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In situ real-time analysis of the MBE growth of CdTe on Ge: A comparison of ellipsometry data analysis techniques

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Abstract

We test an alternative ellipsometry data analysis technique to measure the temperature and submicroscopic surface roughness of CdTe/Ge during growth by molecular beam epitaxy. Such technique is based on a parametric model for the dielectric function and second-order differentiation of the data. It was proposed in order to reduce the effects of roughness and surface contamination, which are detrimental to the run-to-run accuracy of the traditional data analysis. We find that the new technique yields more accurate results than does the traditional analysis in the presence of both microscopic roughness and submonolayers of excess Te at the surface. However, our data indicate that the new method does not improve the run-to-run accuracy of the temperature measurements. We conjecture that this failure is due to the presence of macroscopic roughness on all MBE-grown (2 1 1) CdTe surfaces. We also propose a qualitative method to detect the formation of macroscopic roughness during growth.
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1. Introduction

In recent years, cadmium telluride (CdTe) has received renewed attention as a buffer layer for the growth of large-area mercury–cadmium telluride ($Hg_{1-x}Cd_xTe$) layers on Ge or Si. In our laboratory, CdTe(2 1 1)B/Ge(2 1 1) epilayers are grown by molecular beam epitaxy (MBE) and subsequently characterized and used as substrates for $Hg_{1-x}Cd_xTe$ epitaxy.

Several authors have used spectroscopic ellipsometry to study the MBE growth of $Hg_{1-x}Cd_xTe$ and control the various aspects of the growth process [1–5]. Ellipsometry allows one to control the composition x to better than ± 0.002, and to follow the substrate preparation in real time. In the case of growing CdTe/Ge, ellipsometry yields the surface temperature and the evolution of the microscopic surface roughness in real time. The standard in situ data analysis method is based on a two-layer representation of the dielectric function, which includes a bulk layer and a surface roughness layer modelled in the effective-medium approximation (EMA) [6,7]. The bulk dielectric function is interpolated from a temperature-dependent library [8] and the model fit to the undifferentiated data. The drawback of this method is the poor run-to-run accuracy of the temperature measurement. We measured a temperature spreading of the order of $\pm 5\,°C$ (Fig. 3, points labelled as ‘‘Library’’). A similar spreading has been found for the measurement of the temperature of bulk $Cd_{0.96}Zn_{0.04}Te$, the optical and chemical properties of which are very close to those of CdTe. It has been attributed to the creation of surface states, due to microscopic roughness and nonstoichiometry [9]. Such states induce changes in the measured pseudo-dielectric function, which are interpreted incorrectly by the analysis. Consequently, a new in situ data analysis method was proposed [9] to minimize these effects, based on a fit to the second derivative of the data and a parametric model for

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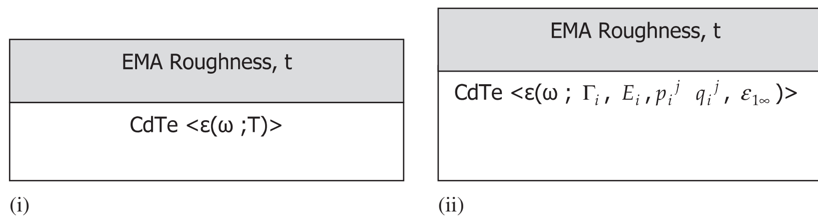

Fig. 1. Model (i): used for the in situ control of the CdTe temperature. The top layer takes into account changes in the surface microscopic roughness (microscopic with respect to the wavelength). Roughness is modelled in the EMA approximation. The bottom layer is based on a temperature-dependent library of dielectric functions. Model (ii): two-layer model including a parametric model for the bulk CdTe dielectric function, and an EMA roughness overlayer.

the dielectric function (Fig. 1). In this note, we apply this new method to the analysis of growing CdTe on Ge to figure out whether it really reduces the temperature spreading.

