Application for NIST Uncertainty Analysis Student Award

Electronic Materials Conference 2022

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Advisor Signature: ____

Advisor signature certifies that the advisor has reviewed the uncertainty analysis and finds no gross errors or misrepresentations of the data, and that the work appears to be original and performed by the student.

Title of EMC Abstract: Influence of Ga flux on high temperature growth of AlGaAs transistors

(1) Brief description of numerical result(s) for which uncertainty analysis has been performed:

The AlGaAs composition of films grown with molecular beam epitaxy was measured with typical result for Al mole fraction x =0.2033 +/- 0.0015 . This uncertainty is based on a single standard deviation confidence interval (k=1).

(2) Describe the type of raw data collected and analyzed in this experiment.

Al and Ga growth rates were measured using RHEED intensity oscillations during molecular beam epitaxial growth. The intensity data were collected with a camera pointed at the RHEED screen and video frame grabber software. The data were collected on a 10 mm test sample immediately prior to growth of the actual transistor films.

(3) Describe the method used to determine the uncertainty in the raw data.

Growth rates were collected for AlAs, GaAs and AlGaAs growth, with three to four data sets acquired per composition. The intensity data were curve fit to locate each extrema in time and then to calculate an instantaneous growth rate. The instantaneous growth rate was averaged over a section at long time (past flux transients), yielding both an average growth rate and a standard deviation for the growth rate from a single curve. The weighted mean μ of the values of the separate data curves were then calculated as

$\mu_y = \mathrm{sum}(y/\ \sigma_y^2)\ /\ \mathrm{sum}(1/\ \sigma_y^2)$. The standard error of the weighted average is the square root of $(1/\ \mathrm{sum}(1/\ \sigma_y^2))$. {Equations 5-6 and 5-10 from P. R. Bevington, *Data Reduction and Error Analysis for the Physical Scientists*.} This result was the main standard uncertainty for the growth rate measurements. Because this is an example, I also show the results of applying Eqns A-4 and A-5 from NIST Technical Note 1297, which would apply if we did not have uncertainty values for each individual data point. The smaller uncertainties associated with using the standard deviation of the values relative to the weighted uncertainty indicates that the data are more reproducible than the noisy values at long time would predict.

Source	Al[*a*]	σ_a	Ga [*g*]	σ_g	AlGa[*b*]	σ_b
Data set 1	0.21244	0.001201	0.82951	0.069453	1.04046	0.08932
Data set 2	0.21211	0.002304	0.82821	0.016829	1.04444	0.00753
Data set 3	0.21242	0.000650	0.84398	0.082639	1.04819	0.03513
Data set 4			0.84769	0.109688		
Weighted Mean	0.21240	0.00056	0.8293	0.016	1.0445	0.0073
TN 1297	0.21232	0.00011	0.8373	0.005	1.0444	0.002

Systematic errors associated with substrate temperature and the reconstruction direction used for intensity measurements were evaluated by repeating the measurements while varying these parameters. There were no observable changes associated with modifying these experimental conditions. I also evaluated the effect of beam position on the final value by adjusting the beam deflection on the RHEED beam. Intensity oscillations were found to include interference beats that increased the intensity decay envelope and changed the phase of the oscillation, leading to a missing half period if peaks are naively counted on either side of the beat. I determined that these beats were due to spatial flux variations along the beam path, and their effect was reduced by using a small substrate (10 mm by 10 mm square). Flux transients associated with changes in cell temperature upon first opening the shutter were significant for the Al cell, and their effect was eliminated by plotting growth rate data as a function of time, and using only data collected after the growth rate had stabilized.

(4) Provide the formulas used to determine the final numerical result from the raw data, and show your propagation of error analysis.

