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CADMIUM TELLURIDE THIN FILMS ON SILICON SUBSTRATES

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This report discusses the epitaxial growth of CdTe films on silicon substrates by the use of a closed hot wall epitaxy (CHWE) system. Deposition parameters were varied in order to determine the growth condition for obtaining good quality CdTe films. The characteristics of the films were investigated by scanning electron microscopy, x-ray diffraction and Auger electron spectroscopy. Experimental data show that no film grows when the source temperature is below 450°C. The film growth changes linearly with source temperature at a rate of 0.025Å/°C, and the best film was grown at a source temperature of 475°C. It was found that the lattice constant of the CdTe films was 6.487 ± 0.004A.

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CADMIUM TELLURIDE THIN FILMS ON SILICON SUBSTRATES

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We report here the epitaxial growth of CdTe films on silicon substrates by the use of a closed hot wall epitaxy (CHWE) system. Deposition parameters were varied in order to determine the growth condition for obtaining good quality CdTe films. The characteristics of the films were investigated by scanning electron microscopy, X-ray diffraction and Auger electron spectroscopy. Experimental data show that no film grows when the source temperature is below 450 °C. The film growth changes linearly with source temperature at a rate of 0.0252 Å s^{-1} $°C^{-1}$, and the best film was grown at a source temperature of 475 °C. We found that the lattice constant of our CdTe films is 6.487 ± 0.004 Å.

1. INTRODUCTION

The growth of high quality CdTe films is important because of their potential applications in solar energy, X-ray detection, γ ray detection and image intensifiers. In addition, its close lattice match and chemical compatibility with $Hg_xCd_{1-x}Te$ ($0 \leqslant x \leqslant 1$) make CdTe an ideal substrate for growth of a variable band gap IR detector material[1,2]. Another important application is high speed heterojunction transistors using the two-dimensional electron gas observed in InSb at the InSb–CdTe interface[3,4]. The current lack of availability of high quality, large area bulk CdTe substrates is generally considered as a major problem for different applications. This problem can be overcome by growing CdTe on an alternative substrate which could then serve as a buffer layer for the subsequent synthesis. Growth of CdTe films on different substrates such as CdTe, InAs, Ge, sapphire and silicon by using metal–organic chemical vapor deposition or molecular beam epitaxy has been reported[5–10].

In this paper, we report initial results for the growth of CdTe buffer films on Si(100) substrates using a closed hot wall epitaxy (CHWE) system.

Silicon substrates are used because of their transparency to IR radiation and their availability as large area wafers with higher structural perfection. In addition,

the processing of silicon integrated circuits is well developed and, as a consequence, selected area CdTe/Si heteroepitaxy offers the possibility of providing the necessary link between InSb/CdTe high electron mobility transistor (HEMT) devices and silicon solid state devices.

The CdTe on silicon deposition was performed with a CHWE system. The transport of the vapor to the substrate occurs as a result of a temperature gradient which exists between the source and the substrate. Temperatures of the various zones of the CHWE system are controlled separately. Films were deposited at different source and substrate temperatures.

2. EXPERIMENTAL PROCESS

2.1. Closed hot wall epitaxy

Deposition of compounds from a single vapor source requires either that evaporation must take place congruently, *i.e.* in the form of a complete molecule, or if dissociation occurs that the constituents are equally volatile. However, relatively few inorganic compounds, alloys or mixtures evaporate congruently because the constitutents which are present in the solid or liquid state usually differ significantly in their vapor pressures. Consequently, the composition of the vapor and hence the composition of the condensate are not the same as that of the source material. For this reason, many techniques have been developed to grow CdTe films[11,12]. In our laboratory, we used CHWE for depositing CdTe thin films.

The design of the CHWE apparatus satisfies the following requirements: (a) no use of compensating material (compensating materials are often used in other kinds of HWE systems[13–18]; (b) closing of the top of the reaction chamber while the film is growing (this reduces the time to reach thermodynamic equilibrium, and reduces the material loss).

The CHWE system is located inside a vacuum chamber with background pressure of about 10^{-7} Torr as shown in Fig. 1. The various temperatures along the CHWE growing chamber are controlled by a temperature controller.

