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Crystal Growth Modeling and Characteristics of Antimony Selenide

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ABSTRACT

Crystal growth is the process in which solids in disordered and irregular state culminate around an embryo forming a solid phase nucleus with regular and periodic structure. This phenomenon can be considered as a first order phase transition. Nucleation occurs due to the presence of a surface wall of an ampoule, foreign particles or an impurity component in a three dimensional manner. In order to grow the antimony selenide (Sb_2Se_3) bulk crystals, the Bridgman-Stockbarger method was employed. Generally, in melt growth methods, two possible types of interfaces occur, namely sharp and diffuse interface. The sharp interface is atomically flat whereas the diffuse interface is atomically rough. The perfection of the grown crystal depends on the type of interface during the liquid-solid transition phase. The critical energy of nucleation and subsequent growth was favored by the free energy of the interface (surface of the nucleus) and the driving force. In the present study, the liquid-solid interface was carefully optimized to obtain atomically smooth interface in order to increase the perfection of the grown crystals. The stoichiometric Sb2Se3 charge was kept in a specially designed quartz ampoule with tapered tip and was placed in the melt growth furnace under 720 °C and the ampoule was translated down at the rate of 4mm/h. The morphological investigations using optical microscopy of the obtained crystal disclosed the absence of imperfections on the surface. The chemical homogeneity of the melt grown Sb2Se3 crystal was assessed by Energy dispersive analysis by X-ray (EDAX) which revealed that the crystals were physically distinct with the right stoichiometric proportions corresponding to orthorhombic phase.

Key Words: Antimony selenide, Nucleation, Liquid-solid transition, Imperfections and stoichiometry

INTRODUCTION

Crystal growth essentially is the transition of a material from a disordered state to an ordered state. Artificially prepared bulk crystals as compared to other habits, proves as a superior ground to understand the nature of material and its novel physical properties that depend on long range geometrical atomic arrangement and symmetry. This is essential in order to meet the ever-growing industrial demand of single crystals as they have high purity and stoichiometry and are best suited for large scale device applications. The surge in semiconductor research and technology gave rise to the necessity of synthesizing and investigating compound semiconducting crystals with enhance device level characteristics[1]. Thorough literature survey revealed the merits of group VI chalcogenides as efficient compounds for applied research particularly, antimony selenide as it has favorable structural, optical and electrical properties and its morphology and growth mechanisms so far have not been studied in detail[2,3]. Therefore, present work focuses on investigating good quality cleaved surfaces of antimony selenide based on the characterizations.

MATERIALS AND METHODS

Antimony selenide (Sb_2Se_3) exhibits orthorhombic crystal structure[4]. In order to efficiently study the characteristics, high levels of purity and stoichiometry are imperative. Therefore a lot of care was taken to avoid contamination by foreign elements. High pure (99.999%) antimony and selenium were weighed in stoichiometric proportions and were loaded into the specially designed and thoroughly cleaned quartz ampoules with a tapered tip in order to facilitate the growth from a single nucleus. These ampoules were sealed under high vacuum pressure of 10^{-6} mbar in order to ensure the absence of contaminants. The Bridgman-Stockbarger method was used for the crystal growth[5]. The materials in the aforementioned tapered ampoules were made to melt using a suitable furnace by raising the temperature above the

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melting point (720 °C). The temperature was steadily increased beyond melting point (770 °C) using the temperature controllers. The ampoule was slowly lowered at the rate in the order of 4mm/hr with respect to temperature gradient so that the melt could be frozen from tip and made to increase in size until it fully occupies the cross-section of the container. A specially designed translation mechanism was employed for slow lowering of the ampoule so as to obtain flat interface between the liquid and solid phases. The ampoules were later cooled slowly back to room temperature and were retrieved for characterization.

RESULTS AND DISCUSSION

The conventional melt growth methods give rise to undesirable structural deformations due to thermal stress at high temperature whereas in the present work, external factors like temperature, translation rate and rate of cooling were optimized to eliminate these types of imperfections. Figure 1a shows the optical image of a cleaved Sb_2Se_3 crystal captured by employing Metallurgical Inverted Microscope. When the translation rate was 4 mm/h, crystalline surfaces were found to possess layer structure. Figure 1b is an optical microscopic image of antimony selenide compound, showing the formation of a smooth surface, indicating the internal ordering of atomic layers. Systematic approach on the crystal growth made it possible to achieve this trait.

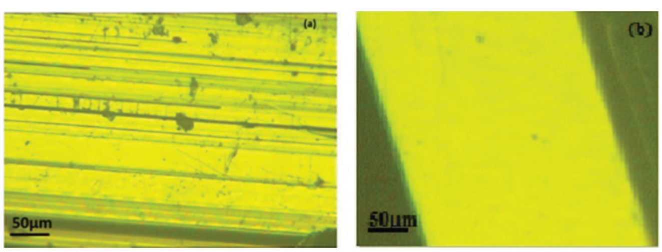

Figure 1: Optical images of Sb_2Se_3 crystal (a) stacked layers and (b) smooth surface.

The chemical composition of the as-grown crystals is critical for device application. Hence the samples were subjected to EDAX analysis and the result revealed that the compound exhibited an agreeable stoichiometry (40.43:59.57) relative to the ideal atomic ratio of 40:60. Figure 3 depicts the EDAX profile of the bulk sample.

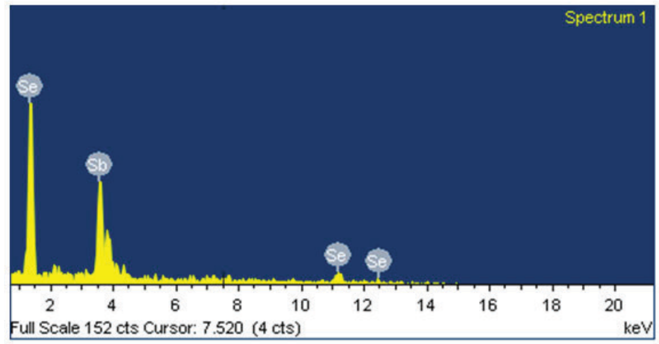

Figure 2: EDAX pattern of Sb_2Se_3 melt grown sample.

CONCLUSIONS

Antimony selenide crystals were grown by Bridgman-Stockbarger method using indigenously fabricated furnace and translation mechanism. The as-grown crystals were examined by microscopy techniques to realize the growth mechanism and defects, which would influence the performance of a crystal for device application. The optical images have revealed the layered structure of crystal and the absence of imperfections. The EDAX profiles confirmed that the compounds have high degree of stoichiometry.

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