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Optical and Microstructural Characterization of the Effects of Rapid Thermal Annealing of CdTe Thin Films Grown on Si (100) Substrates

S. NERETINA,[1,3] N.V. SOCHINSKII,[2] and P. MASCHER[1]

1.—Centre for Electrophotonic Materials and Devices (CEMD), Department of Engineering Physics, McMaster University, Hamilton, ON, Canada L8S 4L7. 2.—Instituto de Microelectronica de Madrid–CNM-CSIC, c/Isaac Newton 8 (PTM), 28760 Tres Cantos, Madrid, Spain. 3.—E-mail: neretis@mcmaster.ca

The effects of rapid thermal annealing (RTA) on CdTe/Si (100) heterostructures have been studied in order to improve the structural quality of CdTe epilayers. Samples of CdTe (111) polycrystalline thin films grown by vapor phase epitaxy (VPE) on Si (100) substrates have been investigated. The strained structures were rapidly thermally annealed at 400°C, 450°C, 500°C, 550°C, and 600°C for 10 sec. The microstructural properties of the CdTe films were characterized by carrying out scanning electron microscopy (SEM), x-ray diffraction (XRD), and atomic force microscopy (AFM). We have shown that the structural quality of the CdTe epilayers improves significantly with increasing annealing temperature. The optimum annealing temperature resulting in the highest film quality has been found to be 500°C. Additionally, we have shown that the surface nucleation characterized by the island size distribution can be correlated with the crystalline quality of the film.

Key words: Infrared (IR) detection, CdTe/Si heterostructures, rapid thermal annealing (RTA), structural characterization

INTRODUCTION

The epitaxial growth of CdTe continues to receive a great deal of attention in the areas of solar-energy conversion, gamma-ray detection, optoelectronics, and integrated optics. Because of chemical compatibility and the close lattice match with $Hg_xCd_{1-x}Te$, which is presently the most important material for infrared (IR) photodetectors, CdTe is also an ideal substrate for the epitaxial growth of high-quality $Hg_xCd_{1-x}Te$.[1] In recent years, CdTe heteroepitaxial layers on Si substrates have been considered as promising alternative substrates for the subsequent growth of $Hg_xCd_{1-x}Te$ over relatively expensive conventional bulk CdZnTe substrates. There are several reasons why there has been much interest in the use of silicon as a base substrate for the epitaxial growth of $Hg_xCd_{1-x}Te$/CdTe multilayer structures. The CdTe films have been grown on various substrate materials including GaAs,[2] sapphire,[3] InSb,[4] and silicon, which are available in large areas of high quality. However, because of low cost and the commercial availability in the form of high-purity large diameter wafers, Si has been recognized as a promising substrate. Moreover, since signal processing is presently only available in silicon, Si-based technology allows the monolithic integration on a single chip of photonic and electronic components. If good-quality $Hg_xCd_{1-x}Te$/CdTe can be grown on Si, it could eventually become possible to integrate the $Hg_xCd_{1-x}Te$ detectors directly to the silicon processor and produce large area monolithic infrared (IR) focal-plane arrays versus a currently used hybrid approach that transfers charge from the $Hg_xCd_{1-x}Te$ detector to the silicon processor through indium bump bonds with all consequent limitations.

There are, however, several difficulties associated with the growth of CdTe on Si. The production of $Hg_xCd_{1-x}Te$ detector arrays,[5] for example, for thermal imaging application, requires producing large

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areas of high-quality CdTe films. High-quality CdTe epitaxial layers on Si substrates have been obtained by several growth methods such as molecular beam epitaxy,[6] metal-organic chemical-vapor deposition,[7,11] and hot wall epitaxy.[8] The growth by vapor phase epitaxy (VPE) has also been considered because of the lower cost, high growth rate, and the capability of producing large area films. Since CdTe/Si structures have a large lattice mismatch ($\Delta\alpha/\alpha \approx 19\%$ at 25°C) and thermal expansion coefficient difference ($\Delta\alpha/\alpha \approx 46.9\%$ at 25°C), the interface region contains dense arrays of dislocations resulting in deteriorating quality of the film. Many attempts have been made to investigate possible ways to improve the surface morphology and structural properties of strained CdTe films grown by different methods using postgrowth treatments. One of them is laser-assisted recrystallization by irradiation with an Ar ion laser beam.[9] In this article, we present the experimental results on the remarkable improvement of the structural quality of the CdTe epilayers by postgrowth rapid thermal annealing.