The CHWE system consists of a fused quartz chamber as shown in Fig. 1. The source material, CdTe powder, is located at the bottom of the chamber. The source material compartment is heated by a halogen projection light bulb rated at 500 W of power. The projection bulb operates at about 100 W in this application. A metal heat shield surrounds the source compartment of the CHWE system to avoid heat radiation loss.

A narrow neck, that prevents a direct path between source and substrate, is located above the source chamber. The substrate is located in the upper portion of the CHWE system. The substrate is suspended from a lid that seals the main chamber of the CHWE system during the deposition process. The CHWE system is placed inside an oven made of a stainless steel square box and heated by four halogen lamps. The lamps are located at the center-lines of the four vertical faces of the box. The substrate temperature is governed by the temperature of the oven.

Three K-type thermocouples are used to measure the temperatures of the three zones, as shown in Fig. 1. The source is the hottest and the substrate is the coolest region of the CHWE system so that the vapor will be transported along the

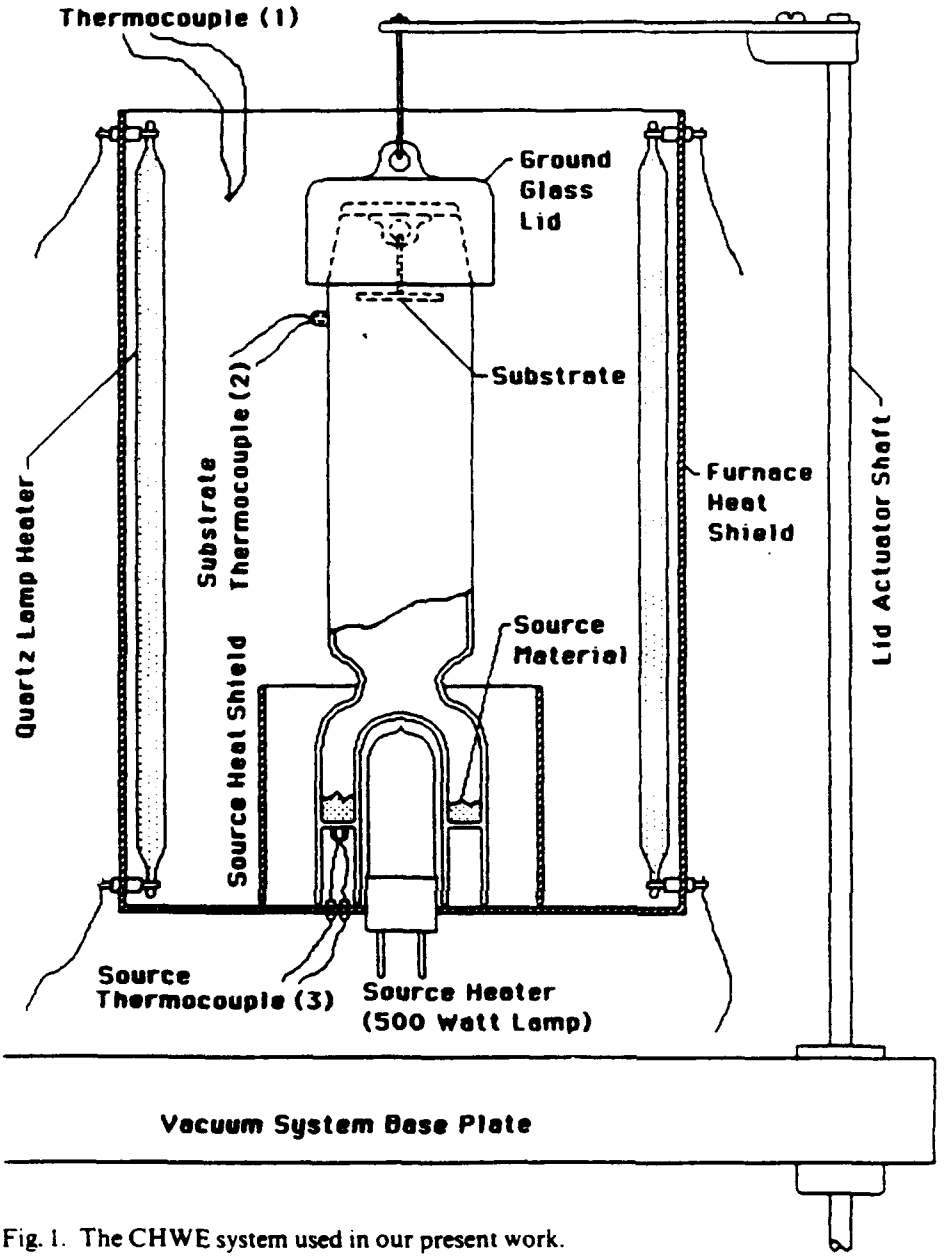


Fig. 1. The CHWE system used in our present work.

temperature gradient from the source to the substrate and deposit a thin film on the substrate.

2.2. Deposition process

First the surface of the Si(100) wafer was polished. Next, the substrate was cleaned using a standard silicon cleaning technique. After the cleaning process, the silicon substrates were suspended from a lid. The quartz CHWE chamber was cleaned and baked inside an oven (60 °C). The chamber was installed in the oven as described in the previous section. The source container at the bottom of the chamber was filled with pure (99.99%) CdTe powder. The top of the chamber was sealed with a dummy lid, and another lid with the substrate was suspended inside the furnace next to the CHWE chamber. All lids were suspended from a stainless steel metal sheet

