Composition Control of Long Wavelength MBE HgCdTe Using In-situ Spectroscopic Ellipsometry

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Improved composition control of $Hg_{1-x}Cd_xTe$ layers grown by molecular beam epitaxy using in-situ spectroscopic ellipsometry is described. This has increased our composition yields from < 40% to approximately 70% for a specification of x to within 0.0015 of target composition. Knowledge of composition during growth also enables corrections to effusion cell temperatures so that the in-depth composition profile can be controlled. Further improvements were obtained after active composition control was implemented whereby the ellipsometer controls the Te cell temperature to maintain the desired composition.

Key words: HgCdTe, spectroscopic ellipsometry, MBE

INTRODUCTION

Accurate composition control is essential for long wavelength Hg_{1-x}Cd_xTe (x ~ 0.22, $\lambda_{co} > 10 \mu m$ at 78 K) where an accuracy of $\Delta x \leq 0.001$ is desired in order to achieve the desired cutoff wavelength for infrared detection. For epitaxial growth by molecular beam epitaxy (MBE), this requires knowledge of the CdTe and Te source temperatures to within ±0.1°C. But this knowledge is lacking because the temperature control thermocouples are not in direct contact with the source materials, and thermal contact between the materials and their crucibles constantly changes due to depletion effects and temperature cycling. Hence, in general, without in-situ real-time monitoring, the layer composition is unknown. This causes yield loss in obtaining the desired average composition, as well as lacking knowledge of the in-depth composition uniformity and profile. Historically, the inability to obtain the desired layer composition is the highest yield loss factor in our MBE growth process.¹

Hence, real-time monitoring of composition is essential to improve producibility. Spectroscopic ellipsometry $(SE)^{2-7}$ has the required sensitivity to measure x to high accuracy for HgCdTe. This paper reports our progress using SE in which we address the issues of how well it works, the impact on composition yield, control of in-depth composition profile, and implementation of real-time active control in which the ellipsometer controls the Te cell temperature to achieve a desired composition.

EXPERIMENTAL

Layers were grown in a Riber 32P MBE system installed in our laboratory in 1999. This system and its operation were discussed in detail by Bajaj et al.8 Substrates were (211)B CdZnTe ($3.5 \pm 1\%$ Zn) with sizes of 3×4 , 4×4 , or 3×5 cm². The substrates were rotated during growth to improve uniformity, and SE data were acquired continuously during rotation. Layer composition is determined by the temperatures of the CdTe and Te effusion cells. The absorbing layers of interest were typically $10-15 \,\mu\text{m}$ thick with compositions in the range 0.205-0.230 depending on application. Layer characterization techniques included room-temperature Fourier transform infrared transmission (FTIR) to determine composition x and layer thickness of the absorber layers. Secondary ion mass spectroscopy (SIMS) was used to independently measure in-depth composition profiles.⁹

SE measurements were performed using a multispectral M-88 ellipsometer system from the J.A. Woollam Co.^{3,10-12} Data were acquired continuously throughout the growth run using 88 wavebands from 1.6 to 4.5 eV. Using an optical constant library built with data from our HgCdTe layers, the data analysis using the 88 separate wavelengths as well as data from the real and imaginary parts of the dielectric function ensured that a unique solution was found for the composition to high accuracy.

RESULTS

As an example of how the layer composition can change unpredictably during a run, Fig. 1 shows the

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Fig. 1. Depth composition profile for the absorber layer from run 3–150. During the time of this growth, all cell setpoint temperatures were constant. The transient from time t = 40-60 m was caused by the transition from a high x buffer layer (off scale).

in-depth composition profile for a 3 h absorber layer during which the CdTe and Te cell temperatures were constant. Off to the left of the graph (t < 40 m), a highx buffer layer was grown. While the composition undershoot around t = 50 m could have been caused by actual temperature overshoot of the Te cell or undershoot of the CdTe cell (but not observed from the controlling thermocouples), the long, sustained decrease in x throughout most of the growth was caused by drifts of the fluxes in either or both of the cells. We have observed that the shapes of profiles obtained for constant cell temperatures can change radically from run to run, which is a major reason for the inability to accurately predict the layer average composition.

To demonstrate that the composition profile of Fig. 1 is real, Fig. 2 shows the profiles of another layer measured by SE and independently by SIMS. The very good agreement between the profiles in terms of features demonstrates the validity of SE.