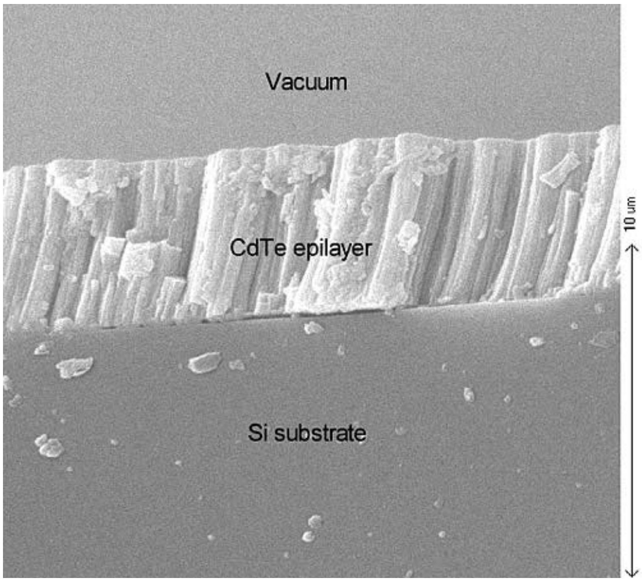

Fig. 1. SEM image of a CdTe/Si interface.

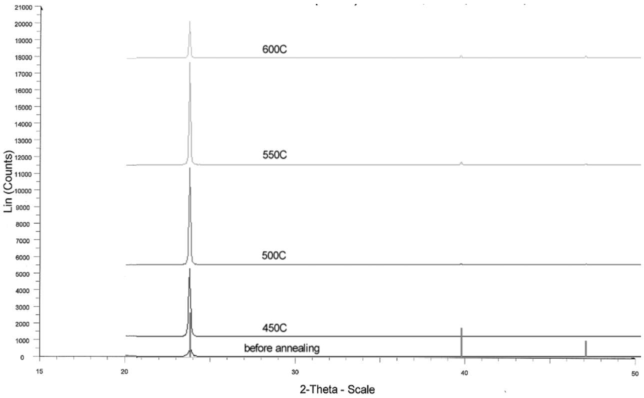

Fig. 2. X-ray 2θ scans of CdTe/Si epilayers as grown and annealed at 450°C, 500°C, 550°C, and 600°C.

EXPERIMENTAL DETAILS

The CdTe epilayers were grown by VPE on Si (100) substrates.[10] The VPE growth was carried out at evaporation temperatures in the range of 700–800°C with no heating system for the substrates. Polycrystalline stoichiometric CdTe grown by the modified Bridgman method was used as a source material. The growth rate was in the range of 0.05–0.2 µm/min. With these conditions, the VPE growth provided planar 1–3-µm-thick CdTe epilayers formed uniformly over the entire substrate area.

The rapid thermal annealing system used in this work is a "heatpulse mini-pulse" built by A.G. Associates (Sunnyvale, CA). Mini-pulse is a rapid thermal processor that uses high intensity visible radiation to heat single wafers for short periods of time at precisely controlled temperatures. Tungsten halogen lamps and cold heating chamber walls allow fast wafer heating (heating rate of 50°C per second) and cooling rates. The rapid thermal annealing (RTA) process was performed in a nitrogen atmosphere. To protect CdTe/Si from any impurities within the mini-pulse system, samples were enclosed in a graphite boat. The RTA process was carried out in a temperature range between 400°C and 600°C at 50°C intervals for 10 sec.

RESULTS AND DISCUSSION

Structural Quality

A Philips scanning electron microscope 515 with a lanthanum hexaboride filament was employed to characterize the film and interfacial microstructure. Figure 1 presents a scanning electron microscopy (SEM) image of a CdTe/Si interface. A cross section of the CdTe/Si structure shows well-defined and flat heterojunction interfaces. The image reveals a good adhesion to the substrate with no evidence of cracks through the bulk.

X-ray diffraction (XRD) techniques were employed to study the structural properties of the CdTe films as a function of annealing temperature. The 2θ scan (Fig. 2) and single-crystal rocking curve (Fig. 3) data were obtained using an automated x-ray diffractometer. The x-ray beam samples large areas of the film; therefore, the results are averaged. The crystallographic orientation of the film was determined to be (111). The lattice constant α is 6.483 Å.