which can be raised, rotated and lowered from the outside of the vacuum system. The whole system is located inside a vacuum chamber with a background pressure of 10^{-7} Torr. The temperatures of the three zones are controlled by our home-made controller. The temperatures were brought to the desired steady state values, and then the dummy lid was removed and the chamber was sealed with the second lid with the substrate hanging from it. After the film was grown, the lid containing the substrate was moved outside the oven box for substrate cooling. The CHWE chamber was sealed, at this time, with a third lid. The heaters were then turned off.

3. RESULTS AND DISCUSSION

Most epitaxial films grow as follows. Depending on the deposition condition, molecules impinging on the substrate lose most of their excess energy and quickly equilibrate thermally with the substrate. Subsequently, they diffuse along the surface until they re-evaporate or, by interacting with each other, form nucleation islands. These nucleation islands grow by capturing the impinging molecules directly from the vapor or from the surface of the substrate until they coalesce and form a continuous layer.

In general, the condition of heteroepitaxial growth to occur depends on the supersaturation ratio P/P_0 where P is the actual pressure over the condensing surface and P_0 is the equilibrium pressure at the surface temperature. For epitaxial growth to occur this ratio has to be greater than unity[13]. Since the substrate temperature was kept constant at 330 °C for several deposition runs, we can assume that P_0 was also constant[19]. The source temperature determines the pressure at the substrate surface. The growth rate at constant substrate temperature as a function of source temperature was measured and is shown in Fig. 2. We note that the growth rate is linearly proportional to the source temperature at 0.0252 Å s^{-1} $°C^{-1}$ for source temperatures between 450 °C and 575 °C. Also, no epitaxial growth occurs below a source temperature of 450 °C. Observing deposition only on the wall of the tube and none on the substrate at source temperatures below 450 °C leads us to believe that the re-evaporation rate from the substrate is higher than the deposition

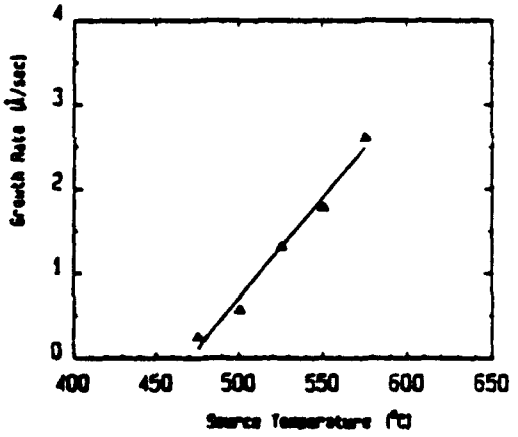
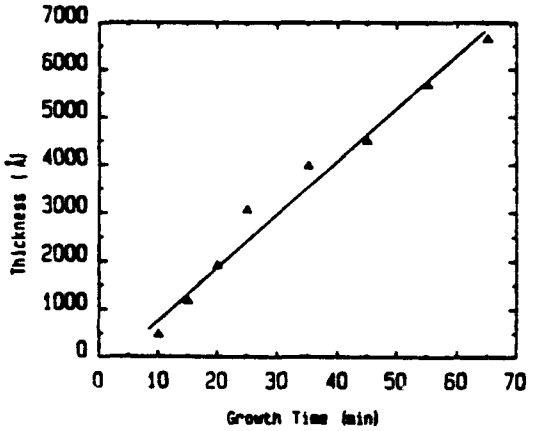


