Correlation of CdZnTe(211)B Substrate Surface Morphology and HgCdTe(211)B Epilayer Defects

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We present results on the surface morphology and recombination lifetimes of molecular-beam epitaxy (MBE)-grown HgCdTe (211)B epilayers and correlate them with the roughness of the CdZnTe substrate surfaces. The substrate surface quality was monitored by in-situ spectroscopic ellipsometry (SE) and reflection high-energy electron diffraction (RHEED). The SE roughness of the substrate was measured after oxide desorption in the growth chamber. The RHEED patterns collected show a strong correlation with the SE roughness. This proves that SE is a valuable CdZnTe prescreening tool. We also found a correlation between the substrate roughness and the epilayer morphologies. They are characterized by a high density of thin elongated defects, “needle defects,” which appear on most samples regardless of growth conditions. The HgCdTe epilayers grown on these substrates were characterized by temperature-dependent, photoconductive decay-lifetime data. Fits to the data indicate the presence of mid-gap recombination centers, which were not removed by 250°C/24-h annealing under a Hg-rich atmosphere. These centers are believed to originate from bulk defects rather than Hg vacancies. We show that Te annealing and CdTe growth on the CdZnTe substrates smooth the surface and lower substantially the density of needle defects. Additionally, a variety of interfacial layers were also introduced to reduce the defect density and improve the overall quality of the epilayer, even in the presence of less than perfect substrates. Both the perfection of the substrate surface and that of its crystalline structure are essential for the growth of high-quality material. Thus, CdZnTe surface polishing procedures and growth techniques are crucial issues.

Key words: Molecular beam epitaxy (MBE), HgCdTe, defects, surface morphology, ellipsometry, reflection high-energy electron diffraction (RHEED)

INTRODUCTION

High-quality mercury cadmium telluride, suitable for device applications, is difficult to obtain by either bulk or epitaxial growth. Compared with other material growth techniques, molecular-beam epitaxy (MBE) growth is most suitable for the growth of high-quality complex heterojunctions and multilayer structures for future, infrared focal-plane arrays.

One of the challenges posed by the MBE growth of HgCdTe is the understanding and control of visible defects on the surface. The defects observed are of several varieties.1,2 Some, such as voids and microtwins, are introduced during growth; others are more related to imperfections or substrate preparation procedures. Even though substrate issues for the growth of HgCdTe have been reported previously,3,4 more studies are needed to fully understand and control substrate-related defects.

Here, we present our results on the surface morphology of HgCdTe epilayers grown by MBE. These
layers are characterized by thin elongated defects ("needle defects"), which, now we believe, are substrate related. The CdZnTe substrates used for these growths were characterized using in-situ spectroscopic ellipsometry (SE) and reflection high-energy electron diffraction (RHEED). Then, the HgCdTe surface morphology was correlated with the CdZnTe substrate properties.

**EXPERIMENTS**

The HgCdTe epilayers were grown in a Riber 32P MBE system (Rueil-Malmaison, France) equipped with RHEED, an 88-wavelength spectroscopic ellipsometer, a pyrometer, and a Hg valved cell. Solid CdTe and Te were used as source materials. Elemental In was used as the n-type dopant.

For this study, front-side-polished CdZnTe (211)B substrates with a Zn mole fraction of 3.5 ± 1% were purchased from Nikko Materials USA, Inc. (Chandler, AZ). Their surface appeared smooth and mirrorlike.

Before growth, the CdZnTe substrates were chemically cleaned using trichloroethylene, acetone, and methanol; etched in a 1% bromine/methanol solution; and rinsed in methanol and deionized water. Then, the substrates were dried and mounted between a spring plate and a graphite thermal diffuser plate on an In-free holder. Extra care was taken to ensure a good mounting repeatability for all substrates.

Once introduced into the growth chamber, excess Te present on the sample surface was stripped at 250°C, and CdTe was deposited to reduce the surface roughness. In-situ SE and RHEED were used to monitor the oxide desorption, interface formation, and growth together with the substrate thermocouple. The pyrometer was used to help monitor the substrate temperature.

Different kinds of interfacial layers were used between the substrate and the epilayer (Fig. 1). It was suggested by our previous qualitative findings that abrupt interfaces interposed between HgCdTe layers of different composition might help block the propagation of substrate-related defects. Most layers were grown with mid-wavelength infrared/very long wavelength infrared interfacial layers. The growth rate of HgCdTe was 6–8 Å/sec; the Cd molar fraction was chosen to be about 0.23.

Our SE is a rotating analyzer ellipsometer that can measure 88 wavelengths in the range from 1.6 eV to 4.3 eV (the Woollam M88, J.A. Woollam, Lincoln, NE). The evolution of the dielectric function during the substrate preparation procedure was recorded in real time. The ellipsometric roughness was measured using the standard two-layer model, comprised of a temperature-dependent library of CdZnTe pseudo-dielectric functions and a surface roughness layer of variable thickness modeled in the Bruggeman approximation (the EMA). This effective medium theory describes well the changes caused by microscopic roughness. Detailed description of the system and the data analysis can be found in our previous paper.

The surface morphology of the HgCdTe epilayers was inspected using a Nomarski optical microscope and an atomic force microscopy (AFM). The minority-carrier recombination lifetimes of these HgCdTe layers were also measured using the photoconductive decay (PCD) method; temperature-dependent lifetime data were fit to extract the density and energy level of the dominant Shockley–Reed recombination centers. X-ray double-crystal rocking curve measurements gave information on the crystalline perfection of the layers grown.

**RESULTS AND DISCUSSION**

Figure 2 shows a comparison of the CdZnTe surface roughness obtained by SE during preparation and the corresponding RHEED patterns. Our CdZnTe substrates were (211)B oriented, and the RHEED patterns were taken from the [111] azimuth. To avoid fitting errors, the SE surface roughness was measured after removing the oxide created by the cleaning procedure.

RHEED is very sensitive to surface imperfections. It is well known that roughness or imperfections in the crystalline structure will make the patterns spotty. However, the quantification of roughness from RHEED patterns is difficult, whereas the SE

![Diagram](image_url)

Fig. 1. The typical structures used for the HgCdTe growth on CdZnTe with different interfacial layers.