The XRD patterns of the CdTe epilayers are shown in Fig. 2. One peak at 23.756° corresponding to the (111) plane appears for all films. Furthermore, the (111) peak becomes sharper and stronger with increasing RTA temperature. The XRD results indicate the progressive improvement in the structural quality of the CdTe films with annealing temperature. It can be explained that CdTe was grown on Si as a highly ordered polycrystalline layer with (111) preferential orientation. As the annealing temperature increases, there is a gradual transition

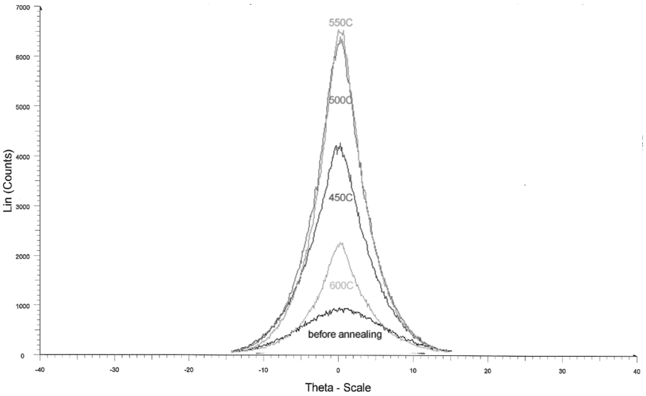

Fig. 3. X-ray rocking curves of CdTe/Si epilayers as grown and annealed at 450°C, 500°C, 550°C, and 600°C.

toward forming a perfect layer resulting in better crystalline quality of the CdTe film.

The rocking curve linewidth (full-width at half-maximum (FWHM)) is considered a measure of the structural perfection of the interface region. The widths of the x-ray rocking curves for CdTe films show dramatic changes as a function of annealing temperature (Fig. 3). The FWHMs of the rocking curves vary from 9.21° for as-grown films to 4.72° for a film annealed at 600°C. This demonstrates a significant improvement in CdTe/Si crystalline quality at higher RTA temperatures.

The quantitative measurements of CdTe/Si structural quality such as the FWHM and net area values obtained from x-ray 2θ scan and single-crystal rocking curve are shown in Tables I and Table II, respectively. It is seen that increasing annealing temperature up to 550°C significantly improves the epitaxial structure. However, as is also evident from Table I and Table II, the peak intensity clearly decreases with further increasing RTA temperatures. This observation indicates the deterioration in the film quality at temperatures above 550°C.

Surface Morphology

Surface morphology has been investigated by employing atomic force microscopy (AFM). The AFM images were collected in the contact mode using a Digital Instrument Nanoscope Scanning Probe Microscope (Santa Barbara, CA).

Figure 4 shows the surface view of CdTe/Si layers as grown and annealed at 500°C. The images exhibit a uniform fine-grained morphology. Because of the large difference in lattice constant and thermal expansion coefficient, accumulated mechanical strains cause the formation of a high density of microcracks in the CdTe epilayers. A large number of surface defects has been observed in as-grown CdTe/Si, which is typical for surface morphology of a strained layer. Further, we can see that rapid thermal annealing greatly reduces, but does not completely eliminate, the defect density. In addition, at higher annealing temperatures, the CdTe grains crystallize to form larger grains (Fig. 5), which are consistent with the XRD patterns in Fig. 2. However, increasing the temperature above 550°C results in a deterioration of the surface quality.

Crystal growth is a complex heterogeneous process involving bulk diffusion, surface absorption, surface diffusion, and finally integration of molecules or ions into the crystal lattice. Figure 5 shows that both surfaces consist of many islands that seem to reflect nucleation, which can be explained by the presence of native Si oxide due to a relatively poor vacuum of only 10^{-7} Torr during VPE. Surface nucleation can be studied with AFM and correlated with crystalline quality.[11] It has been shown that nuclei with less density correspond to higher crystalline quality. Figure 5 shows the surface nucleation of an as-grown film and the annealed one at 550°C. It is seen in Fig 5 that as annealing temperature increases, the density of nuclei decreases, which, according to the Ref. 11, results in the improved crystalline quality.