Composition of the film can be extracted from the RHEED measurements of the AlAs, GaAs, and AlGaAs growth rates, a, g, and b, respectively. These three growth rates can be combined to calculate the Al mole fraction x in four different ways, which are: a / b, $(b-g)/b$, $a / (a+g)$, and $(b-g) / (a+g)$. Using Taylor-series expansions, the standard deviation in Al mole fraction x is estimated in terms of the mean and variance of the growth rates a, g, and b, for each of the four equations listed above. The equation $(b-g) / (a+g)$ gives higher mean square error than at least one of the other equations regardless of the values of the standard deviations of the average growth rates. The standard deviations σ for x based on the other equations can be estimated as follows (see attached paper):

$\sigma(a/b) \approx (a/b)\,\mathrm{sqrt}\{ (\sigma_a / a)^2 + (\sigma_b / b)^2 \}$

$\sigma((b-g)/b) \approx (a/b)\,\mathrm{sqrt}\{ (\sigma_b^2 + \sigma_g^2)/ a^2 + (\sigma_b / b)^2 - 2\,\sigma_b^2 / ab\}$

$\sigma(a/(a+g)) \approx (a/b)\,\mathrm{sqrt}\{ \{ (\sigma_a / a)^2 + (\sigma_a^2 + \sigma_g^2)/ b^2 - 2\,\sigma_a^2 / ab \}$

Applying all three equations for calculating the aluminum mole fraction x from the growth rate data, I obtain:

Method	x	σ
a/b	0.2033	0.0015
(b-g)/b	0.2061	0.0162
a/(a+g)	0.2039	0.0031

All three values agree to within their experimental uncertainty. The value with the lowest uncertainty is the method in the first row, hence the best estimated value for *x* is 0.2033 with standard uncertainty of 0.0015, or 0.7% of the mole fraction value.

(5) Provide a table of uncertainty analysis that summarizes the above steps.

Factor	Standard Uncertainty	Comments
Overall uncertainty	0.0018	Nonzero errors added in quadrature
Growth rate measurement	0.0015	Standard error
Electron beam within 1mm of center	0.001	Depends on flux spatial distribution
Flux transients	No contribution	Restrict analysis to long times
Temperature	No contribution	595 to 622 °C
Reconstruction (2x vs. 4x)	No contribution	Assumes beam on same spot after substrate rotation

(6) If applicable, attach a paper or thesis chapter that provides further information. [The pdf on the next page in this example was inserted using the Insert | Text | Object command with word, using the Create from File option. The full file can be seen by double-clicking on the rectangle that appears when clicking on the first page.]

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Accuracy of AlGaAs growth rates and composition determination using RHEED oscillations ☆

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Abstract

We investigate the sources of uncertainty in the measurement of the reflection high-energy electron diffraction (RHEED) intensity oscillations during growth of AlAs, GaAs, and AlGaAs on GaAs substrates, and the resulting effects on predicted growth rates and composition. Sources of error examined include beam positioning, flux transients, substrate size, 'beat' phenomena in the RHEED oscillations, substrate temperature, and incident beam direction. We find that flux transients and flux nonuniformity are the dominant systematic errors in predicting growth rates and composition with RHEED. From flux uniformity measurements, we estimate the beam positioning error for our growth system to be 0.2–0.6%/mm, and substrate size to impact the uncertainty by as much as several percent. In addition to these errors, flux transients can cause an uncertainty of up to 1%. We also present a procedure that uses the measured variance in the growth rates to calculate the composition with the smallest mean square error.

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Keywords: A1. Reflection high energy electron diffraction; A2. Molecular beam epitaxy; B2. Semiconducting III–V materials

1. Introduction

The use of reflection high-energy electron diffraction (RHEED) intensity oscillations has proven to be a powerful tool to understand growth mechanisms of GaAs, AlAs and AlGaAs in molecular beam epitaxy (MBE). Early studies [1–3] of RHEED patterns generated discussion of the surface constructions and growth mechanisms of the GaAs system, but one important feature, immediately recognized by all, is the close relationship between the RHEED intensity oscillations and the growth rate of their films. Specifically, the period of the intensity oscillations of the specular diffraction spot corresponds to the time required to grow exactly 1 ML of crystal over a broad range of growth conditions. Great effort has gone into understanding the RHEED intensity oscillations [4,5], and their usefulness in monitoring MBE growth. Nevertheless, there is considerable variability in how the RHEED technique is applied. The purpose of this paper is to critically examine

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