Fig. 2. Variation in the growth rate of the CdTe films with source temperature: the substrate temperature is kept at 330 °C and the growth time is 45 min.

rate. Thus, we can assume that P must be less than P_0 for source temperatures less than 450 °C.

Figure 3 shows the thickness of the epitaxial CdTe films grown at a constant rate as a function of time at a source temperature of 525 °C and a substrate temperature of 330 °C. For this experiment the substrates were preheated to 280 ± 2 °C. The average growth rate is defined as TH/T where TH is the film thickness and T is the time. No deposition occurred for approximately 5 min; after the initial period the films seem to grow at a steady rate of 101.96 Å min^{-1}.

The growth rate was also measured as a function of substrate temperature at constant source temperature. The result of the experiment is shown in Fig. 4. The source temperature was kept at 500 °C and the substrate temperature was varied from 250 °C to 350 °C. The maximum growth rate occurred at 300 °C. No film could be observed at substrate temperatures above 350 °C. We assume that P/P_0 is less than unity at a substrate temperature above 350 °C.



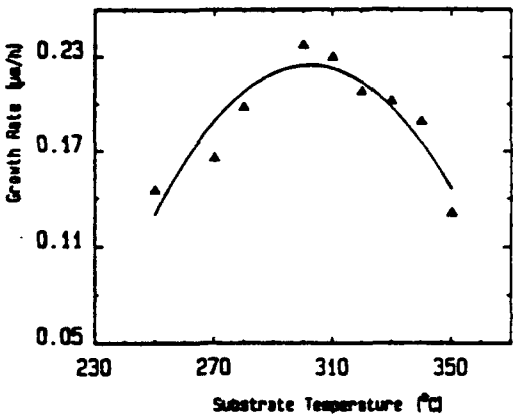


Fig. 3. Variation in the thickness of the films as a function of time: T_{source} = 525 °C and $T_{substrate}$ = 330 °C.

Fig. 4. Variation in the growth rate of the CdTe films with substrate temperature: the source temperature is kept at 500 °C and the growth time is 80 min.

The surface morphology of CdTe films grown on Si(100) substrates was investigated at different source temperatures and at a substrate temperature of 330 °C. The surface roughness, as observed on high magnification scanning electron microscopy (SEM) pictures, seems to increase with the increase in source temperature[20].

However, the growth rate is linearly proportional to the source temperature at constant substrate temperature, as shown in Fig. 2. A number of SEM pictures taken at a magnification of 10 000 of the surface of our epitaxial CdTe films are shown in Fig. 5. Each picture shows a film grown at a different source temperature. We observed that the film grown at the lowest source temperature has the least roughness. Ideally, epitaxial growth proceeds monolayer by monolayer. However, as the supersaturation ratio increases, random nucleation will become dominant and the number of nucleation islands containing more than one monolayer also increases. Since the lattice constant of CdTe is about 20% larger than that of silicon, there should be mismatched boundaries where the islands coalesce. Also, the thermal expansion coefficient of CdTe is about twice as large as that one of silicon[21].