Table I. FWHM and Net Area Values from X-ray 2θ Scans of CdTe/Si Epilayers As-Grown and Annealed at 450°C, 500°C, 550°C, and 600°C

Annealing Temperature	Max. Int. Cps	FWHM 2θ°	Net Area Cps × 2θ°
CdTe/Si before annealing	435	0.268	127.4
CdTe/Si annealed at 450°C	2013	0.119	290.0
CdTe/Si annealed at 500°C	2912	0.101	354.8
CdTe/Si annealed at 550°C	3045	0.091	332.6
CdTe/Si annealed at 600°C	1079	0.086	111.9

Table II. FWHM and Net Area Values from X-ray Rocking Curves of CdTe/Si Epilayers As Grown and Annealed at 450°C, 500°C, 550°C, and 600°C

Annealing Temperature	Max. Int. Cps	FWHM θ° Rocking Curve	Net Area Cps x θ°
CdTe/Si before annealing	443	9.21	4201.8
CdTe/Si annealed at 450°C	2090	5.86	14402.0
CdTe/Si annealed at 500°C	3158	5.09	19636.3
CdTe/Si annealed at 550°C	3230	4.88	19115.5
CdTe/Si annealed at 600°C	1096	4.72	6503.6

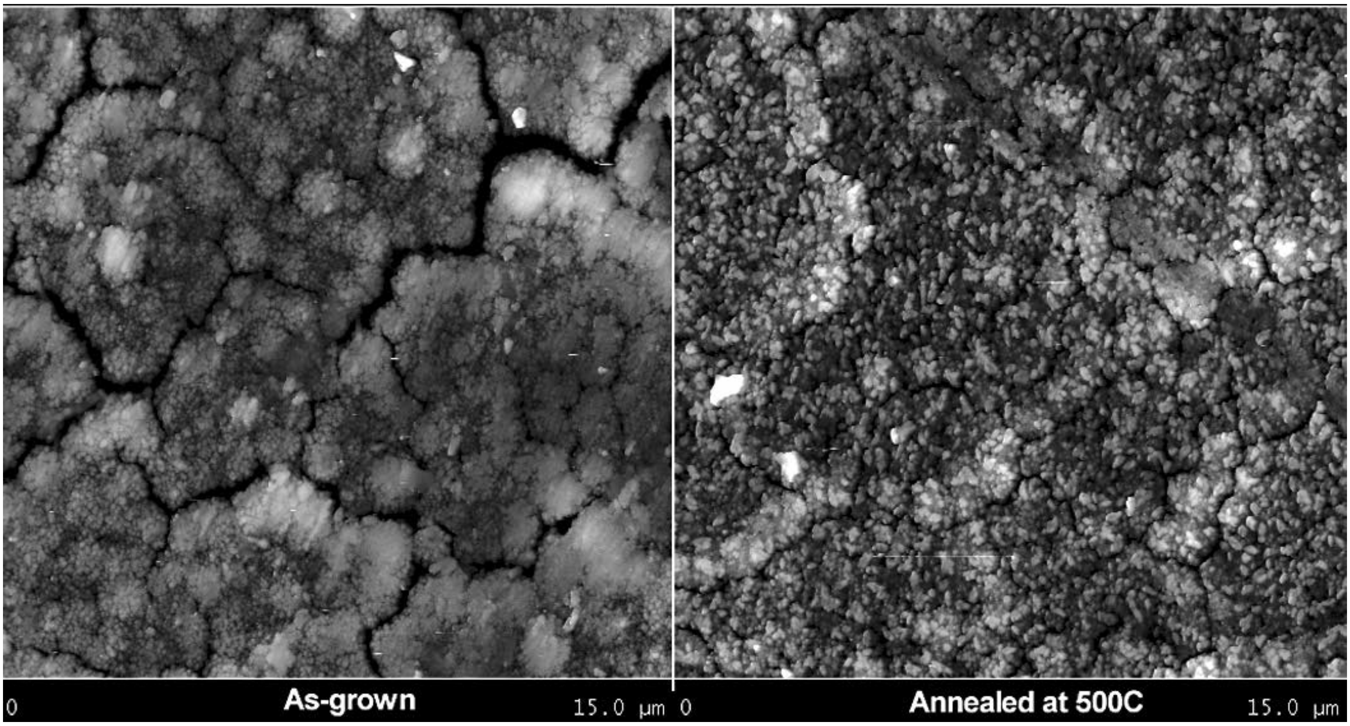

Fig. 4. AFM images of CdTe/Si epilayers as grown and annealed at 500°C, 15-µm scale.

