation damage of the sample. Hence, by avoiding problems of crystal to crystal scaling, comparisons concentrate on the film scanning and processing methods and with a relatively small computing effort finally arrive at a merged data set with an R sym in each case. Three different types of scanners, the Joyce-Loebl Scandig-3 (used at 50 μm and 100 μm raster) the Optronics Photoscan (100 μm raster) and a flying spot densitometer are being compared. In total, four Scandigs and three Optronics instruments are being separately used at the various institutions involved in this project. The separate data processing software packages involved utilize both off-line and on-line methods.