Electrical Properties and Compositional Distributions of CVT and PVT Grown Hg$_{1-x}$Cd$_x$Te Epilayers

YI-GAO SHA,* M.P. VOLZ, and S.L. LEHOCZKY

Space Science Laboratory, NASA Marshall Space Flight Center, Huntsville, AL 35812

Epitaxial layers of Hg$_{1-x}$Cd$_x$Te were grown on CdTe substrates by the chemical vapor transport technique using HgI$_2$ as a transport agent. The epilayers were of nearly uniform composition both laterally and to a depth of about one-half of the layer thickness. By comparison, the composition varied continuously throughout the depth of the layer for epilayers grown by the physical vapor transport technique. Layers were grown both p- and n-type with carrier concentrations on the order of 10$^{17}$ cm$^{-3}$. Low-temperature annealing was used to convert the p-type layers into n-type. The room-temperature carrier mobilities of as-grown and converted n-type layers ranged from 10$^3$ to 10$^4$ cm$^2$/V-s depending on the composition and are comparable to previous literature values for undoped Hg$_{1-x}$Cd$_x$Te crystals.

Key words: Chemical vapor transport (CVT) technique, HgCdTe, physical vapor transport (PVT) technique

INTRODUCTION

The mercury-cadmium telluride (Hg$_{1-x}$Cd$_x$Te) alloy system has been used for many years as a primary device material for infrared applications because of its high electron mobility, long lifetime of carriers, and electronic band gap that can be varied to cover the spectrum from near- to far-infrared. Epitaxial layers of Hg$_{1-x}$Cd$_x$Te have been successfully grown recently on CdTe substrates by chemical vapor transport (CVT) and by physical vapor transport (PVT) in a closed system using a single source material. These epilayers had reasonably good morphological and compositional uniformity and relatively low etch-pit-density (EPD) values.$^{1,2}$ In CVT, mercuric iodide (HgI$_2$) was used as a transport agent to enhance the transport of Cd whose partial pressure is otherwise so low that the Cd atoms are practically absent from the vapor. It has been shown that HgI$_2$ can be effectively used to grow Hg$_{1-x}$Cd$_x$Te epilayers with desired alloy compositions.$^1$ It has also been shown that the composition of the source material may be selected different from that of the epilayer to enhance the overall growth rate in this method.$^2$ In PVT, relatively high interdiffusion rates in the Hg$_{1-x}$Cd$_x$Te/CdTe system were utilized to allow Cd to diffuse from the substrate into the epilayer grown on it. Therefore, the alloy composition of the epilayer was mainly effected by the growth temperature. The main concern so far about the CVT technique is the unavoidable iodine doping of the epilayer during growth, which may deteriorate the electronic properties of the epilayer. Earlier work indicated that iodine in HgCdTe is a slowly diffusing donor in occupying Te lattice sites.$^{3,4}$ Reported carrier mobilities of iodine doped bulk Hg$_{0.9}$Cd$_{0.1}$Te crystals were of the same order of magnitude as those of indium doped ones, about 1 x 10$^4$ cm$^2$/V-s at 77K.$^{4,5}$ However, the electronic properties of CVT grown HgCdTe epilayers have not been investigated in connection with the iodine doping.
In this work, a series of HgCdTe epilayers have been grown using both CVT and PVT methods and their electronic properties are measured and compared. The composition profiles perpendicular to the epilayer surface, determined by electron microprobe analysis, and the lateral compositional uniformity, examined by infrared transmission measurements, are also presented.

**EXPERIMENTAL PROCEDURES**

**Materials Synthesis**

Stoichiometric amounts of elemental Hg (99.9998% with respect to metals and 99.9997% overall), Cd, and Te (both 99.999% with respect to metals), corresponding to about 30 g of Hg0.5Cd0.5Te (x = 0.2, 0.4, or 0.6) were loaded into a pretreated fused silica ampoule of 15 mm ID and about 12 cm long. The loaded ampoule was sealed at a pressure of 2 x 10^{-6} Torr while the sample-end was cooled with liquid nitrogen. The synthesis reaction was carried out at increasing temperature up to about 650°C over a period of 15 h. The sample was then annealed at this temperature for 15 h, and subsequently at about 20°C below the solidus temperature for 48 h, at 600°C for 12 h, and finally at about 500°C for 10 h. The synthesized product was further homogenized by grinding and mixing. No elemental Hg was visible during this step. The possible loss of elemental Hg to the vapor phase (at 500°C) was less than 3 mg and can be practically ignored in view of the amount of the sample.

Commercially available HgI₂ (99.99%+) was used as the chemical transport agent. It was further purified in-house by repeated sublimation under dynamic vacuum prior to use.

Commercially available CdTe single crystal wafers (ρ ~ 100 Ω-cm) of (100) or (111) orientation were used as substrates for the epitaxial growth. These substrates were about 1.5 mm thick and about 10 x 5 mm in size. The growth side was mechanically polished finishing with 0.1 μm alumina powder.

**Growth Ampoule Design and Preparation**

A detailed description of the design and preparation of the double-ampoule-sample assembly used for the epitaxial growth experiments is given in Ref. 1.

**Growth Conditions**

The epitaxial growth experiments were performed in a vertical, stabilizing orientation (hot end on top, density gradient parallel to the gravity vector). The growth furnace and the temperature profile used along the ampoule were similar to those used in the previous work. The ampoule was placed in a position such that the source material was at a temperature of about 590°C and the substrate at about 540°C. The amount of HgI₂ used as a transport agent corresponds to a HgI₂(g) partial pressure of 0–0.1 atm at the temperature used during growth. These partial pressure values were calculated by knowing the amount of HgI₂ added to the sample, the volume of the ampoule, and by assuming the ideality of the HgI₂ vapor. During growth, the ampoule remained stationary. The growth time used in this work ranged from 4 to 18 h. The distance between the surface of the source material and the substrate was about 9.5 cm.

**Characterizations**

Optical microscopy using Nomarski differential interference contrast illumination was used to examine the surface morphology of the epilayers. The epilayer-substrate interface and the layer thickness were examined by SEM microscopy. The alloy composition profiles normal to the surface of the epilayer were measured by using energy dispersive x-ray (EDX) spectroscopy at a spacial resolution of about 3 μm. Pseudobinary solid solution samples were used as standards. Hall effect measurements were made using the van der Pauw technique at temperatures between 14 and 300K and with a field strength of 6 kG. Contacts were made on freshly etched samples with indium solder. The ohmic character of the contacts was verified by examining the I-V curves. The carrier concentrations and mobilities were derived from the measured Hall coefficients and resistivities of the sample. Infrared (IR) transmission-edge measurements were used to determine the lateral compositional variations of the epilayers. The diameter of the IR-beam was 800 μm. The composition x was obtained by measuring the 1% absolute transmission cut-on wavelength and using the expression for energy gap given by Hansen et al.

**RESULTS AND DISCUSSION**

The Hg₁₋ₓCdₓTe epitaxial layers grown in this work generally had smooth surface morphology and well defined layer-substrate interfaces as observed in the previous investigations. The growth rates observed for different compositions of source materials and for different pressures of transport agent and the temperature dependence of the surface morphology were consistent with those already reported. They are