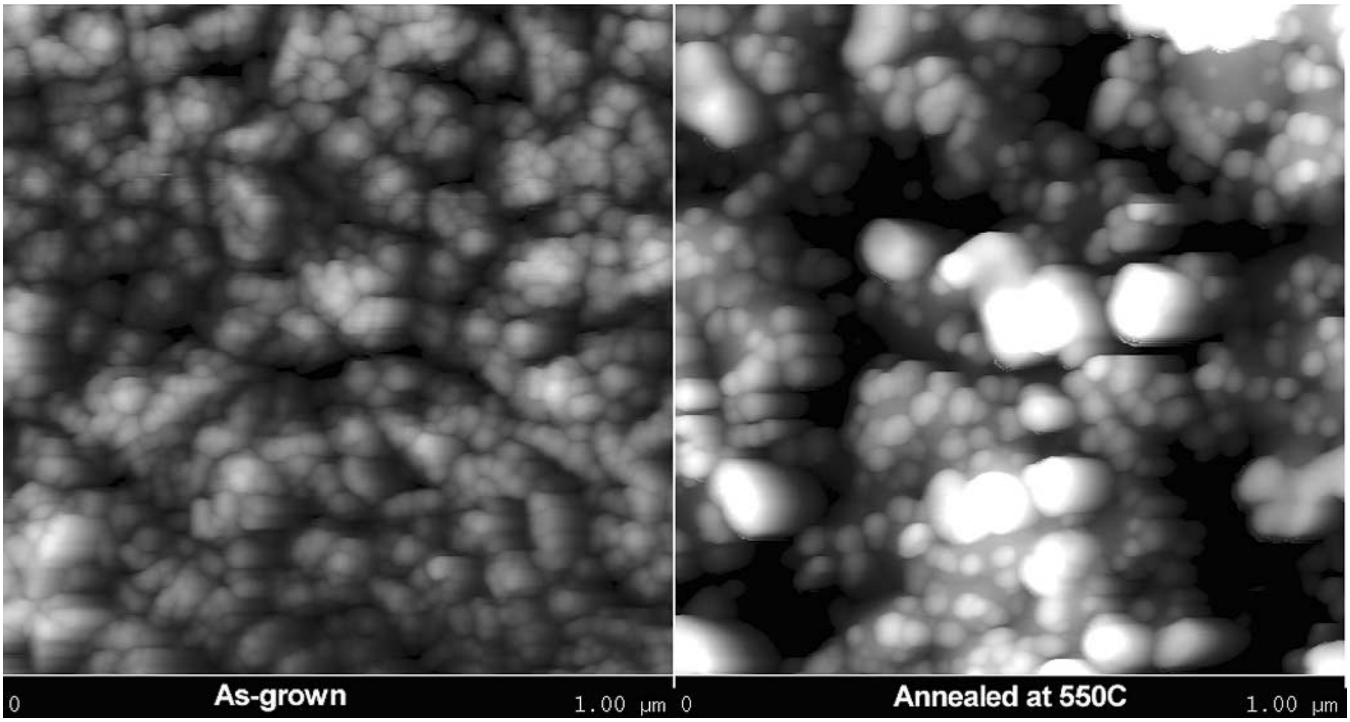

Fig. 5. AFM images of CdTe/Si epilayers as grown and annealed at 550°C, 1-µm scale.

These observations are in good agreement with XRD studies, which prove the improvement in crystallinity with increasing annealing temperature.

CONCLUSIONS

In conclusion, the quality of CdTe thin films grown by VPE on Si (100) substrates can be remarkably improved by postgrowth rapid annealing, which improves both the crystalline structure and surface morphology. The XRD results show that the FWHM values of 2θ scans and rocking curves decrease with increasing annealing temperature. This indicates higher crystalline perfection of the annealed films. The AFM shows better surface morphology with increasing annealing temperature. The density of surface defects is greatly reduced, and the grain size becomes larger at higher, RTA temperatures.

The improved structural quality of CdTe opens possibilities for the subsequent epitaxial growth of high-quality $Hg_xCd_{1-x}Te$. Moreover, the achieved high crystalline quality results in a good optical quality, which is adequate for light-guiding applications. Therefore, the heteroepitaxial layer can also be used as an active medium for device application, for example, fabricating optical waveguides in integrated optics devices.

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