Preparation and characterization of Pb_{1-x}Sn_xTe pseudo-binary alloy semiconductors

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Abstract. A p-type pseudo-binary alloy semiconductor, Pb_{0.5}Sn_{0.5}Te, has been prepared from p-type specimens of PbTe and SnTe and lattice constants determined with an accuracy of 0.0001 nm. Vacuum annealing of Pb_{0.5}Sn_{0.5}Te reveals two new x-ray powder diffraction lines bearing indices (444) and (800), while others become more sharp. CuKα-doublets get clearly resolved and the lattice constant is increased by ~0.0002 nm. Slight deviation from Vegard's law linearity is observed showing that the sample must be considered as ternary in nature. Thin films deposited on mica and glass substrates kept at room temperature are found to have a little higher SnTe content. The effective carrier concentration calculated from Hall measurements at room temperature is ~3.4 × 10^{21} m^{-3}.

Keywords. Narrow-gap semiconductors; pseudo-binary alloys; x-ray analysis.

1. Introduction

The alloy semiconductor Pb_{1-x}Sn_xTe is being extensively studied nowadays, as it has small and controllable band-gap ($\textit{E}_g$), depending on Sn-content ($x$), temperatures (Dimmock et al 1966) and hydrostatic pressure (Melngailis et al 1970) etc. Thus the emission wavelength of the sources (light-emitting diodes) based on this material is within the IR-region of the spectrum (6-32 μm). This makes the material potentially useful as IR-detectors and lasers (Butler et al 1966), specially in the cryogenic range.

The variation of the band gap of Pb_{1-x}Sn_xTe with $x$ has been explained with a band-inversion mechanism (Dimmock et al 1966) which has also been verified by several experiments viz. measurements of electrical conductivity as a function of temperature for several alloys near the crossing. (Bis and Dixon 1968).

The alloy Pb_{1-x}Sn_xTe with $x > 0.5$ has not been so widely studied and so in this work we choose $x = 0.7$ because it is very close to, and on the SnTe-side of, the band-crossing point at room temperature.

2. Preparation

Both PbTe and SnTe have the same rock-salt structure and they exhibit complete solid solubility over the entire composition range. Hence a pseudo-binary assumption is justifiable for Pb_{1-x}Sn_xTe for $x = 0$ to 1.
Here a polycrystalline ingot of $p$-$Pb_{0.3}Sn_{0.7}Te$ is prepared from $p$-$PbTe$ and $p$-$SnTe$. For $p$-$PbTe$, the bulk specimen is obtained from Bhabha Atomic Research Centre, Trombay and $p$-type $SnTe$ bulk is prepared from 99.99% pure semiconductor grade tin and tellurium.

Crushed samples of $p$-$PbTe$ and $p$-$SnTe$ are taken in proportions appropriate to their molecular weights for $x=0.7$. The relation is $[w_1/w_2 = 1.3593 (1-x/x)]$ where $w_1$ and $w_2$ are the masses of $PbTe$ and $SnTe$ respectively and $x$ is the mol fraction of $SnTe$. Weights are taken in an electronic microbalance and then the samples are placed in a quartz tube, which is subsequently evacuated to $\sim 8 \times 10^{-6}$ Pa and sealed. The sealed ampoule is then heated to $\sim 975^\circ C$ in a furnace for 6 hr, thorough mixing of the components is ensured and finally it is quenched in cold water.

3. Experiments

The ingot thus prepared is powdered in an agate mortar, sieved through a 270 ASTM mesh and then a small amount of it is taken in a glass (corning) capillary of internal diameter $\sim 0.25 \times 10^{-3}$ m. The (capillary and the sample) assembly is then kept mounted in a Debye-Scherrer camera (i.d. = 0.1145 m) for 40 hr and an x-ray powder photograph of the combination is obtained from which different lines for the sample are clearly identified. The same combination is then annealed at 500°C for 6 hr at a vacuum of $\sim 1.3 \times 10^{-2}$ Pa (Hewes et al. 1973), after which another powder photograph of the combination is taken with the same exposure time.

By the same procedure, x-ray powder photographs are also taken for $PbTe$ and $SnTe$. In all cases, CuK$\alpha$-radiation (from a NORELCO unit using Ni-foil as $\beta$-filter) is used.

Then, with glass and mica as substrates (kept at room temperature), thin films of $Pb_{0.3}Sn_{0.7}Te$ are deposited by thermal evaporation, using a heating current of 70 amps and a vacuum of $6.6 \times 10^{-8}$ Pa, the rate of deposition being $\sim 20-30$ nm/min. The substrates are kept at room temperature and so the films are expected to be polycrystalline. Diffractometer analysis with these films shows that only few peaks appear and they do so at a slightly higher angle ($\theta$) than the corresponding powder diffraction lines. This reveals (using Vegard's law) that the films have a slightly increased $SnTe$-content as compared to the bulk sample.

4. Measurements

For annealed $Pb_{0.3}Sn_{0.7}Te$, interplanar spacings ($d$) of different crystallographic planes and lattice parameter ($a$) of the crystal are calculated from measurements on its powder photograph. Using the Taylor-Sinclair function $\frac{1}{2} \cos^2 \theta (1/\sin \theta + 1/\theta)$ (obtained from tables), the most accurate value of $a$ is determined by the extrapolation method (figure 1) with an accuracy of $\sim 0.0001$ nm. Similar measurements are performed with the powder photographs for only unannealed $Pb_{0.3}Sn_{0.7}Te$, $PbTe$ and $SnTe$. In all cases, lines with $\theta \geq 29^\circ$ only are considered for graphical extrapolation.