2. Experiment

We used 4″ CdTe/Ge samples grown routinely in our lab by MBE. For each sample, in situ ellipsometry data were acquired during growth. The growth chamber is a Riber Epineat reactor equipped with standard effusion cells; the sample mounting system provides a good thermal contact between the substrate and a thermocouple placed at the back of the holder. We believe the thermocouple values to be reproducible within better than $\pm 2.5\,^{\circ}\mathrm{C}$. The growth recipe was detailed elsewhere [10,11]. A monolayer of Zn was used to control the polarity before CdTe growth. The nominal growth conditions were the same for all samples, except for the Zn flux. Manipulating the Zn flux allowed us to change the surface morphology significantly from run-to-run, to test the response of our data analysis to this parameter.

The chamber is equipped with strain-free windows for in situ ellipsometry (SE) measurements. The ellipsometer we used is a commercial rotating compensator instrument [12] operating in the 1.2–5.0 eV range.

X-ray diffraction revealed the excellent and highly reproducible crystalline quality of the layers grown, with a full-width at half-maximum (FWHM) of the order of 100 arcsec (Fig. 2). Both visual inspection and Nomarski phase contrast microscopy confirmed the presence of macroscopic roughness on most wafers. Stylus measurements yielded a rms roughness varying from 100 Å to the low measurement limit of 50 Å, with a correlation length of the order of the micrometer. No obvious correlation was found between the surface morphology and the FWHM. The thickness of the layers was determined by FTIR spectroscopy. It varied between 5.4 and 7.0 μm.

To investigate the response of each model to changes in the surface stoichiometry, we charged an as-grown sample that had been stored in air for over a month. The sample was etched with bromine and methanol before introducing it into the chamber. The oxides were stripped in situ at 300 °C for several minutes, and the sample cooled down to room temperature. Then, without extracting it from the chamber, the sample was ramped in steps to 150, 250, 300, 350 and 400 °C (nominal thermocouple temperature), and ramped down in the same fashion. Ellipsometry data were recorded throughout the procedure. We repeated the sequence twice using the same sample; in the first run (a), we subjected the sample to a Te flux at 400 °C for approximately 10 min, to obtain a smooth, Te-rich surface. In run (b) we did not expose the surface to Te, ensuring a rough surface close to stoichiometry or slightly Cd-rich.

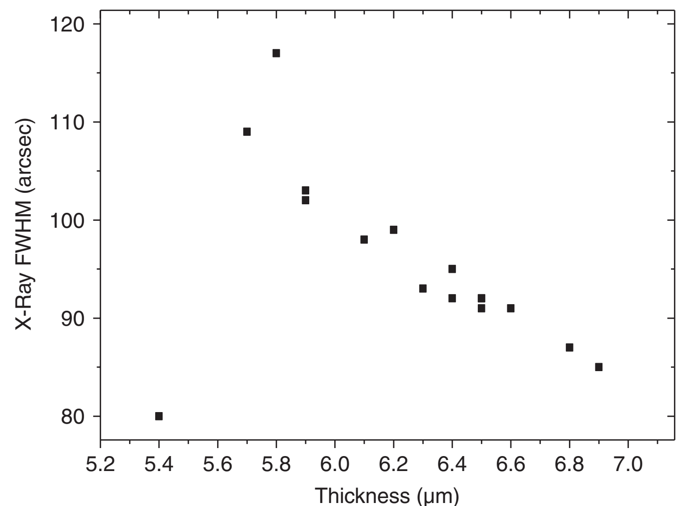

Fig. 2. Correlation between the FWHM of the CdTe layers used in this discussion and their thicknesses. The two dots that lie outside of the curve correspond to a sample that was annealed in situ after the growth (down left) and another that was grown at a much higher substrate temperature (run number 24389).

A calibration based on the position of E_1 and the curves given in Ref. [13] indicates that 400 °C is approximately equal to ~260–280 °C. This difference is due to the thermal resistance of the substrate holder. The data were fit using both methods (i) and (ii), which we are now describing.

3. Data analysis

3.1. Method (i)

Here, three parameters are left free in the fit: the angle of incidence, the EMA surface roughness t and the

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