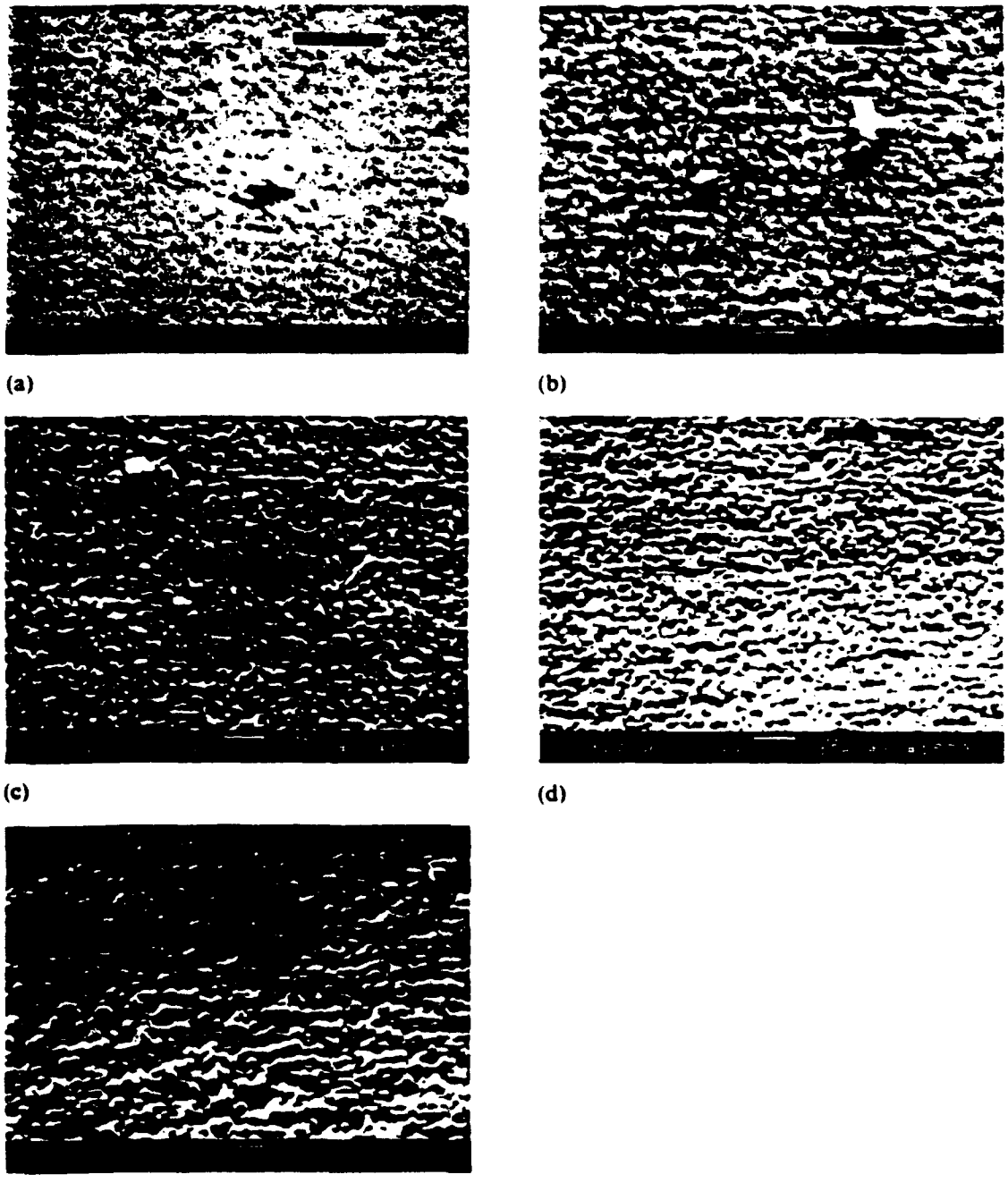


Fig. 5. SEM micrographs of the CdTe epitaxial films grown at different source temperatures ($T_{substrate}$ = 330 °C: (a) 475 °C; (b) 500 °C; (c) 525 °C; (d) 550 °C; (e) 575 °C. Some large dust particles are also visible in some of the photographs.

Thus stretching stresses will be induced in the CdTe films as the film and substrate cool[7,22-24]. All these phenomena contribute to the roughness of the CdTe films.