Figure 3 shows a comparison of run-to-run x control with and without SE. With SE, the large outliers are completely eliminated and the distribution is noticeably tighter. The standard deviation improved from 0.0081 to 0.0018, a factor of 4.5 improvement. A discussion of the resulting improvements in cutoff wavelength control and factors affecting it can be found in Ref. 13.

Figure 4 shows the relationship between compositions measured by in-situ SE and room temperature transmission measurements for 50 layers. A relatively constant offset ($x_{SE}-x_{FTIR}$) of -0.0025 is observed (and accounted for during growth), with 90% of the layers having an accuracy of $\Delta x < \pm 0.002$ from the desired composition. x_{SE} represents an average using nine time slices equidistantly spaced from the beginning to end of the layer. For a given layer, the accuracy of this parameter is ~ ± 0.0005 , which depends on the exact time slices selected. Consistency of this offset parameter is now the key driver controlling the yield of layers having the desired composition. This parameter is plotted in Fig. 5 for 144 of the most recently grown layers. A similar accuracy of ~0.0005



Fig. 2. Depth composition profile for the absorber layer from run 3–99, comparing measurements from in-situ SE and post-growth SIMS.



Fig. 3. Comparison of x control for hundreds of x-0.2 layers grown without SE compared with recent layers grown with SE. With SE, the large outliers are completely eliminated and the distribution is noticeably tighter. The standard deviation improved by a factor of 4.5.

mated for the determination of x_{FTIR} . However, due to the strong sensitivity of geometrical factors on the SE measurements and their analysis (e.g., substrate rotation wobble, layer morphology, etc.), we believe x control is primarily limited by the SE measurements rather than how accurately x can be determined by FTIR.

Implementation of Active Control

Figures 1 and 2 above show that the layer composition cannot be predicted merely by knowing the CdTe and Te cell temperatures. Run-to-run variations in in-depth composition complicate achieving the desired average composition as measured by FTIR, and are potentially detrimental to detector performance due to reduced quantum efficiency. These factors have made it desirable to implement active control whereby the Te cell temperature (which controls x) is controlled by the output signal of the ellipsometer.

Automated feedback control was achieved through



Fig. 4. Relationship between compositions measured by in-situ SE and room temperature transmission measurements for 50 layers. A relatively constant offset ($x_{SE}-x_{FTIR}$) of -0.0025 is observed (and accounted for during growth), with 90% of the layers having an accuracy of $\Delta x < \pm 0.002$ from the desired composition. These layers were grown without active control.





real-time SE data and a control program written using *LabVIEW* software from National Instruments.¹³ The user inputs the desired starting and ending composition and corresponding growth time. The program then determines a target composition value using a linear fit. A proportional feedback algorithm makes adjustments during the growth run to the Te effusion cell temperature in response to the deviation of composition measured from SE with respect to the target composition.

Consider the case where a linear composition profile is desired. Without active control, using a linear Te cell temperature ramp during growth will generally result in an approximately linear composition profile. However, the slope of the profile varies from run to run due to time-dependent cell characteristics,



Fig. 6. Depth composition profile for the absorber layer from run 3–243, comparing the linear composition profile with the Te cell temperature that was required to achieve it. The deviation from a linear temperature profile approximately represents the degree of active control necessary to achieve the linear composition profile.

and it can even change during a run which then causes a deviation from linearity in the composition profile. Using active control, Fig. 6 shows the profile for one layer with the corresponding Te cell temperature profile. The cell temperature is determined by a linearly ramped setpoint plus a correction setpoint term determined from the ellipsometer output sufficient to maintain a linear composition profile. The deviation from linearity in the temperature profile approximately represents the amount of active control correction that was necessary to keep the composition profile linear. As Fig. 6 shows, the correction necessary can be significant.

SUMMARY AND CONCLUSIONS

Accurate control of HgCdTe composition during MBE growth has been a challenge, but thanks to the combined efforts of many in the HgCdTe MBE and SE communities, the goal is now within reach. In the work reported here, using SE resulted in a standard deviation improvement in x control from 0.0081 to 0.0018 for more than 200 layers grown using SE, a factor of 4.5 improvement. Active control of Te cell temperature by the ellipsometer was implemented to further improve control regardless of drifts in effusion cell characteristics. The reproducibility of the offset parameter, ($x_{\text{SE}}-x_{\text{FTR}}$), is now the key driver controlling the composition yield. Work is now underway to understand the factors that limit this reproducibility.

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