

Furnace design for the mercuric iodide crystal growth for new semiconductor radiation detector

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1. Introduction

Mercuric iodide has been attracted an interest for 40 years due to its efficiency as room temperature detector for X and γ -rays. It is worthy to note that commercial γ -ray detectors such as Ge semiconductor detectors should cool down to liquid nitrogen temperature. Compared to other semiconductor detectors such as CdZnTe and CdTe, mercuric iodide has higher efficiency, lower leakage current and less degradation. In addition, mercuric iodide has useful properties such as large band gap of 2.15 eV, low electron-hole pair creation energy of 4.2 eV, and high atomic number (Hg : 80 and I : 53) [1-2]. However, it is difficult to obtain high quality single crystals and the long term reliability problem in devices so that the applications of α -HgI₂ are limited.

Mercuric iodide undergoes a structural phase transition from an orthorhombic yellow phase (β -HgI₂) to a tetragonal red phase (α -HgI₂) at 127 °C. In addition, the melting temperature of HgI₂ is 259 °C. Thus, when it grows through a melting method over 259 °C, the β -HgI₂ phase can be included in the final crystals in the room temperature. In general, in order to grow α -HgI₂ single crystals, the operating temperature is below 127 °C. Note that the crystals from the solution method have contamination problems and the crystals from the physical vapor method usually display a higher quality with a well defined structure. A good thing for the physical vapor method is that α -HgI₂ has high vapor pressure (~0.1 Torr at 120 °C) [3] indicating that α -HgI₂ can be grown in closed ampoules.

2. Methods and results

2.1 Crystallographic structure

The crystal structure of α -HgI₂ is very unique, which has not been found other compounds. The structure is tetragonal whose space group is P4₂nmc. The lattice constants for a and c are 0.4361 nm and 1.245 nm, respectively. As shown in Fig. 1, a mercury ion is surrounded by 4 iodine ions which compose of a tetrahedron. Along c axis, the tetrahedra are weakly bonded by the van der Waals force. The Hg-I distance is 0.2783 nm within the tetrahedra, while Hg-I bond length in vapor phase is approximately 0.26 nm which is smaller than the sum of tetrahedral covalent radii of mercury and iodine. Mass spectrometric investigations for the equilibrium vapor pressure reveal two transitions

at 127 °C and 70 °C. The former one is a structural transition from an orthorhombic phase to a tetragonal phase and the latter is a phase transition at the surface of crystals.

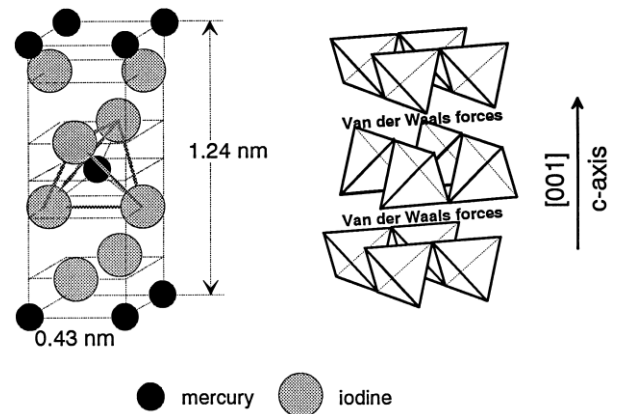


Fig. 1. Crystal structure of α -HgI₂ (tetragonal).

2.2 Phase diagram

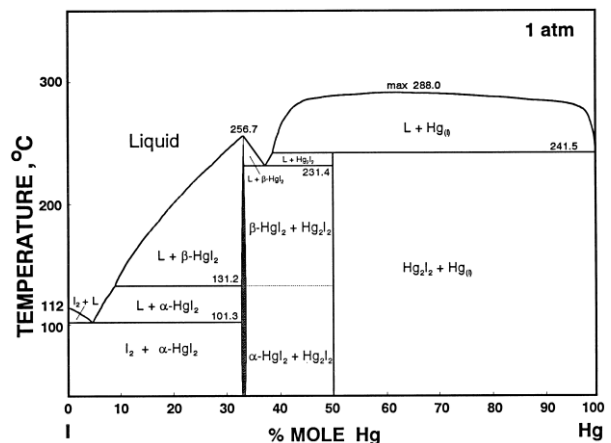


Fig. 2. Phase diagram of I-Hg system [4]

According to the phase diagram of I-Hg system [4], HgI₂ melts congruently at 256.7 °C while Hg₂I₂ melts incongruently at 241.5 °C. Below 33 % Hg mole, eutectics (I₂ and α -HgI₂) are formed at low temperature while eutectics (α -HgI₂ and β -HgI₂) are formed between 33% and 50 % Hg mole. Incongruent melting for Hg₂I₂ leads to the disproportion between iodine rich HgI₂ melt at 37.7 mole % Hg and mercury rich melt at > 99.0 mole % Hg. These two melts form a miscibility gap up to 288 °C, which shows quite flat immiscibility. Total

miscibility of I and Hg is observed above 288 °C. Note that mercury and iodine are more volatile elements than their compound HgI_2 .

2.3 Furnace

In order to grow $\alpha\text{-HgI}_2$ single crystals, the operating temperature for the solution growth or vapor growth methods should be below 127 °C where the structural phase transition occurs from an orthorhombic phase to a tetragonal phase. However, the crystal growth from the solution method is known for having contamination problems. In contrast, a physical vapor technique gives rise to a higher purity with a well defined structure. Figure 3 shows a simple furnace structure for the physical vapor technique. This oil bath furnace gives a stable temperature profiles to operate at temperature around 120 °C [2]. Furthermore, an additional heating coil generates non-uniform temperature profiles, which has two advantages. One is to generate the large temperature gradient at crystal growth side dT/dx , which can effectively reduce the sidewall nucleation. The other is to yield a larger value of crystal temperature which can enhance the mobility of the adhered molecules.



Fig. 3. Schematic figure of the oil-bath furnace. (1) controller; (2) heating plate; (3) heating coil; (4) thermal couples; (5) rotating and pulling motors.

2.4 temperature profiles

The furnace produces a larger temperature gradient near the crystal growth region. The obtained temperature profiles are shown in Fig. 4 where T_{sou} , T_{cry} , and T_{max} are the temperature at source, crystal, and heating coil, respectively.

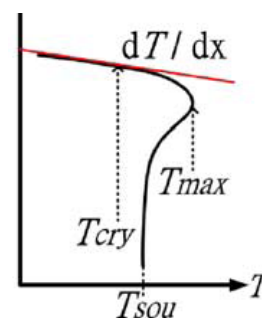


Fig. 4. The temperature profile of the oil bath furnace.

3. Conclusions

We design a furnace for $\alpha\text{-HgI}_2$ crystal growth by the physical vapor method. The obtained temperature profile shows the large temperature gradient near the heating coil. By using grown crystals, the further analysis should be performed for these crystals. In addition, the performance for the room temperature radiation detector should be checked.

Acknowledgements

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