We also investigated the crystalline properties of the CdTe film with X-ray analysis. The penetration depth of Cr Kα X-rays is less than the thickness of the CdTe film[25]. Therefore, the dots in the Laue back-reflection pattern of Fig. 6(b) are due to the CdTe film and not due to the silicon substrate. Figure 6 also includes the Laue patterns of silicon substrate, CdTe film, CdTe powder source and cadmium

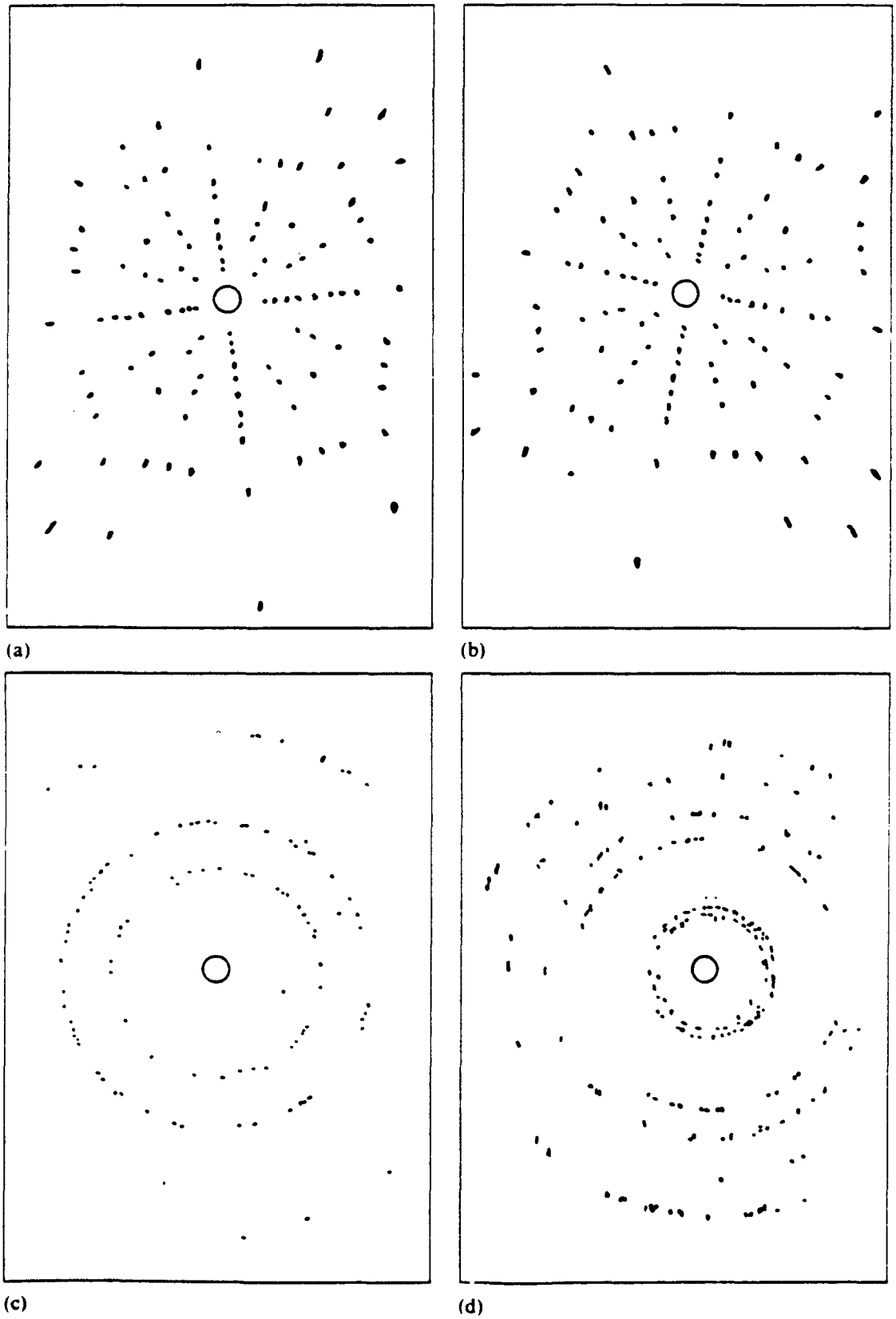


Fig. 6. Cr Kα X-ray diffraction patterns for (a) Si(100) substrate, (b) CdTe epitaxial film on an Si(100) substrate (T_{source} = 525 °C and $T_{substrate}$ = 330 °C), (c) CdTe powder source and (d) cadmium film on Si(100).

