for each specimen. These values of the integrated scattering intensities were taken as equal to one. Wide-angle X-ray patterns taken after aging of 15 h clearly showed the existence of the metastable state ε′ (h.c.p.). Wide-angle X-ray study of liquisol-quenched Al–Ag–Zn alloys is still in progress.

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References


X-ray diffraction from one-dimensional superlattices in GaAs1−xPx crystals: erratum. By Armin Segmüller and A. E. Blakeslee, IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598, U.S.A.

(Received 16 May 1973)

The second harmonic strain amplitude A2 in Tables 1 and 3(a) of Segmüller & Blakeslee [J. Appl. Cryst. (1973) 6, 19-25] should be doubled.

Owing to a program error the computed value of the second harmonic strain amplitude A2, given in our paper (Segmüller & Blakeslee, 1973), is too small by a factor of 2. All values of A2 in Tables 1 and 3(a) should be doubled. The symmetry ratio χ in Table 3(a) should read 2-7 and 1.4 rather than 2 and 1.2 for Crystals 1 and 2 respectively, resulting in a better agreement between the two models. In Table 4 the lattice spacings for the extreme composition d1 and d2 should read 5.62 and 5.55 for Crystal 1 rather than 5.61 and 5.54 respectively.

Reference


Crystal Data


Crystal data for thallium gallium diselenide, TlGaSe2. By T. J. Isaacs, Westinghouse Research Laboratories, Pittsburgh, Pennsylvania 15235, U. S. A.

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Crystals of TlGaSe2 were grown by solidification from melts. The space group a = 7.60, c = 31.36 Å, β = 90° 20′, is P21/m.

Origin of specimen

The compound TlGaSe2 was made from high-purity elements (at least 99.999 %) obtained from American Smelting and Refining Company. These were weighted out in stoichiometric proportions, and were sealed in an evacuated silica-glass tube which was then heated slowly past the melting point of the compound. The melt was held at ap-
proximately 900°C for several hours, was shaken vigorously a number of times to ensure thorough mixing, and then was cooled slowly to room temperature.

**Crystal morphology**

There is one prominent cleavage which causes the crystals to be platy. There are also two lesser cleavages perpendicular to the main cleavage and to each other.

**Crystal geometry and crystal physics**

Small crystals were examined using the precession method with Mo Kα radiation. Zero, first and second-level photographs were taken with the beam normal to each of the three crystallographic axes. The density was determined by pycnometer.

The compound is monoclinic (class 2/m), but shows pseudo-tetragonal symmetry. Zero-level photographs taken perpendicular to the prominent face show pseudo-fourfold symmetry, and it is only in upper-level pictures that the non-tetragonal nature is seen. The c axis is perpendicular to the major cleavage and it is the twofold axis. Indexing of these films showed that there were systematic absences when 00l was odd which would make the space group either P2₁ or P2₁/m. The piezoelectric test was negative, a result which is not diagnostic by itself, but Raman and infrared studies were made which show the material to be centric, as there were no vibrational modes which were simultaneously Raman and infrared active.

**Discussion**

This compound was first reported as a semiconductor (Offergeld, 1963). A later study by Hahn & Wellman (1967) implied possible tetragonal symmetry with lattice parameters of a = 7.8, c = 30.5 Å, and Z = 16. In the work reported here, it has been found to be pseudo-tetragonal, but actually monoclinic with a small deviation of the interaxial angle β from 90°, and with a superstructure producing a cell doubled along the c axis.

Examination of the cell parameters shows that c is four times a (or eight for the doubled cell). The overall structure could be viewed as a stacking of cubes along the c axis, arranged such that there is a small deviation of the axial angle β from 90°.

**References**

Hahn, H. & Wellman, B. (1967). Naturwissenschaften, 52, 42.


**Crystal data for CuInSe₂**

By J. Parkes, R. D. Tomlinson and M. J. Hampshire, Department of Electrical Engineering, University of Salford, Salford 5, England

(Received 2 March 1973; accepted 1 May 1973)

X-ray data is presented and analysed for the semiconducting compound CuInSe₂, prepared by zone levelling. Values of a = 5.782 and c = 11.620 Å have been determined and intensity calculations have been used in the evaluation of interatomic separation and bond angles. Some aspects of stoichiometry, related to electrical characteristics, are discussed and it seems probable that the structure of the compound is modified by a small concentration of Se vacancies.

**Origin of specimens**

CuInSe₂ was initially produced by the fusion of a stoichiometric mixture (by weight) of the elements. The purest commercially available elements were used in this process (99.9998% pure Cu bars and Se pellets and 99.9999% pure In pellets), every effort was made to avoid impurity contamination. The mixture was contained in a clean quartz capsule and vacuum sealed in a measured pressure of 10⁻⁹ torr. The compound was formed at 1050°C and zone levelling was employed to produce a homogeneous rod (as evidenced by four-point-probe resistivity measurements made along the length of the sample). Material used in the X-ray analysis was crushed, passed through a 300 mesh screen, and heat treated (one hour at 790°C) in an evacuated quartz capsule. The heat-treatment temperature was chosen in order to avoid a phase transformation which occurs at 810°C, [first reported by Palatnik & Rogacheva (1967) and later confirmed by differential thermal analysis in our own laboratories].

**Crystal geometry**

The structure of the compound was first reported briefly by Hahn, Klinger, Meyer & Storger (1953) to belong to the chalcopyrite family (I42d), with a = 5.77 Å and c/a = 2.00.

Atomic positions in this tetragonal structure are as follows (International Tables for X-ray Crystallography, 1952):

| 4 Cu: | 0 0 0, 1/2 0 1/2, 0 1/2, 1/2 0 1/2 |
| 4 In: | 0 1/2, 1/2 0, 1/2 1/2 |
| 8 Se: | 1/4 1/4 1/4, 1/4 1/4 1/4, 1/4 1/4 1/4, 1/4 1/4 1/4 |

In this investigation Debye–Scherer X-ray photographs were obtained with a 114-83 mm diameter camera employing Straumanis film mounting. A diffractometer was also used in order to obtain the intensity values which were required for a determination of the u parameter. Filtered copper radiation was used with a working tube voltage of 15-20 kV and values of θ₁K₂₁ = 1.54051, θ₂K₂₂ = 1.54433 Å or