LATTICE PARAMETERS OF $CuInSe_2$ IN THE 10-295 K TEMPERATURE RANGE

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Copper indium diselenide, $CuInSe_2$, is a subject of investigation in many laboratories because of opportunity of its application as an efficient absorber in polycrystalline-thin-film solar cells. The absorbing-layer thickness is much lower (several micrometers) than that of polysilicon based solar cells (several hundred micrometers). This compound crystallizes in a tetrahedral chalcopyrite-type structure (space group $I\text{-}42d$), related to the zincblende structure type. It exhibits a considerable range of off-stoichiometry **[1]**, attributed to remarkably low formation enthalpy of defect pairs **[2]**. Its axial ratio, c/a, is very close to the ideal value, 2.

In the present study, unit-cell dimensions for $CuInSe_2$ in the temperature range 10-295 K were determined. The crystals studied in this paper were grown at Warsaw University of Technology using the vertical Bridgman method without seed from stoichiometric amount of 5.5N or 6N purity components. The ingots were cooled from 1080°C down to 750°C at 1°C/h and then down to 500°C at 5°C/h (for more details, see Ref. [3]). Composition of the crystals was determined with the use of a JEOL electron microprobe. Phase analysis did not reveal any foreign phases in the crystal.

The low-temperature XRD measurements were carried out at a powder diffractometer [4] at the B2 beamline using the Debye-Scherrer geometry. The powder was mounted within a thin-wall capillary in a He-closed-cycle cryostat allowing capillary rotation. The experiment consisted in data collection using temperature steps starting from the lowest available temperature, 10 K. A scintillation counter was applied for the data collection. The wavelength was determined to be λ=1.13363 Å by least-squares refinement of five reflections of silicon (NIST 640b diffraction standard, a=5.43094 Å).

Early work on thermal expansion of $CuInSe_2$ is limited to temperatures above 30 and 60 K for a and c lattice parameters, respectively [5], and - for both parameters - to 80 K [6] and 90 K [7]. The present results of investigation of the unit-cell dimensions for $CuInSe_2$ in the temperature range 10-295 K are presented in Fig. 1. The obtained dependencies on temperature show, in agreement with those reported by Deus *et al.* [5], that there is a vanishing tendency of the thermal expansion at the lowest temperatures. However, the thermal expansion coefficients are found to be lower in the a direction and higher in the c direction than those reported in Ref. [5]. This is manifested by different slopes of the $a(T)$ and $c(T)$ runs. Minima at about 70 K in $a(T)$ and $c(T)$ are encountered.

The discrepancies between the present results and those of Ref. [5] can be due to both, difference in samples studied and differences in experiment details. In the cited paper, single crystals were investigated, while in the present study a powdered crystal was used. In Ref. [5] the dependencies for (001) and (011) oriented single crystals have been measured, the result for $c(T)$ was derived from these two curves. In powder diffraction studies (unlike in single crystal studies), a single measurement gives both lattice parameters simultaneously. Slight difference in the value of tetragonal distortion factor (1.00485 in the present work and 1.0051 in the cited paper) might indicate that the deviation from stoichiometry of these samples is different. Some influence of defects introduced by powdering on thermal expansion behaviour is not excluded.

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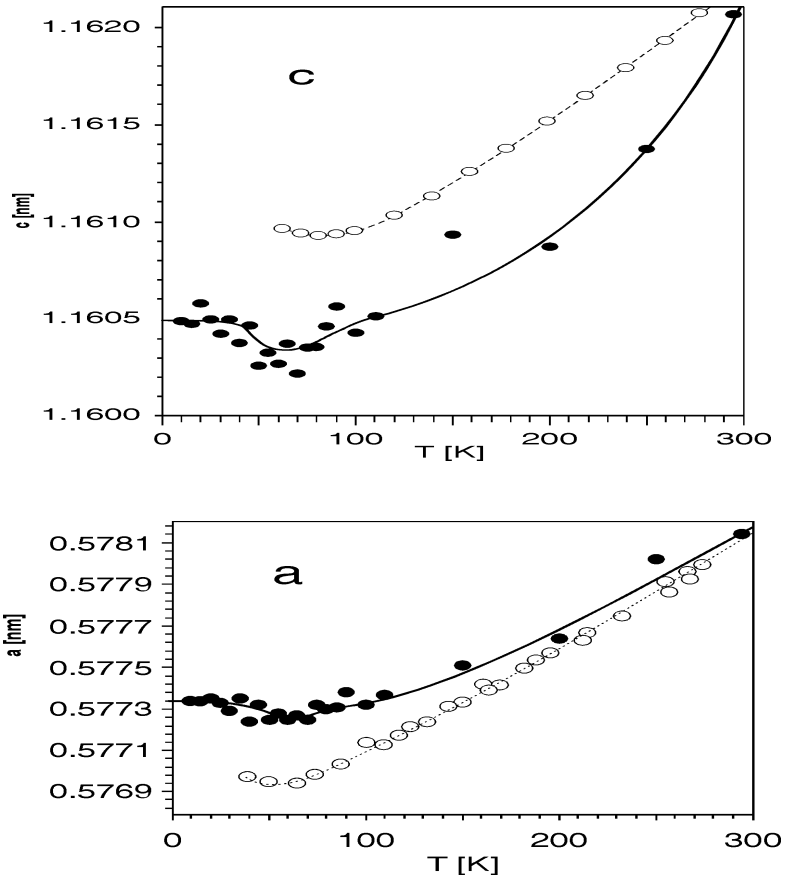

Figure 1: Lattice parameter dependence on temperature for $CuInSe_2$. Present data (full circles) are compared to the data from Ref. [5] (open circles).

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