metal film. Similar to the CdTe film, the Laue patterns, as shown in Figs. 6(c) and 6(d), are solely from the CdTe powder source and the cadmium metal film, supporting our calculation. It is clear from the back-reflection patterns that the films are single crystalline and oriented in the (100) direction with the same four-fold symmetry as the silicon substrate but with a different lattice spacing. Experimental results indicate a lattice spacing of 6.487 ± 0.004 Å which is in good agreement with previously reported values[2].

The composition of our films was analyzed with a scanning Auger probe. We compared the Auger peaks obtained from our films with those obtained from the 99.99% pure CdTe source material purchased from Alpha Chemicals and found that the ratios of the heights of the cadmium and tellurium Auger peaks in both films and source material were identical. From this we conclude that the films and the source material have the same compositon. An Auger depth profile, shown in Fig. 7, reveals that the films are compositionally uniform throughout their cross-section.

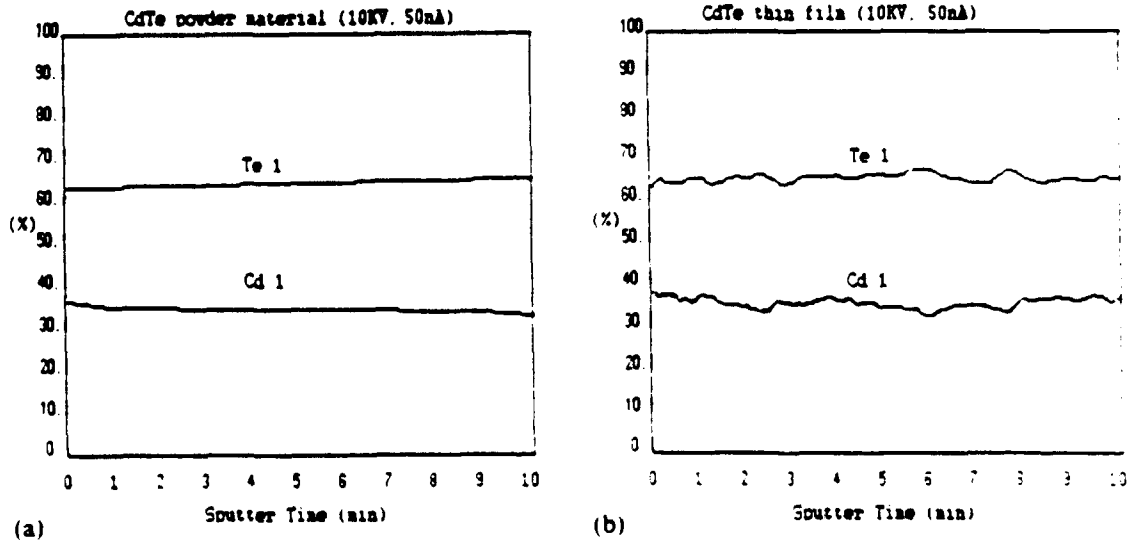


Fig. 7. The composition of CdTe film was analyzed by using Perkin–Elmer Auger electon spectroscopy equipment. The Auger depth profiles show that both (a) source material and (b) CdTe epitaxial film have the same composition (T_{source} = 525 °C and $T_{substrate}$ = 330 °C).

4. CONCLUSION

Although the lattice mismatch and thermal expansion coefficient mismatch between CdTe and silicon are as large as 20% and 50% respectively, single-crystal CdTe films were grown on a silicon substrate in a CHWE system without any compensating material. The films were characterized by means of SEM, X-ray diffraction and Auger electron spectroscopy. The results show that the films are single crystalline and stoichiometric.

The growth rate increased with increasing source temperature because of the higher supersaturation and nucleation rate. The film's surface roughness is a function of the growth rate, lattice mismatch and thermal expansion coefficient mismatch. The only controlled factor in this experiment is temperature and the best surface condition was obtained at a source temperature of 475 °C.

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